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# 구두발표논문

Oral session abstract

## Status of JSNS<sup>2</sup> and JSNS<sup>2</sup>-II

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### Abstract:

The JSNS<sup>2</sup> experiment aims to search for the existence of sterile neutrinos at J-PARC. A 1 MW beam of 3 GeV protons incident on a spallation neutron target produces an intense neutrino beam from muon decay at rest. The experiment searches for muon anti-neutrino to electron anti-neutrino oscillations which are detected by the inverse beta decay interaction, followed by gammas from neutron capture on Gd. There was a 1st physics run in 2021, and a 2022 physics run has been ongoing since this January. Currently, studies on 2021 and 2022 data are in progress. We also have a plan to construct a second detector for the 2<sup>nd</sup> phase of the JSNS<sup>2</sup> experiment, named JSNS<sup>2</sup>-II. In this talk, the status of JSNS<sup>2</sup> detector and studies are reported and the plan and the expected results for JSNS<sup>2</sup>-II are introduced.

### Keywords:

JSNS2, sterile neutrino, J-PARC

## Status of the KDAR neutrino search with JSNS<sup>2</sup>

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### Abstract:

Kaon Decay-At-Rest (KDAR) provides a neutrino signal with well-known neutrino energy, which is an important probe for measuring the neutrino cross-section in an energy range that is otherwise difficult to access experimentally. The J-PARC Sterile Neutrino Search at the J-PARC Spallation Neutron Source (JSNS<sup>2</sup>) experiment is in a unique place for measuring monoenergetic neutrinos at 236 MeV from KDAR. JSNS<sup>2</sup> is located at the J-PARC's Material and Life Science Facility (MLF) where the world's most intense source of KDAR created by a 3 GeV proton beam incident on a liquid mercury target. In this presentation, We will present the first result of the search for the KDAR neutrinos conducted with the JSNS<sup>2</sup> experiment with the data during the JSNS<sup>2</sup>'s first long-term physics run during 2021, consisting of more than 115 days of data and  $1.45 \times 10^{22}$  POT.

### Keywords:

JSNS2, Neutrino, KDAR, J-PARC, Sterile neutrino

## Measurement of the HCAL hit time at CMS

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### Abstract:

At CMS, knowing the hit time of the particles can provide additional information to reject backgrounds and to identify signatures of new physics. With the hadron calorimeter (HCAL), hit time can be extracted from the result of the local reconstruction algorithm. But, it is not reliable because the algorithm is designed to optimally extract energy. This motivates the development of methods dedicated to the measurement of hit time. In this talk, the ongoing effort to define the HCAL hit time will be discussed.

### Keywords:

HCAL, CMS, Hit time

## Status of CMS LGAD Sensor Testing in Korea

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### Abstract:

As part of the CMS Phase 2 upgrade, MIP Timing Detector is planned to be installed in order to mitigate the impact of pileup that is expected to reach 200 in HL-LHC. In the endcap region, silicon-based Low Gain Avalanche Detector (LGAD) sensors that allow timing resolution of a few tens of picoseconds are used. The sensor design needs to be optimized considering several factors, including radiation resistance, uniformity of gain, and long-term stability. Korea University is participating in the test of market survey sensors and the highlights of the test will be discussed in this talk.

### Keywords:

CMS, MTD, LGAD, Market survey, ETL

## Implementation of MHT trigger algorithm on the FPGA for CMS Phase-2 Level-1 trigger

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### Abstract:

The CERN LHC will be upgraded for the high-luminosity LHC (HL-LHC) with an increasing luminosity by a factor of 10 in order to maximize the potential for the discovery of new physics. This brings significant increasing data and needs for improvement of the CMS detector performance and trigger algorithms. The Level-1 (L1) missing transverse energy (MET) trigger algorithm based on the field programmable gate array (FPGA) is being developed for newly introduced L1 correlator trigger for the HL-LHC. Furthermore, The L1 missing vector sum of Hadronic energy (MHT) trigger algorithm can improve the signal selection capability of the CMS Phase-2 L1 trigger. The CMS L1 trigger is being developed using Xilinx Vivado high-level synthesis (HLS) to implement the firmware of the MHT trigger algorithm on the FPGA board. We present the optimization of the MET and MHT algorithms with respect to the latency and resource usages based on both the HLS simulation and hardware system.

### Keywords:

CMS, L1 trigger, FPGA

# The CMS Muon High Level Trigger with Machine Learning for the High Luminosity LHC

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## Abstract:

The High Luminosity LHC (HL-LHC) is designed to operate with the maximum peak instantaneous luminosity of  $7.5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$  with a cost of the average number of proton-proton collisions per bunch crossing (pileup) up to 200. In these challenging conditions, the CMS Muon High Level Trigger (Muon HLT) aims to reduce the event rate from the order of tens of kHz, accepted by the Level-1 (L1) muon system, to 1.5 kHz by preferentially selecting muons from decays of the W, Z, and H bosons. Due to an excessive detector hit multiplicity at high pileup, a significant increase of computing time for muon trajectory reconstruction is expected. We present a novel development of a "seed classifier" designed to efficiently select high quality initial states for the muon pattern recognition utilizing machine learning techniques, leading to a significant reduction of computing time while preserving the high muon reconstruction efficiency.

## Keywords:

LHC, CMS, Trigger

# An optimal way of exploiting collider variables using machine learning

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## **Abstract:**

We introduce a new method of building machine learning models with which the exploitation process of various collider observables from particle detectors can be optimal and maximally interpretable. We demonstrate the algorithm for various collider variables using Monte-Carlo simulation data of the Standard Model Higgs production and decay at the LHC.

## **Keywords:**

machine learning, collider data analysis, Higgs at the LHC, exploitation

## Physics Analysis Tools in the Python ecosystem for the HL-LHC

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### **Abstract:**

One of the biggest challenges in the High-Luminosity LHC (HL-LHC) era will be significantly more data to be recorded and analyzed from the collisions at the ATLAS and CMS experiments. Novel approaches when interacting with the data and performing physics analysis are being developed by the High Energy Physics (HEP) community in the Python ecosystem, and rely on the development of the required cyberinfrastructure to be executed at scale. Various tools and services primarily from Institute for Research and Innovation in Software for High Energy Physics (IRIS-HEP) will be discussed. An ongoing Run-2 physics analysis workflow that employs new software components will be presented to assess performance and to understand potential practical issues in deployment, interoperability, collaboration, and interface stability.

### **Keywords:**

Computing, High Energy Physics, HL-LHC, Physics Analysis

## Cubic Closed String Field Theory on a Double Layer

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### Abstract:

Various studies have attempted to extend the Witten's cubic open string field theory to the cubic closed string field theory, which may describe Einstein gravity in the low energy sector consistently. In the present study we propose a cubic closed string field theory, introducing a double layer to describe the closed string world-sheet as an extension of the open string world-sheet of the Witten's cubic open string. We mapped the closed string world-sheet onto the complex plane, of which the lower half plane is completely covered by the extended part of the string world-sheet. Using the Green's function on the complex plane, evaluated the Polyakov string path integral, from which we extracted the Neumann functions and the vertex operators. We obtained the one and two string vertices (identities) following this procedure and finally the cubic string vertex operator. It is notable that the obtained cubic string scattering amplitude coincide with the cubic graviton interaction of the Einstein gravity. Thus, the resultant cubic closed string field theory consistently describes the Einstein gravity. We also show that the Kawai-Lewellen-Tye (KLT) relations of the first quantized string theory may be manifested in the cubic closed string field theory.

### Keywords:

string field theory, closed string, Witten's cubic open string field theory

## 2d (0,2) gauge theories and families of toric Calabi-Yau 4-folds

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### Abstract:

A special class of 2d (0,2) supersymmetric gauge theories, named as Brane Brick Models (BBM), is obtained by the low-energy limit of world-volume theories of D1 branes probing toric Calabi-Yau 4-fold. Among the various combinatorial tools BBM involves, this talk will focus on orbifold reduction and 3d printing, which generate the Lagrangian data of 2d gauge theory from the geometric data of Calabi-Yau 4-folds. For an illustrative example, we explicitly construct the gauge theories corresponding to two families of integer-labeled toric Calabi-Yau 4-folds, called  $Y^{p,k}(P^2)$  and  $Y^{p,k}(P^1 \times P^1)$ , respectively, with these. This talk is based on an ongoing project with R.-K Seong (UNIST) and S. Franco (CUNY).

### Keywords:

supersymmetry, D-brane, string theory, Calabi-Yau manifold, toric geometry

## Perturbative Gravity from Double Field Theory

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### Abstract:

We construct the perturbative gravity around a curved background including the entire massless NS-NS sector from the perturbative double field theory (DFT). We present the perturbative DFT action and equations of motion (EoM) including all-orders around curved background. From the perturbative DFT, we deduce the perturbative gravity to all-orders in fluctuations. This framework is equivalent usual perturbative gravity up to field redefinition but much simpler from the aid of the  $O(D,D)$  structure and doubled Lorentz group of DFT. The perturbative action and EoM are derived to arbitrary order for the entire massless NS-NS sector and pure gravity case.

### Keywords:

Perturbative Gravity, Double Field Theory

## Dynamical Symmetry and the Thermofield State at Large N

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### **Abstract:**

We discuss Thermofield Double QFT at real time, in the large N limit. First, we establish a (dynamical) symmetry which we argue holds in general on the real time portion of the Schwinger-Keldysh contour. At large N this symmetry is seen to generate a one parameter degeneracy of stationary collective solutions. The construction is explicitly worked out on the example of  $O(N)$  vector QFT. As a nontrivial application we describe construction of the corresponding (large N) Thermofield Double State in real time collective formalism.

### **Keywords:**

QFT at finite temperature, Large N, TFD

## Hydrodynamics with dynamical gauge fields and holography

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### Abstract:

We study the magneto-hydrodynamics in (2+1) dimension with dynamical gauge fields and confirm that it is consistent with the quasi-normal modes of the (3+1) dimensional holographic model at finite magnetic field. In holography, we analyze the dynamical gauge fields using two different ways, by implementing the Legendre transformation or the Power-law Maxwell model, finding agreement between the two methods within quasi-normal modes (sound, charge diffusion, shear diffusion, EM wave mode). Our result not only shows the non-trivial consistency between hydrodynamics and quasi-normal modes in holography, but also is useful for the complete understanding of the magneto-hydrodynamics in that the previous literature mainly considers hydrodynamics with the external gauge fields.

### Keywords:

Holography, Hydrodynamics, Black hole, Quasi-normal mode, Dynamical gauge field

## Holographic teleportation with conservation laws: diffusion on traversable wormholes

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### Abstract:

We study the effects of conservation laws on wormholes that are made traversable by a double trace deformation. After coupling the two asymptotic boundaries of an eternal AdS-Schwarzschild black hole with U(1) conserved current operators, we find that the corresponding quantum matter stress-energy tensor violates the averaged null energy condition (ANEC) in the bulk, rendering the wormhole traversable. We discuss how the wormhole opening depends on the charge diffusion constant and how this affects the amount of information that can be sent through the wormhole.

### Keywords:

Gauge-Gravity Correspondence, Holography and Condensed Matter Physics (AdS/CMT)

## Multilayered graphenes in holography

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### Abstract:

We have previously computed the spectral function for the fermion bilinear is dual to bulk meter field  $\Phi_I(r, x)$ . Among them, we found that a flat disk band that was formed by the tensor order  $B_{xy}$ , which corresponds to the flat band, which is the surface mode of ABC stacked multilayer graphene, and the strength of the  $B_{xy}$  interaction is proportional to the number of layers, that is stacking order  $N$  in ABC stacked multilayer graphene.

### Keywords:

ABC stacked multilayer graphene, Holography, Flatband, Spectralfunction

## Holographic Realization of Lieb Lattice and Its Gapping

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### Abstract:

We study gapped and non-gapped flat band phase transition with a solvable model in the holographic principles. By considering the real scalar field on the fermion and changing the boundary action, we discover similarities between our holographic result and the Lieb lattice flat band dispersion. We also show that it is possible to interpret the scalar interaction as a gap generating parameter like the staggered hopping parameter in the tight binding model of Lieb lattice.

### Keywords:

Holography and Condensed Matter Physics (AdS/CMT), Lieb Lattice, Flat Band, Gapped and Non-gapped Phase Transition

## Revisited "photoemission experiments in holographic superconductors" : Superconducting Dome from holographic spectral function

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### Abstract:

By modifying a flow equation, we revisit "photoemission experiments in holographic superconductors". Also, we find similarities between our interaction term and BCS-theory's model. From this result, we match our complex scalar field as superconducting gap parameter. Furthermore, we show superconducting dome phase by adding both real and complex scalar field with proper criteria defined by fermionic spectral density.

### Keywords:

Holographic Superconductor, Fermion Spectral Function, Superconducting Dome, Phase Diagram

## Present status of the ISOL beam lines of Rare Isotope Science Project

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### Abstract:

Construction of Isotope Separation On-Line (ISOL) beam line at Rare Isotope Science Project (RISP) was completed and now is commissioning with stable ions produced from Target Ion Source(TIS). The ISOL beam transportation line is mainly composed of 4 components, which are the pre-mass separator beam line, a RF cooler buncher for beam bunching, a electron beam ion source (EBIS) for charge breeding, and the A/q separator. After the optical component alignment was carried out on 2020, the beam commissioning of ISOL transport line has started by using  $^{133}\text{Cs}$  stable ions from an surface ionizer at the TIS from 2021. As a result, we found a pre-mass separator beam line setting condition with a required mass resolving power ( $> 400$ ) and 100% beam transmission efficiency. Although the beam commissioning of the A/q separator is still undergoing, the beam was able to transport from the TIS to the end of ISOL beam line, that is the entrance of RFQ accelerator system. In this presentation, the beam commissioning results for the pre-mass separator, and the A/q separator including the RF cooler buncher and EBIS will be reported. In addition, some future test plans also will be discussed.

### Keywords:

ISOL, low energy beam transport, beam line commissioning

## Status of LAMPS Start Counter

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### Abstract:

LAMPS 실험의 모든 검출기가 동기화된 데이터를 얻고, 빔 입자의 종류를 구별하며, 충돌 후 생성된 입자의 종류를 알아내려면 100 ps 수준의 높은 시간분해능을 갖는 검출기가 필요하다. Start Counter는 LAMPS 실험에서 입사하는 입자의 기준 시간을 측정하는 검출기이다. 입자가 Start Counter의 얇은 신틸레이터와 만났을 때 생성된 광신호의 데이터는 다중 픽셀 광자 검출기(Multi-Pixel Photon Counter, MPPC)를 통해 수집된다. 이 연구에서는 LAMPS Start Counter 제작 및 설치 과정과 아메리슘 소스를 통하여 측정한 신호와 시간 분해능에 대하여 발표한다.

### Keywords:

LAMPS, Start Counter, MPPC, RAON

## Development of time-of-flight detector in LAMPS at RAON

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### Abstract:

We have developed a time-of-flight (TOF) detector for triggering and timing measurements in RI beam experiments with LAMPS at RAON. The LAMPS TOF detector consists primarily of the barrel TOF (BTOF) and forward TOF (FTOF) arrays placed in the LAMPS solenoid magnet. The BTOF array covers  $2\pi$  azimuthal angles surrounding the LAMPS TPC with 46 fast plastic scintillators. The FTOF array is positioned downstream of the TPC, which comprises 48 ultrafast scintillators of trapezoidal shape. The timing and attenuation properties of the scintillators are measured using cosmic-ray muons and  $\beta$  rays from  $^{90}\text{Sr}$ . The cosmic-ray muon events are triggered in triple coincidence with trigger scintillators. In this talk, we will report the assembly of the LAMPS TOF and the intrinsic time resolutions of the LAMPS TOF detector compared to the results obtained from the prototype test. We will also discuss the geometrical and momentum acceptance of the detector.

### Keywords:

MPPC, ToF, LAMPS, RAON, Scintillator

## Development of an Active Target Time Projection Chamber for low-energy rare isotope beam experiments

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### Abstract:

An Active Target Time Projection Chamber (AT-TPC) is designed to measure nuclear reactions at low-energy rare isotope collision experiments at Rare isotope Accelerator complex for ON-line experiment (RAON). We are planning a new experiment using the AT-TPC as the main component to measure a scattering of alpha particles and heavy ions, particularly associated with the formation of alpha cluster resonance. Before the main experiment, we develop the prototype AT-TPC with Gas Electron Multipliers (GEM). The prototype AT-TPC has a active volume of  $10 \times 10 \times 15 \text{ cm}^3$ , and the 256 read-out pads are used for data acquisition. We plan to use the quasi-free scattering of proton to carbon target for the performance test, using a 100 MeV proton beam at KOMAC. In this presentation, we present the progress of R&D for the prototype ATTPC, hardware assembly, construction of a DAQ system, and AT-TPC performance.

### Keywords:

TPC, AT-TPC, LAMPS, RAON

## Simulation of an Active Target Time Projection Chamber for low-energy rare isotope beam experiment

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### Abstract:

Active Target Time Project Chamber(AT-TPC) is a novel type of TPC in which the drift gas is used as the collision target. As the collision happens in the active volume of TPC, tracks can be reconstructed with 4- $\pi$  acceptance. To investigate the performance of AT-TPC for the low-energy LAMPS experiment at RAON, we build the simulation package based on Geant4 and GARFIELD++. We use a toy Monte Carlo to calculate the electron showers, the effective gain for the fast simulation. We expect this simulation package to facilitate the use of AT-TPC detector for the low-energy experiments at RAON. In this presentation, we report the progress of the simulation tools for the prototype detectors (  $10 \times 10 \text{ cm}^2$  and  $20 \times 20 \text{ cm}^2$  for active areas) and the main detector (a cylindrical shape with a diameter of 40cm).

### Keywords:

Active Target Time Project Chamber(AT-TPC), LAMPS experiment

## Multi-gap RPCs for measurement of beam-induced photons

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### Abstract:

In the present R&D, multi-gap resistive plate chambers (MRPCs) are studied for dose verification in particle therapy. Here, we apply the MRPC technology to measure beam-induced gamma rays with SPECT (single photon emission computer tomography) and in-beam PET (positron emission tomography) detector systems for the therapeutic-beam verification. Two six-gap RPCs with a gap thickness of 0.52 mm were constructed using 0.55-mm-thick soda-lime glass and tested with  $^{137}\text{Cs}$  (662 keV) and  $^{22}\text{Na}$  (511 and 1,274 keV) sources with current activities of 4.8 GBq and 125 kBq, respectively. The measured efficiencies for the gamma rays emitted from the two gamma sources agree well with the simulation result performed by using a GEANT program. In order to demonstrate the uniformity of the detector sensitivity, we utilize the six-gap RPCs and reproduce gamma-transmission images for various objects such as scissors, a spanner, and a two-fold pressure gauge whose spatial resolution is on an order of 2 mm.

### Keywords:

Dose verification, Particle therapy, Multi-gap RPCs, Beam-induced gamma rays

## Cosmic-ray Muon Spectrometer (COSMUS)

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### Abstract:

A new cosmic-ray muon spectrometer(COSMUS) aims to measure the long-term variation in cosmic-ray flux. The COSMUS consists of a cylindrical array of 24 trapezoidal prism-shaped scintillators, sandwiched by four layers of large-area plastic scintillators, Cherenkov counters, and a drift chamber. We constructed a tall support structure to arrange the detectors effectively and completed installing half of the detectors. With the COSMUS, we will study cosmic rays' momentum and angular distributions over a wide zenith range. We will present the design, installation, and results of the detector commissioning in detail.

### Keywords:

cosmic-ray, muon

## Opportunity of Korean GEM manufacturing infrastructure for building MPGD at EIC

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### **Abstract:**

Electron-Ion Collider (EIC) is a planned facility capable of colliding polarized electrons and polarized protons or various nuclei up to uranium at high luminosity. EIC is expected to play a leading role in various precision QCD studies. Among detector plans of EIC, are plans for the use of micro pattern gas detector (MPGD) such as gas electron multipliers (GEM) or micro resistive well (uRWELL). For CMS phase-2 upgrade, Korea CMS collaboration has equipped facilities for GEM production and trained person power. Using those facilities, the production of not only GEM but also uRWELL is possible, which can contribute to EIC. This is one of the few opportunities for Korea to participate in international collaboration with its original technology. Ideas on those opportunities is presented.

### **Keywords:**

EIC, MPGD, GEM, uRWELL

## Pair-breaking effect of magnetic field on Nb thin films studied with terahertz time-domain spectroscopy

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### Abstract:

We studied the terahertz properties of superconducting niobium thin films under in-plane magnetic fields up to 7 T at 1.5 K by using terahertz time-domain spectroscopy. Our measurement technique can experimentally determine both the real and imaginary parts of the optical conductivity without Kramers-Kronig analysis. Under the magnetic field, the superconductivity is systematically suppressed, eventually entering the gapless superconducting state near the upper critical field value. Utilizing the Skalski, Betbeder-Matibet, and Weiss (SBW) theory, which considers the time-reversal symmetry breaking due to general external perturbations, we determined the pair-breaking parameter over the entire range of the magnetic fields up to the upper critical field, including the gapless regime.

### Keywords:

Terahertz time-domain spectroscopy, niobium, superconductivity

# Enhancement of critical current density and strong vortex pinning in high entropy alloy superconductor $Ta_{1/6}Nb_{2/6}Hf_{1/6}Zr_{1/6}Ti_{1/6}$ synthesized by spark plasma sintering

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## Abstract:

We synthesized the high entropy alloy (HEA)  $Ta_{1/6}Nb_{2/6}Hf_{1/6}Zr_{1/6}Ti_{1/6}$  compound by a planetary ball milling and spark plasma sintering method. The sintered HEA sample shows a BCC crystal structure with small secondary phases. The superconducting phase transition is observed in the electrical resistivity ( $T_c \sim 7.8$  K) and magnetic susceptibility ( $T_c \sim 7.6$  K) measurements, which the  $T_c$  is similar to the one of the arc-melted sample. The zero-temperature limit of the upper critical magnetic fields  $H_{c2}(0) = 10.5$  T and coherence length  $\xi = 5.66$  nm is a little bit decreased or comparable with the arc-melted HEA sample ( $H_{c2}(0) = 12.05$  T and  $\xi = 5.23$  nm). The field-dependent isothermal magnetization hysteresis  $M(H)$  shows the typical type-II superconducting behavior with flux avalanches at low magnetic field regions. The calculated critical current densities  $J_c$  ( $73,200$  A  $cm^{-2}$  at  $T = 4$  K,  $H = 0.01$  T) are significantly increased by 286 % (at 2 K) ~ 687 % (at 4 K) as compared to the one of the arc-melted HEA sample. The enhanced  $J_c$  of the sintered HEA sample is caused by the enhancement of pinning force due to point pinning as well as surface pinning effect. The vortex relaxation measurements show stable remanent magnetization after magnetic fields are turned off for over 10,000 s, which is contrary to the conventional superconducting vortex relaxation behavior. The strong pinning force in the SPS sintered  $Ta_{1/6}Nb_{2/6}Hf_{1/6}Zr_{1/6}Ti_{1/6}$  compound has beneficiary on the practical applications because of the significantly enhanced critical current density  $J_c$  with stable remanent magnetization  $M_{rem}(t)$ .

## Keywords:

high entropy alloy, superconductor, spark plasma sintering, critical current density, pinning force and flux jump

## Large Enhancement of Spin Hall Conductivities in W-N Alloys

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### Abstract:

Recently in spintronics, W compounds have attracted attentions owing to large spin Hall angle [1]. Motivated by recent experiment [2], we investigate spin Hall conductivities (SHC) of W-N alloys using first-principles calculations. Among various compositions of W-N alloys [3], W<sub>2</sub>N and WN are considered from energetics. Without N, SHC of  $\alpha$ -W and  $\beta$ -W are -744 and -818  $\hbar/e$  S/cm, respectively, consistent with previous study [4]. With N, W<sub>2</sub>N exhibits large SHC of -937  $\hbar/e$  S/cm, which is enhanced by 14.54 % over  $\beta$ -W, respectively. The large SHC of W<sub>2</sub>N is elucidated by the large Berry curvature around  $2/3\Gamma$ . On the other hand, in WN case, SHC of NaCl-type and hexagonal structures are -619 and -696  $\hbar/e$  S/cm, respectively, whereas NbO-type possesses quite small SHC of -194.49  $\hbar/e$  S/cm. This tendency is in good agreement with the experimental study [2].

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### Keywords:

first-principles calculations, spin Hall angle, spin Hall conductivities

## Unprecedented lattice dynamics in a primary insulator-metal transition magnet $\text{NiS}_{2-x}\text{Se}_x$

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### Abstract:

$\text{NiS}_{2-x}\text{Se}_x$  [1] is a prototypical strongly correlated system, exhibiting a complex phase diagram including an insulator-metal transition [2], magnetic phase transitions, and quantum criticalities with Se ions. Although it has been studied for decades, understanding the nature of underlying electronic phases is still unclear. Here, we present polarised Raman and Inelastic x-ray Scattering (IXS) measurements on  $\text{NiS}_{2-x}\text{Se}_x$  ( $x = 0 \sim 1$ ) single crystals upon temperature [3]. Our careful Raman measurements reveal the subtle, but clear softening of optical phonons for the first time. This observation is completely beyond the expectation since this does not take place with the transition, which could be a consensus for decades. We perform the inelastic x-ray scattering measurement to better understand this peculiar phenomenon by measuring the phonon dispersions in the full momentum space. We will discuss the possible implications of our new observations, followed by the relevance to two basic mechanisms for the insulator-metal transition (Mott and Anderson localization) [4] with the revised perspective on the complex interplay between phonons, charges, and spins.

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### Keywords:

Insulator-Metal Transition, Phonon, Magnet, Raman, Inelastic X-ray Scattering

# Development of Sagnac interferometer for magneto-optical measurement and its applications to superconductivity and magnetism

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## Abstract:

Magneto-optical (MO) measurement of condensed matter systems plays a key role as it reveals if the time-reversal symmetry of a system is broken. Among the various MO techniques, Sagnac interferometer possesses the unique property of rejecting all the reciprocal effects, thus giving definite evidence for time-reversal symmetry breaking (TRSB) [1]. This property of Sagnac interferometer enables sensitive measurement without any magnetic field modulation. Recent studies using Sagnac interferometer have revealed ferromagnetism in the two-dimensional van der Waals materials [2] and TRSB in many unconventional superconductors [3]. So far, most studies using Sagnac interferometers, however, have been focused on the intrinsic property of a sample at equilibrium state. In this talk, we introduce further application and development of Sagnac interferometer from two perspectives. First, we present measurements of mesoscopic superconducting structures with various nontrivial geometries. The sensitivity of Sagnac interferometer enables observation of a magnetic flux jump due to individual vortex entries into a micro-size superconductor [4]. Second, we present a modified Sagnac interferometer for time-resolved MO measurement which was unable in the static Sagnac interferometer. For illustration, we show ferromagnetic resonance of a Permalloy film caused by a magnetic field pump [5].

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- [4] H. Heo et al., in preparation
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## Keywords:

Sagnac interferometer, Magneto-optical effect, Time-reversal symmetry breaking, Superconductivity

## Switchable Ferroelectric Bias and Ternary Polar States

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### **Abstract:**

Interaction between dipoles has created intriguing physical phenomena, such as exchange bias in the magnetic heterostructures and magnetoelectric effect in multiferroics, which lead to advances in multifunctional electronic devices. Among constituents of dipole pairs, however, the defect-dipole tends to be considered as the undesired to deteriorate the functionality of the electronic devices. In this talk, we present that a new substrate enables inaccessible strain engineering to ferroelectric BaTiO<sub>3</sub> and demonstrates deterministic control of defect-dipole to reveal three in-plane polar-ordering states characterized by biased/pinched hysteresis loops, more than the magnetic exchange bias. A combination of the first-principles calculations and comprehensive experimental studies propose a physical mechanism of the multiple polar states via interplay between the defect-dipole and the spontaneous polarization.

### **Keywords:**

ternary polar states, switchable ferroelectric bias

## Magnetic Skyrmion-Based Spintronic Device

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### **Abstract:**

In spintronics, essential building blocks have been established and enable realization of multifunctional spintronic devices. In this talk, I will briefly introduce important spintronic building blocks and discuss how to design each ingredient to meet the requirements for a device with specific functionalities. As an example of such spintronic devices, magnetic skyrmion-based memory will then be discussed in detail including material design and operation principle. Also, several intriguing features reside in the magnetic skyrmions will be presented.

### **Keywords:**

spintronics, spin-torque, Dzyaloshinskii-Moriya interaction, Magnetic skyrmion, Topology

## Design of flat band materials

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### **Abstract:**

We introduce a systematic scheme for the construction of flat band systems by using the compact localized state, which is the fundamental eigenstate of a flat band. We show that the geometric properties of the eigenstate of the flat band can also be controlled in this construction method. Finally, we propose a novel band engineering to realize such flat or nearly flat band systems.

### **Keywords:**

flat band, band engineering

## Rational Molecular Design for Triboelectric Materials Toward Efficient Triboelectric Energy Harvesting

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### Abstract:

Halogenic elements have the largest electron affinity (EA=-270~-349 kJ/mol) which can accommodate extra electrons. So that it is often considered as a strong matter of triboelectric applications. However, halogenic elements are not homopolymerizable that carbon (EA=-122 kJ/mol)-based polymers (i.e. PTFE, PVDF) are often employed for structural use and mechanical integrity at the expense of reduced electron affinity, intrinsically sacrificing triboelectric energy harvesting. Herein, we report the first example of triboelectric energy harvesting with sulfur backbone-based inorganic polymers synthesized via inverse-vulcanization process with elemental sulfur, a by-product (annual surplus of ~7 million tons) of petroleum refining processes. Fluorinated polymeric sulfur demonstrated 3 folds increase in triboelectric energy outputs in both voltage and currents in comparison with commercial PTFE film. Such high energy harvesting was achieved by high electron affinity of sulfur (-200 kJ/mol) and by its hypervalency and expanded-octet, providing two additional bonding coordination with halogens compared to carbon with 4 coordination number.

### Keywords:

Halogen element, Energy Harvesting, Triboelectric, Sulfur Polymer

## Systematical analysis of SrTiO<sub>3</sub>/SrRuO<sub>3</sub> superlattice by vertical transport study

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### Abstract:

Resonant tunneling which is a quantum mechanical process has been attracting both scientific and technological attention because of its interesting physics and application for next-generation electronics. This phenomenon accompanies negative differential resistance (NDR) in current-voltage characteristics and has various physical properties that are used in many electronic circuits such as multi-level logic devices. In this study, we studied electrical transport properties of SrRuO<sub>3</sub>/SrTiO<sub>3</sub> [SRO/STO] superlattices having different STO thicknesses to make the quantum-well structure of SrRuO<sub>3</sub>. In the DC and pulse electrical measurements considering thermal effects, the SRO/STO superlattice sample of two unit-cell STO thick shows the direct tunneling current behavior. And that of four unit-cell thick gives the strong NDR behavior. However, that of six unit-cell or thicker shows the hysteresis and much weaker NDR characteristic. We carefully analyzed these experimental results in terms of the resonant tunneling mechanism where the thickness of insulating STO layer is critical.

### Keywords:

oxide, resonant tunneling, superlattice

## Development of a superconducting quantum computer : 5 qubits and more

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### **Abstract:**

Here we report our recent result of the 5-qubit superconducting quantum computer development. We successfully demonstrated a system-level operation of multiple qubit gate operations, from the device to the analysis, based on the 5-qubit Josephson quantum processor. We will also present a future direction to more than 100 qubit level scaling up of the superconducting quantum computer system. This work is done by the superconducting quantum computer development team led by SKKU, in a close collaboration of SKKU, KRISS, UNIST, Kyungpook National Univ., Seoul National Univ., Korea Univ., Yonsei Univ.,

### **Keywords:**

Superconducting quantum computer

## High-fidelity iToffoli gate for fixed-frequency transmon qubits

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### Abstract:

Several three-qubit gates have been implemented for superconducting qubits, but their use in gate synthesis has been limited due to their low fidelity. Here, using fixed-frequency superconducting qubits, we demonstrate a high-fidelity iToffoli gate based on two-qubit interactions, the so-called cross-resonance effect. As with the Toffoli gate, this three-qubit gate can be used to perform universal quantum computation. The iToffoli gate is implemented by simultaneously applying microwave pulses to a linear chain of three qubits, revealing a process fidelity as high as 98.26(2)%. Moreover, we numerically show that our gate scheme can produce additional three-qubit gates which provide more efficient gate synthesis than the Toffoli and iToffoli gates.

### Keywords:

Quantum computing, Superconducting qubits, Quantum gate

## Superconducting qubits with epitaxially-grown nitride Josephson junctions

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### Abstract:

In superconducting qubits composed of aluminum-based Josephson junctions (JJs), the decoherence from microscopic two-level systems in amorphous aluminum oxide has long been a concern. As an alternative material for the qubits, fully epitaxial NbN/AlN/NbN JJs are an attractive candidate with the potential to solve the above problems because of crystal quality, chemical stability against oxidization, and relatively high transition temperature ( $\sim 16$  K) of NbN. Early studies of superconducting qubits using epitaxially grown nitride JJs have shown significant potential, but their coherence time was limited due to dielectric loss from the MgO substrate [1]. To improve this, we have employed a Si substrate with TiN buffer layer for the epitaxial growth of the nitride JJs and fabricated an all-nitride capacitively-shunted flux qubit coupled to a half-wavelength coplanar waveguide resonator [2]. As the results, this nitride qubit has demonstrated a significant improvement in coherence times, such as  $T_1 = 16.3$  ms and  $T_2 = 21.5$  ms as the mean values of a hundred measurements, which are more than an order of magnitude longer than those reported in the literature using MgO substrates [1]. We explain that this improvement in coherence times is attributed mainly to the reduced dielectric loss when replacing the MgO substrate with the Si substrate. These results are an important step towards constructing a new platform for superconducting quantum hardware.

This work was supported by Japan Science and Technology Agency Core Research for Evolutionary Science and Technology (Grant No. JPMJCR1775), JSPS KAKENHI (JP19H05615), JST ERATO (JPMJER1601) and partially by MEXT Quantum Leap Flagship Programs (JPMXS0120319794 and JPMXS0118068682).

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### Keywords:

Superconducting qubit, Nitrides, Epitaxial growth, Josephson junctions, Coherence time

## Prediction of the ground structure based on majority voting

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### **Abstract:**

First-principle density functional theory calculations have been widely used to predict the atomic structure of materials and to understand their electronic structure. Recently, there have been many attempts as well to construct databases of DFT calculations for screening and machine learning. However, there is no exchange-correlation functional that always accurately predicts the ground structure of materials. Therefore, even if we obtained a material with high stability by using a specific exchange-correlation functional, we cannot completely trust whether it is really the preferred structure in the experiments.

In this presentation, we discuss whether the ground structure of materials can be more accurately predicted by using the law of the majority. We obtained the ground structure of 68 binary materials using 16 methods. Zinc-blende, wurtzite, NaCl, and CsCl structures were considered. Interestingly, the most accurate methods were SCAN+rVV10 and PBE+D3 which correctly predict the ground structure 65 times over 68 materials. We also found that the accuracy in predicting the ground structure can be improved by applying the majority voting rule for several sets of calculation methods.

### **Keywords:**

exchange-correlation, density functional theory, ground structure, van der Waals

## A cost-effective hybrid density functional theory calculation for defect calculation: an application to diamond Si

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### Abstract:

Many physical properties of materials should be considered to make efficient semiconductor devices. Among them, the defect property is very necessary for controlling the electrical properties. Recently, hybrid density functional theory [1] has been widely used for defect calculations. However, this method has been difficult for high-throughput defect calculations due to the high computation cost. To reduce the cost, we downsampled the k-point grid for the Hartree-Fock (HF) exchange than that for the generalized gradient approximation (GGA) exchange-correlation [2,3]. In comparison with the conventional hybrid calculation without the downsampling, the computation time was reduced by about 20 times without losing much accuracy. Using this approach, we obtained the defect formation energy and charge transition levels of P dopant, Si self-interstitials, and Si vacancy defects in diamond silicon. We also discuss how defect formation is affected by P doping.

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### Keywords:

density functional theory, semiconductor, defect, hybrid density functional

## Ab initio Tight-binding Model of Monolayer Transition Metal Dichalcogenides without Mirror Reflection Symmetry

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### Abstract:

In this talk we present the ab initio tight-binding (TB) model to describe monolayer transition metal dichalcogenides when the mirror reflection symmetry is broken. First we review the Slater-Koster scheme based on energy integrals including up to three-center contributions, contrasting with the two-center approximation. The TB model, constructed by truncating Wannier functions, is compared with the density functional theory calculations as the truncation range increases. We further present improved TB models by applying additional optimization procedures to the model. We discuss physical properties derived from the TB models and their applicability.

### Keywords:

tight-binding model, density functional theory, transition metal dichalcogenide

## Accelerating density functional theory calculations by predicting charge density using convolutional neural networks

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### Abstract:

Density functional theory (DFT) has been established as a standard methodology for describing the electronic and structural properties of solids and molecules in materials science. However, the practical use of the DFT is limited to systems containing less than a few hundred atoms, since the computational costs extremely increase with respect to the system size. Here we propose a machine learning (ML) approach based on the three-dimensional (3D) convolutional neural networks to accelerate the DFT calculation by predicting electronic charge density, which is one of the key ingredients for DFT calculation. Since we directly use the 3D grid-based physical properties as input feature vectors, the proposed model is simple and intuitive not requiring any artificial descriptors. Utilizing the CNN architecture, the model is transferable to translational and rotational variance and also can be applied to periodic systems, like polymer and DNA. We finally validate performance that the predicted charge density is accurate enough to capture the other electronic properties, such as the density of states. Our findings provide insight towards the future direction for accelerating the materials simulations based on the ML approach.

### Keywords:

Density functional theory, Machine learning, Convolutional neural networks, Charge density

## Electrolyte-mediated nanograin intermetallic formation enables superionic conduction and electrode stability in rechargeable batteries

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### Abstract:

Toward realizing the high-energy-density rechargeable batteries, self-supporting aluminum (Al) foil has been explored as an emerging anode to replace the graphite anode. However, the implementation of Al foil anodes into the rechargeable batteries has been plagued by limited charge-carrier kinetics, substantial volume variation, and poor electrochemical reversibility. Herein, we introduced an electrolyte-mediated mechanical prelithiation method at relatively low pressure, resulting in a gradient and nanograins intermetallic LiAl layer onto the Al under the consideration of matrix hardness to circumvent the large volume change. The designed electrode can provide superionic conduction, structural integrity, as well as high Coulombic efficiency compared with those of bare Al anode, as evidenced by theoretical calculations and battery experiments. This electrode showed fast-charging (112.3 mAh g<sup>-1</sup> at 5 C), ultrastable capacity retention (~100.0% at after 600 cycles), and high Coulombic efficiency > 99.7% at 10 C under the high-capacity loading condition in the dual-ion battery. When paired with LiFePO<sub>4</sub> cathode, the gradient and nanograins intermetallic electrode render conventional lithium-ion battery long-lasting for 200 cycles, demonstrating the decent interfacial and architectural design for the foil-type electrodes.

### Keywords:

battery, fast-charging, structure instability

## Camera based Lock-in detection of magnetic field using an ensemble of nitrogen vacancy in Diamond

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### Abstract:

Lock-in based nitrogen vacancy (NV) magnetometers have successfully detected bio-magnetic fields from neurons, a live mammalian muscle, and a live mouse heart. These measurements bring up a possibility that NV magnetometers could image microscopic distributions of the bio-magnetic fields. Here, we demonstrate a lock-in camera based wide-field NV microscopy which mean per pixel volume-normalized magnetic field sensitivity is  $43.9 \text{ nT}\cdot\mu\text{m}^{1.5}/\text{Hz}^{0.5}$ . A continuous wave excitation of laser and microwave is adopted and a double resonance with hyperfine driving is applied. An external magnetic field is aligned along the  $\langle 001 \rangle$  of the NV diamond to exploit 4 NV axes. Additionally, sub-ms temporal resolution (2500 Hz) is achieved at the cost of lower signal to noise ratio. This could be a step forward to image neuronal connectivity which requires nanotesla sensitivity at micrometer spatial resolution. Defects and current flows in integrated chips and battery cells could also be imaged using our technique.

### Keywords:

diamond nitrogen vancancy, lock-in detection, widefield magnetometer

## Photon-magnon coupling in YIG/ISRR hybrid systems

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### Abstract:

Understanding and exploitation of robust interaction between different physical systems are the keys to the development of information-processing devices [1-2]. For example, photon-magnon coupling in a variety of hybrid systems has been the focus of increasing research attention [3-11]. Herein, we report an experimental observation of coupling modes and characteristic dispersions in hybrid systems consisting of Yttrium Iron Garnet (YIG) film and inverted patterns of split-ring resonators (noted as ISRR) in planar geometry. To understand the fundamental interaction characteristics of those hybrid systems, anti-crossing dispersions and linewidth evolutions are analyzed with the help of analytical derivations based on electromagnetic interactions. We also report a novel phenomenon of the coexistence of coupling-induced transparency (CIT) and absorption (CIA) of transmission signals in a hybrid structure consisting of YIG film and three concentric ISRRs. The observation of both CIT and CIA is ascribed to magnon-mediated photon-photon coupling between decoupled ISRRs. An analytical model developed based on the balance between the coherent and dissipative multiple-paths interactions precisely reproduces both the CIT and CIA experimentally observed from a single hybrid system [12]. This work, promisingly, can provide a guidance for design of efficient, flexible, and well-controllable photon-magnon hybrid devices that are highly in demand for applications to quantum technologies.

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### Keywords:

Photon-magnon coupling

## 반도체 점결함을 이용한 스핀-광자 인터페이스 연구

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### Abstract:

고체 점결함은 양자광원으로 사용할 수 있을 뿐 아니라, 바닥 상태의 스핀은 수명이 긴 양자 메모리로 사용할 수 있어서 양자통신, 양자컴퓨팅 등 양자정보 기술 개발에 적극적으로 사용되고 있다. 광자 큐비트와 스핀 큐비트 간의 양자 상태 전환이 가능한 경우 양자 컴퓨팅 네트워크와 양자 중계기 네트워크의 기반인 스핀-광자 인터페이스로 사용될 수 있는데, 고체 점결함은 포획 이온, 원자, 양자점 등과 함께 양자 중계기 개발이 가능한 물리계로 평가 받고 있다. 최근에는 점결함을 이용한 확정적 원격 양자 얽힘 뿐 아니라 최초로 양자 네트워크의 확장 가능성을 입증하기도 하여 양자 네트워크 실현을 앞당길 수 있는 물리계로 평가 받고 있다. 이 발표에서는 점결함을 이용한 큐비트 구현과 같은 기초 원리부터 시작하여 스핀-광자 인터페이스 구현 및 이를 이용한 양자 중계기 연구개발의 최신 동향을 소개하고자 한다. 또한, 양자 정보 소자 개발에 장점이 있는 실리콘 카바이드 같은 반도체의 점결함을 이용한 스핀-광자 상호 작용에 대한 최근 연구 진행 상황을 소개할 계획이다.

### Keywords:

큐비트, 점결함, 스핀-광자 인터페이스

## Magnon-photon coupling and magnon entanglement in compensated ferrimagnets

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### Abstract:

We theoretically show that the coupling between magnons in an antiferromagnetically coupled ferrimagnet and microwave photons in a cavity is largely enhanced at the angular momentum compensation point ( $T_A$ ) when  $T_A$  is distinct from the magnetization compensation point [1]. The origin of the enhanced magnon-photon coupling at  $T_A$  is identified as the antiferromagnetic spin dynamics combined with a finite magnetization. Moreover, the strong magnon-photon coupling can be achieved at high excitation frequency in a ferrimagnet, which is challenging to achieve for a ferromagnet due to low magnon frequency and for an antiferromagnet due to weak magnon-photon coupling. If time is allowed, we will also discuss magnon-magnon entanglement in compensated ferrimagnets [2].

### References

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[2] J. Shim and K.-J. Lee, in preparation

### Keywords:

Magnon-photon coupling, Magnon-magnon entanglement, Compensated ferrimagnet

## Revised Michaelis-Menten rate law and its application to time-varying biomolecules

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### Abstract:

Michaelis–Menten rate law has been used for describing biomolecular interactions and has made important contributions to advances in biochemical and biomedical research. It is based on the approximation that the biomolecular complex concentration can approach the equilibrium fast enough each time, so-called the quasi-steady-state approximation. However, molecular concentrations change over time actively in numerous biomolecular interactions. Thus, the quasi-steady-state assumption cannot be strictly applied to such systems. In this study, we presented the revised Michaelis–Menten rate law for the interactions of time-varying biomolecules. Our revised rate law, characterized by rigorously-derived time delay effects in molecular complex formation, improves the accuracy of models especially for protein-protein and protein-DNA interactions. Michaelis-Menten rate law has been used for describing biomolecular interactions and has made important contributions to advances in biochemical and biomedical research. It is based on the approximation that the biomolecular complex concentration can approach the equilibrium fast enough each time, so-called the quasi-steady-state approximation. However, molecular concentrations change over time actively in numerous biomolecular interactions. Thus, the quasi-steady-state assumption cannot be strictly applied to such systems. In this study, we presented the revised Michaelis-Menten rate law for the interactions of time-varying biomolecules. Our simulation and empirical data analysis show that the improvement is not limited to the quantitatively better characterization of the dynamics, but also allows the prediction for qualitatively new patterns in the systems of interest.

### Keywords:

Michaelis–Menten rate law, time-varying biomolecules

## 인공지능을 통한 가치 발굴: 헤도닉 가격 모형과 머신러닝

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### Abstract:

인공지능 모델은 데이터 간 비선형적 구조를 포착하는데 유리하여 부동산 가격 추정에 높은 정확도를 보인다. 그러나 전통적 방식과 같이 분석 결과를 해석하는 것이 어렵기 때문에 black-box 모형으로도 불려왔다. 이러한 인공지능 모델의 단점을 극복하기 위해, 본 논문은 부동산 가격 추정에 있어서 분석 결과를 해석하기 위한 새로운 접근법을 제안한다. 우리의 연구에서 최소자승회귀와 공간회귀에 근거한 전통적인 헤도닉 가격 모형과 랜덤 포레스트 및 심층신경망 모델인 머신러닝 결과를 비교한다. 각 모델의 정확도를 비교한 결과, 심층신경망은 높은 정확도를 얻기 위해 데이터 전처리가 중요한 과정으로 작용하는 반면, 랜덤 포레스트는 데이터 전처리와 관계없이 심층신경망 및 헤도닉 가격 모형에 비해 높은 정확도를 보여주는 것이 확인되었다. 또한 각 헤도닉 변수들이 결과에 미치는 영향을 해석해 보기 위해 랜덤 포레스트 모델에 Gini 중요도와 SHAP value를 적용하였다. 이 방법을 통해 개별 변수의 중요도와 가격에 미치는 영향력의 방향을 유의하게 확인할 수 있었다. 본 연구의 결과는 랜덤 포레스트는 부동산 가격 추정에 있어서 헤도닉 가격 모델만큼 충분한 해석가능성이 있음을 보여주고 있다. 본 연구에 적용한 접근법은 다른 연구에도 쉽게 적용될 수 있어 그 확장성을 바탕으로 다양한 분야에서 사용될 수 있을 것으로 기대된다.

### Keywords:

Hedonic price model, Importance measure, Machine learning, Real estate appraisal

## Energy-threshold-based dynamical stability of power-grid systems

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### Abstract:

Basin stability is a widely used approach for assessing the stability of dynamic systems. Observing the system's response to various perturbations, it effectively quantified a node's ability to maintain its synchrony from external stimulation. Even if the methodology provided much insight on the understanding of the dynamic system it has a few small issues about physical implications. Since most complex dynamic systems reveal diverse chaotic and non-chaotic regions sensitive to perturbation conditions, the scheme of basin stability has difficulty capturing each region's detailed characteristics. In the present work, we propose an energy-based methodology to estimate the system's boundary between chaotic and non-chaotic regions. Extending the result of stability analysis for a two-body system, we approximate each node's minimum energy threshold to break the synchronization of the entire system. Numerical results on several model networks show that our methodology suitably estimates the actual energy threshold, representing the local vulnerability of synchronization dynamics.

### Keywords:

Power grid, synchronization, dynamic stability, network science

## Motion of self-propelled particles in vibrated granular matter close to jamming

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### Abstract:

Self-propelled particles immersed in a dense granular medium provides an interesting way to build a self-organizing system with both structural stability and flexibility. Here we experimentally and theoretically investigate the dynamics of such a system, namely a few self-propelled polar particles placed among a crowd of densely packed nonpolar disks in a two-dimensional circular confinement. First, we observe that each self-propelled particle exhibits anomalous diffusion within the granular medium, eventually reaching and sticking to the boundary of the system. The anomalous diffusion is accompanied by the  $1/f$  noise and the power-law interevent time distribution, whose characteristics depend on the aspect ratio and the polarity of the self-propelled particles. Second, we observe that multiple self-propelled particles eventually form a stable cluster at the boundary, which persistently moves in one direction if the number of constituent self-propelled particles are below a certain threshold. We propose a simplistic model describing how the motile cluster can be maintained via symmetry-breaking mechanism and why the motility cannot be maintained when the cluster becomes too large. These results show that merely changing the particle shape and number can effectively modulate the collective motion of a self-organized structure.

### Keywords:

self-propelled particles, vibrated granular matter, anomalous diffusion, spontaneous symmetry breaking

# Terahertz metasurfaces for electro-photonic nano-tweezers and their applications

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## Abstract:

Most existing optical sensors require labeling target small materials or bio-species, which has limitations that may change the properties of the measuring material and induce a risk of side effects in vivo if the target is a biomaterial. Terahertz waves themselves are sensitive to the intrinsic molecular vibration modes of various biomaterials, so a label-free sensing is possible. Indeed, to increase the detection sensitivity and selectivity, various design of metasurfaces can be suggested especially in the form of vertically aligned double layers of metal gaps for tweezing performance. By employing vertically-aligned metal nanogaps as electrodes, fluid convection-assisted delivery and low-voltage capturing of extremely diluted nanoparticles into electric trapping sites were performed. At the same time, the real-time probing of captured nanoparticles in an aqueous environment can be investigated by greatly induced terahertz electric field within optical hotspot sites, the same region with the trapping sites.

## Acknowledgements

NRF-2020R1A2C2007077 & 2019M3A6B3030638

## Keywords:

Terahertz metasurfaces, Electro-photonic nano-tweezers, Label-free biosensors

## 테라헤르츠 메타물질을 이용한 고민감도 생체조직 이미징

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### Abstract:

테라헤르츠 전자기파는 다양한 생체 분자의 다양한 진동모드와 에너지 수준이 일치하고, 또한 meV 수준의 낮은 광 에너지에 의해 대상을 이온화하지 않으므로, 광대역 광원과 검출기를 통해 분광학 기반으로 생체시료 분석에 폭넓게 연구되고 있다. 그러나 생체내의 다양한 분자들은 매우 낮은 농도로 존재하기 때문에 일반적인 광학적 방식으로는 검출 및 영상화가 어렵다. 본 연구에서는 테라헤르츠 영역에서 동작하는 메타물질 센서를 통해 극미량 저농도 분자검출을 구현한다. 근접장 영역에서 발생하는 전자기파 증폭에 의한 테라헤르츠파와 물질 사이의 상호작용 증폭을 이용하여, 기존의 방식으로 검출이 어려운 수준의 저농도 시료 또는 극미량의 변화를 민감하게 측정할 수 있다. 또한 메타물질 센싱 소자의 공진주파수를 검출하고자 하는 대상물질의 흡수공진에 일치시킴으로써, 매우 유사한 특성을 가지는 생체 분자들을 추가적인 표지 없이 선택적으로 구분할 수 있다. 이러한 센싱 소자는 일반적인 반도체 공정을 통해 제작할 수 있으므로, 이를 대면적화하고 테라헤르츠 이미징 장치와 결합하여 고민감도의 비표지 영상장치를 구현하여 질병의 모니터링에 적용한다. 메타물질을 통해 비선형적으로 증폭된 신호로부터 시료의 광학적 특성을 정량화하기 위한 알고리즘을 도입하고, 이를 통해 생체조직 내의 질병과 관련된 바이오마커의 변화를 영상으로 관찰할 수 있다.

### Acknowledgements

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### Keywords:

terahertz, metamaterial, bioimaging

## Terahertz spectroscopy on nanoconfined molecules using metallic nano-trenches

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### Abstract:

Recent advance in nanofabrication has enabled nanophotonic devices operating at arbitrarily long wavelengths, opening a new field of terahertz nano-optics. A metallic nano-trench is a unique nanophotonic platform that simultaneously provides strong electromagnetic field enhancement and confinement of target system to  $\sim 1$  nanometer scale. Therefore, it is an ideal testbed for systematically studying size-dependent dynamics of gap-filling material systems. In this talk, we share our progress in fabrication of metallic nano-trenches as narrow as 1.5 nm and their application in spectroscopic studies on nanoconfined molecules. We demonstrate label-free detection of various liquids filled in 10 nm-wide metallic nano-trenches and discuss anomalous optical properties of water molecules observed at sizes smaller than 5 nm.

### Keywords:

Terahertz, Nano-trenches, Nanoconfinement, Water, Sensing

## Terahertz generation using a two-color laser pulse in a gaseous medium

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### Abstract:

A two-color laser pulse is used to investigate terahertz (THz) wave generation in a gaseous medium. The two-color laser field is made by the superposition of the fundamental laser field and its second harmonic. We observe a shift in terahertz amplitude and ionization yield simultaneously with respect to the relative phase between the fundamental and second harmonic laser beams. The electron dynamics in the intense two-color laser field are analyzed to understand THz wave generation. We discuss the optimal condition for intense THz wave generation.

### Keywords:

Terahertz, two-color laser pulse

## Analysis of the Low-Temperature Terahertz Response of Red Lead Pigment

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### Abstract:

Pigments are the principal material component of paintings. In order to accurately date paintings and explore the artistic techniques employed, detailed information about the constituent pigments is crucial. Among many analysis techniques for artwork, terahertz spectroscopy is useful as a non-destructive tool for studying artists' pigments. To identify the terahertz spectral features of historically important pigments, we have performed low-temperature transmission measurements on Red Lead (Minium,  $Pb_3O_4$ ), which is one of the earliest red color pigments widely used in paintings. Our Red Lead pigment samples prepared in polyethylene-mixed form exhibit several absorption peaks that are much clearer at low temperatures than at room temperature. The terahertz methods introduced here should help identify and analyze the topographic distribution of pigments in historical artwork.

### Keywords:

pigment, painting, minium, red lead, terahertz spectroscopy

## Simulating Strong Field Physics using Attosecond Pulses

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### Abstract:

We demonstrate a strong field simulator (SFS), an attosecond method capable of resolving strong field processes into their constituent parts by separating ionization from rescattering steps. Our SFS consists of a phase locked, spectrally shaped extreme ultraviolet (XUV) attosecond pulse train (APT) precisely synchronized to a strong near-infrared (NIR) pulse. We use experiment and theory to study the delay-dependent effect the NIR field has on the photoelectron distribution from helium and argon atoms ionized by the XUV-APT. We find that as the APT is delayed with respect to the NIR field, the electron and double ion distributions are modulated at the fundamental NIR frequency and its second harmonic frequency. This demonstrates that different trajectories are populated at different delays. We will show that (1) the SFS has indeed transitioned into the strong field regime and (2) double ionization of helium and argon supports the mechanism for (e, 2e) field driven rescattering. Our analysis also demonstrates that the SFS approach is compatible with tunnel ionization when the SFS wave functions are coherently added. Thus, the SFS method is a powerful tool for studying rescattering in a more diverse set of conditions than those produced by the tunneling process.

### Keywords:

Attosecond, strong field, ionization, interferometry

## Sampling Few-Cycle Laser Waveforms in Space and Time

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### Abstract:

Knowledge of the space-time properties of ultrafast laser pulses is necessary both for characterizing spatiotemporal distortions and for applications using structured beams. In attosecond science, knowledge of the laser intensity envelope is not sufficient, however, as the electron dynamics are governed by the sub-cycle electric field variation. In this talk, I will present my group's progress in completely characterizing – in space and time – the electric field waveforms of near- to mid-infrared few-cycle laser pulses. By spatially resolving the electronic and/or optical signals driven by few-cycle laser pulses in the multiphoton and tunneling regimes, we demonstrate single-shot measurement of optical waveforms undergoing dynamical wavefront rotation [1] as well as the characterization of structured light fields. As an example of the utility of such measurements, we apply waveform sampling to interpret the results of high-order harmonic measurements in solids [2].

### References:

- [1] Y. Liu, et al. Nature Photonics **16**, 109-112 (2022).
- [2] S. Gholam-Mirzaei, et al. J. Opt. Soc. Am. B **35**, A27-A31 (2018).

### Keywords:

Attosecond, Ultrafast, Solid-state, High-order harmonic

# Ultrafast spectroscopy of materials via high-order harmonic generation

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## Abstract:

Dynamics of electrons in atoms, molecules and solids occur on attosecond time scale ( $1 \text{ as} = 10^{-18} \text{ s}$ ), which is too fast to capture in standard pump-probe spectroscopy settings. High-order harmonic generation (HHG) is a non-linear optical method, where samples emit attosecond bursts of light that are synchronized with the driving laser field to their sub-cycle timing levels. Because of such a unique attosecond synchronization high harmonic could either be used for the self-probing of the structure and dynamics of the material, or they can be transported and tailored to generate isolated attosecond pulses. In this talk, I will give a brief overview of how HHG can be used for self-probing of molecules, bulk crystals, atomically thin 2d-crystals, and most recently three-dimensional topological insulators [1-5]. This approach requires an advanced understanding of the HHG mechanism, the dependence to the crystallographic orientation of the sample, including the identification of the unique signatures of symmetry breakings and non-trivial topology. In three-dimensional topological insulators, we find that signatures of non-trivial topological states are manifested in the enhanced generation efficiency when the driving laser fields are circularly polarized [4,5].

## Selected Publications:

1. S. Ghimire *et al.*, Observation of high-order harmonics in a bulk crystal, *Nature Physics* 7, 2, 138 (2011)
2. S. Ghimire and D. Reis, Review: High-order harmonic generation from solids, *Nature Physics* 15, 10-16 (2019)
3. H. Liu *et al.*, High-harmonic generation in atomically thin semiconductor, *Nature Physics* 13, 262-265 (2017)
4. D. Baykusheva *et al.*, All-optical probe of three-dimensional topological insulators based on high-harmonic generation by circularly polarized laser fields, *Nano Lett.* Oct. 22, 2021
5. D. Baykusheva *et al.*, Strong-field physics in three-dimensional topological insulators, *PRA* 103, 023101, 2021

## Blue-green emitting CsPb<sub>1-x</sub>Cd<sub>x</sub>Br<sub>3</sub> nanocrystals with tunable shape and phase control

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### Abstract:

Colloidal CsPbX<sub>3</sub> (X = Br, Cl, and I) perovskite nanocrystals (NCs) have been attracted intense attention as phosphors and photovoltaic materials with thermal durability owing to their promising optoelectronic properties. Various tactics have been presented in the band gap modulation of metal halide perovskite nanocrystals while controlling their structure and composition and especially conserving spectral stability of the emission color. However, a perspective that has been scarcely investigated is how the composed type of two different M<sup>2+</sup> cations affects the shape evolution and phase transition of AMX<sub>3</sub> perovskite NCs, in which A is a monovalent ions, M is a divalent ions, and X is a halide. Specifically, the elongation phenomenon in AMX<sub>3</sub> perovskite NCs can be attributed to the electrostatic repulsions between adjacent divalent ions within the linear metal chains. Furthermore, nanoscale one-dimensional morphology is characterized with both optical and electrical properties and the presence of Cd in the AMX<sub>3</sub> structure can induce phase transformation. In the present work, we explore influence of different Cd mole fractions on optical properties and carrier dynamics of CsPb<sub>1-x</sub>Cd<sub>x</sub>Br<sub>3</sub> NCs. These results can give the way to a number of applications in the fabrication of specialized nanostructures.

### Keywords:

CsPb<sub>1-x</sub>Cd<sub>x</sub>Br<sub>3</sub>, Band gap modulation, Shape evolution, Phase transformation, Carrier dynamics

## Optical and Electrical Benefits of Au-Nanopillar Electrodes for MoS<sub>2</sub>-Based Optoelectronic Devices

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### Abstract:

Transition metal dichalcogenide (TMD) materials have been intensively studied due to its fascinating physical characteristics, including sizable bandgap energy and large absorption coefficient. Therefore, there have been many research works to develop TMD-based optoelectronic devices. However, the absorption in TMD monolayers is very limited due to the extremely small physical thickness. Plasmonic metal nanostructures can be integrated with ultrathin TMD layers to improve the optical absorption in TMD active layers. In TMD/metal hybrid systems, excitation of surface plasmons can give rise to enhanced light-matter interactions and tuning of the spectral responses of the TMD layers. In this work, MoS<sub>2</sub> monolayers, grown by chemical vapor deposition method, were wet-transferred on Au-coated SiO<sub>2</sub> nanopillar (NP) arrays. The SiO<sub>2</sub> NP arrays were fabricated by electron-beam lithography and dry etching processes. We measured reflectance and photoluminescence spectra of MoS<sub>2</sub> monolayers on Au NP arrays. Absorption in MoS<sub>2</sub> monolayers was calculated using finite-difference time-domain simulation method. Optical characteristics of the MoS<sub>2</sub> monolayers on the NP arrays were compared with those on the flat Au surfaces based on experiments and calculation results. For the electrical characterizations, Kelvin probe force microscopy was used to measured contact potential difference contrast of MoS<sub>2</sub> on the Au NP arrays. The spatial distribution of photo-generated carriers on the MoS<sub>2</sub> surface suggested that the Au NP arrays efficiently collect charge carriers under light illumination. This work will help us to propose novel optoelectronic devices based on TMD/metal hybrid nanostructures.

### Keywords:

MoS<sub>2</sub>, surface plasmon, Kelvin probe force microscopy

## Vacancy doping effects on MoS<sub>2</sub> nanoflakes in various shapes and vacancy concentrations

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### Abstract:

Vacancy engineering is a common doping technic in thin-film semiconductor physics. Atomic defects can be made in various ways, such as using an electron beam. In particular, we studied systems with defects in sulfur sites. MoS<sub>2</sub> has a structure in which two sulfur atoms are attached to one molybdenum atom, so it can be referred to as VS1 without one sulfur atom and VS2 without both sulfur atoms. MoS<sub>2</sub> layers with sulfur atomic defects are known to have no significant change in the lattice structure and to be able to withstand about 10 percent of the external stress. We use KWANT within a six-band tight-binding model to study the electronic properties of MoS<sub>2</sub> nanoflakes with VS2. In this work, we considered different types of nanoflakes that have various shapes and edge conditions. Like many two-dimensional materials with honeycomb structures such as graphene, the edge condition of MoS<sub>2</sub> nanoflake shows different characteristics. Sulfur vacancies also create additional localized states in the energy gap region. By combining these features and modulating the vacancy concentration, its properties could be applied to future low dimensional spin and valleytronics devices

### Keywords:

MoS<sub>2</sub>, Tight-binding KWANT, vacancy engineering, FET

## The observation and identification of charge transfer exciton in hydrothermally synthesized 2D Tellurium

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### Abstract:

The 2-dimensional (2D) semiconductors have been studied in optoelectronic and electronic fields due to excellent optical and electrical properties. The rarity of p-type semiconductor triggered many studies of black phosphorus (BP) with p type semiconductor properties even though it has instability under ambient condition.

The field effect transistor with hydrothermally synthesized 2D Tellurium have been reported in 2018[1]. The 2D Tellurium demonstrated high field effect mobility ( $\sim 500 \text{ cm}^2/\text{Vs}$ ) with p type semiconducting property ( $E_g \sim 0.4 \text{ eV}$ ), comparing with BP, it also showed outstanding stability under ambient. The PVP, which is widely used as a capping ligand in the synthesis of nanomaterials, is known to give an n-doping effect due to the electron donating group of long carbon chain. In the case of 2D Tellurium synthesized by hydrothermal method, PVP is used as capping ligand, indicating the interaction of PVP and 2D Tellurium existed. In this work, the unique Photoluminescence (PL) in hydrothermally synthesized 2D Tellurium was observed at different position of pure PVP. The newly observed PL peak was confirmed as charge transfer exciton between LUMO of PVP and valence band of 2D Tellurium via Raman scattering, IR nanoscopy, and AFM.

### References

[1] Yixiu Wang et al., Nat. Electron., 1 (2018), 228–236.

### Keywords:

2D tellurium, P type semiconductor, laser treatment

## Reversal of anomalous Hall conductivity by perpendicular electric field in 2D WSe<sub>2</sub>/VSe<sub>2</sub> heterostructure

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### Abstract:

Anomalous Hall effect and valley polarization are attracting tremendous interest for device applications in spintronics and valleytronics technologies [1-3]. Here, we investigated the possibility of the electric field induced switching of the anomalous Hall conductivity (AHC) and the valley polarization due to the magnetic proximity effect in the two-dimensional (2D) WSe<sub>2</sub>/1T-VSe<sub>2</sub> heterostructure. We found that two possible stackings of the WSe<sub>2</sub>/VSe<sub>2</sub> heterostructure could happen due to their small total energy difference (namely C-I and C-II stackings). The WSe<sub>2</sub> layer had a valley polarization of 3 (-19) meV in the C-I (II) stacking. The valley polarization was further increased up to 8 (-28) meV in C-I (II) stacking when the electric field was applied from the VSe<sub>2</sub> layer to the WSe<sub>2</sub> layer. Also, we obtained an AHC of 75 (80) S/cm in the C-I (II) stacking, and no substantial change was found by applying the electric field without any carrier doping. However, we found a sign change from positive AHC to negative value under the electric field in the hole doped system in C-II stacking with physically acceptable doping concentration. We attribute this reversal of the AHC to the electric field dependent Berry curvature variation. Particularly, the minority spin states of the WSe<sub>2</sub> layer had a major contribution to the reversal of the AHC. Our finding suggests that the electric field control of the AHC switching can be possible in the 2D heterostructure, and provides potential spintronics and valleytronics device application.

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### Keywords:

2d, anomalous Hall effect

## Optical property investigation of two-dimensional transition metal dichalcogenide defect sites using tip-enhanced spectroscopy

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### Abstract:

Atomically thin transition metal dichalcogenides (TMdC) shows excellent behaviors with optical and electrical properties which could lead the substantial promising application in various field. Because the quality of TMdC sample decides the performance of each device, quality evaluation and understanding the defect site features of TMdC is the key point to advance the commercialization of TMdC devices.

Tip-enhanced spectroscopy (TESC), that is the combined technique with scanning probe microscopy and spectroscopy such as photoluminescence (PL) and Raman scattering. The improved nano scale spatial resolution and high sensitivity make TESC can detect the nanoscale defect feature such as defect bound exciton and dark exciton etc. from monolayer WSe<sub>2</sub>.

Here we present the correlation between the PL and Raman scattering of WSe<sub>2</sub> defect site such as edge and cracks with nanoscale spatial resolution. Investigation of TEPL and TERS at same site could give powerful insight for understanding TMdC in depth.

### Keywords:

two-dimension TMD, tip-enhanced spectroscopy, TERS, TEPL

## Enhanced Physical Properties of Transition Metal Dichalcogenides by Passivating the Surface Defects of Substrate

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### Abstract:

The optical and electrical properties of 2D materials such as transition metal dichalcogenides (TMDs) are sensitive to the surface defects of the substrate. Silicon dioxide, a widely used dielectric substrate, has a charge puddle inducing the inhomogeneity to 2D materials. Thus, the high quality of dielectric materials such as h-BN or Al<sub>2</sub>O<sub>3</sub> has been applied for homogeneous and enhanced properties. The S10, one of Perfluorinated Polyether (PFPE), is commercially used as a coating material. It can passivate the surface charge puddle and also provide a weak p doping effect due to fluorine atoms of S10. Here we report a facile way of passivation for surface charge puddle at SiO<sub>2</sub> substrate. The effect of surface passivation and p doping were confirmed by photoluminescence (PL) mapping of TMDs. TMDs on S10 coated area enhanced (six times in the case of MoS<sub>2</sub>) homogeneous PL intensity.

### Keywords:

Surface Defects, Passivation, TMDs, 2D materials, Perfluorinated Polyether

## Complete trion conversion and waveguiding in atomically thin semiconductors

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### Abstract:

Dynamically controllable complete conversion dynamics of the excitonic quasiparticles in 2D semiconductors is a pressing matter to realize the new types of excitonic devices. Here, under the ambient condition, we present the complete exciton-to-trion conversion at the nanoscale strain-gradient facilitated by the propagative surface plasmon polariton (SPP) of the nano-gap based waveguide. The obtained excitation- polarization-dependent spatial distributions of the plasmon and the trion confirm the contribution of the plasmon-induced hot electron generation in this complete conversion process. Moreover, we show the electrically switchable activation of the SPP mode at the desired location by employing a sequence feedback algorithm of the spatial light modulator (SLM), which in turn leads to the dramatic increase of the trion density. This work provides a new strategy to facilitate the fully optically operating excitonic devices with the efficient generation, deterministic positioning, and dynamic tunability of the trion conversion under the ambient condition.

### Keywords:

trion conversion, waveguide, plasmonics

## Role of h-BN encapsulation in excitonic properties of 2D semiconductors

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### Abstract:

The intriguing physical properties of transition metal dichalcogenides (TMDs) can be significantly altered by the extrinsic disorders surrounding TMDs. The encapsulation of TMDs using hexagonal boron nitride (h-BN) has been proposed to show the narrowing of the excitonic linewidth and the suppression of the exciton annihilation process. However, the role of h-BN encapsulation has not been understood clearly. In this work, we demonstrate that the h-BN encapsulation prevents the desorption of the adsorbed gas molecules on monolayer WS<sub>2</sub> crystal. We prove that the h-BN encapsulation effectively passivates the defects in WS<sub>2</sub> by fixating the adsorbed gas molecules onto WS<sub>2</sub> crystal, allowing us to observe the intrinsic excitonic properties of monolayer WS<sub>2</sub>.

### Keywords:

Transition metal dichalcogenides, Hexagonal boron nitride, Passivation, Defects

# Surface/Interface Engineering of 2D Materials via Chemical Functionalization

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## Abstract:

Over the last three decades, carbon (one of the most abundant materials found on earth) and carbon nanomaterials (carbon allotrope forms such as 0D fullerenes, 1D carbon nanotubes, and 2D graphene) have attracted significant attention due to their unique electronic, thermal, mechanical, and chemical properties. Recent advances in the synthesis and assembly techniques have renewed interest in employing carbon nanomaterials as the basis of electronic applications, and the flexibility and the low cost of these materials provide the opportunity for many applications such as wearable, disposable, and next-generation electronics. In addition, in these material systems, we can dramatically change their properties by engineering the surface, defect, phase, and interface.

In this talk, I will deliver the recent progress regarding the synthesis of carbon nanomaterials and provide related applications for functional nanocomposite materials and electronic devices. Especially, this talk mainly affords studies on the chemical functionalization of graphene and introduces how to modify the surface and interface of 2D vdW heterostructures and control the defects for a broad range of practical applications such as electronics, spintronics, bio-sensors, and energy harvesting.

## Keywords:

2D materials, Surface engineering, Interface engineering, Chemical functionalization

# Giant 2D Single-Crystalline Metallic Nanosheets: Synthesis and Applications

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## Abstract:

In this study, we report hierarchical porous Cu film via assembly of single-crystalline, nanometer-thick, and micrometer-long copper nanosheets and their use in EMI shielding. Layer-by-layer assembly of Cu nanosheets enabled formation of a hierarchically-structured porous Cu film with features such as multi-layer stacking; 2D networking; and a layered, sheet-like void architecture. The hierarchical-structured porous Cu foil exhibited outstanding EMI shielding performance compared to the same thickness of dense copper and other materials, exhibiting EMI shielding effectiveness (SE) values of 100 and 60.7dB at thicknesses of 15 and 1.6  $\mu\text{m}$ , respectively. In addition, the EMI SE of the hierarchical porous Cu film was maintained up to 18 months under ambient conditions at room temperature and showed negligible changes after thermal annealing at 200°C for 1 hr. These findings suggest that Cu nanosheets and their layer-by-layer assembly are one of the promising EMI shielding technologies for practical electronic applications.

## Keywords:

metal nanosheet, EMI shielding, hierarchical porous Cu film

## Substitutional doping approaches for the functionality tuning in two-dimensional SnSe<sub>2</sub>

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### Abstract:

Substitutional atomic doping is one of the most convenient and precise routes to modulate semiconducting material properties. Although two-dimensional (2D) layered transition metal dichalcogenides (TMDs) have been of great interest as a prominent semiconducting material due to their unique physical/chemical properties, such a practical atomic doping is still rare, possibly due to the intrinsic localization nature of conduction paths based on d-band states. Here, I introduce the halogen element substitution on anionic site in 2D SnSe<sub>2</sub> as the efficient electrical tuning approach ranged from semiconducting to metallic conductivity. Non-doped SnSe<sub>2</sub> shows semiconducting transport behavior dominated by 2D variable range hopping conduction, exhibiting relatively strong localization of carriers at low-temperature regions. Moderately electron-doped SnSe<sub>2</sub> by substitution on Se with higher valent halogen exhibits superior electrical conductivity even than the heavily doped one owing to the higher electron mobility of the former ( $167 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  at 2 K). Combined with Raman spectra, temperature dependence of mobility clearly evidences the effective screening of homopolar optical mode phonon compared to typical TMD materials. By utilizing the wide electrical tunability in 2D SnSe<sub>2</sub>, various kinds of practical application such as thermoelectric, chemical sensing, and pinning-free contact are discussed.

### Keywords:

two-dimensional (2D) materials, doping, material synthesis, electrical transport

## **A new proteomics tool for uncovering putative proteins associated with protein-mutation linked diseases**

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### **Abstract:**

In this seminar, I will introduce a new chemical tool that can reliably detect the proximal proteins of lamin A and its mutant that causes laminopathies. Furthermore, I will discuss the feasibility of this new proteomics tool and its immense potential for discovering biomarkers associated with protein mutation-linked diseases.

### **Keywords:**

Host-guest chemistry, proximal chemical labelling, laminopathy, proteomics

## Physics and Chemistry of Water Molecules at Heterogeneous Interfaces

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### Abstract:

Water is one of the most abundant molecules found on the earth and living organisms. Water is considered a passive component of life due to the relatively inert and stable nature of water molecules. We found that water molecules are rendered to be highly reactive at the interface of micron-sized water droplets (microdroplets). Vibrational Stark spectroscopy coupled with stimulated Raman excited fluorescence microscopy revealed the presence of an intrinsic interfacial electric field formed at the water-air interface of the microdroplet. This strong electric field on the order of  $10^7$  V/cm induces the formation of reactive oxygen species (ROS), including hydrogen peroxide, hydroxyl radical, and superoxide from water molecules. The FRET analysis showed that molecules are highly localized at the nanoscale regime near the water surface. This molecular enrichment at the water surface accelerates various reactions, including protein unfolding, redox reactions, hydrogen-deuterium exchange, and crystallization, by the factor of  $10^3$  or higher. Those heterogeneous interfaces, including water-air, water-oil, and water-phospholipid membrane, provide an environment where biomolecules are in a highly ordered state, which can lower the entropic barrier of thermodynamically unfavorable reactions such as phosphorylation and nucleoside formation at room temperature. This talk will describe how the unique properties of water molecules at heterogeneous interfaces are employed to address various biological questions.

### Keywords:

Water Molecules, Microdroplet, Interfacial Phenomenon, Biological Membrane, Entropic Barrier

## Single-molecule FRET approach to develop more potently engineered CRISPR-Cas12a genetic scissor

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### Abstract:

CRISPR-Cas12a has emerged as an attractive molecular scissor alternative to Cas9 owing to its unique features and advantages, including fewer off-target effect, an alternative PAM sequence, pre-crRNA processing, and indiscriminate single-stranded DNase activity. Notably, the indiscriminate DNase activity enables Cas12a to be used as a platform for nucleic acid detection. However, despite these advantages, Cas12a has not been well utilized as recently reported base and prime editors because it does not have complete nickase variants, unlike Cas9. Herein, we provide a thorough understanding of the mechanisms that govern the generation of complete double-stranded DNA breaks by a single catalytic site of Cas12a using single-molecule FRET assays to improve our ability to develop a rational design for more potently engineered Cas12a. This would extend the range of applications of Cas12a genetic scissor in the future.

### Keywords:

CRISPR, Cas12a, Single-molecule FRET, Genetic scissor, DNA cleavage

## The Michaelis-Menten Rate Law beyond the Steady State and Its Application to Circadian Dynamics

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### Abstract:

The Michaelis-Menten (MM) rate law has been applied to a wide range of problems to describe the chemical reaction dynamics. Despite being the dominant paradigm, MM rate law has limited applicability for the systems with fast-varying substrate concentrations. This is due to the requirement, often called the quasi-steady-state (QSS) condition, that the concentration of the reaction intermediates should approach the equilibrium much faster than the substrate concentrations, which is not the case for the systems with oscillatory dynamics. In this study, we present the revised MM rate law for the time-varying bio-molecular concentrations by relaxing the QSS condition. Particularly for the mammalian circadian system, we show that our revised MM rate law better captures the conditions of oscillations, the oscillation periods, and the emerging rhythmicity in protein degradation rates.

### Keywords:

chemical reaction dynamics, Michaelis-Menten, quasi-steady-state, mammalian circadian system

## Alternation of replication protein A binding mode on single-stranded DNA by NSMF potentiates RPA phosphorylation by ATR kinase

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### Abstract:

Replication protein A (RPA) is a eukaryotic single-stranded DNA (ssDNA) binding protein. RPA dynamically interacts with ssDNA in various binding modes depending on the DNA length occupied by RPA. RPA plays essential roles in DNA metabolism including replication, repair, and recombination. Especially, accumulation of RPA on ssDNA due to replication stress initiates DNA damage response (DDR) by activating ATM and RAD3-related (ATR) kinase, which phosphorylates downstream DDR proteins including RPA. On the other hand, it was recently reported that N-methyl-D-aspartate receptor synaptonuclear signaling and neuronal migration factor (NSMF) promotes RPA2 phosphorylation in response to replication stress. However, the detailed mechanism underlying the ATR-mediated RPA2 phosphorylation by NSMF remains elusive. Here, we observed that NSMF colocalizes with RPA at DNA damage sites and physically interacts with RPA in vivo and in vitro. From biochemical assays using purified RPA and NSMF, we found that NSMF dislodges RPA from ssDNA in part. Single-molecule assay allowed quantitative analysis on the RPA dissociation induced by NSMF, suggesting that NSMF rearranges RPA binding modes from unstable state to stable one. Furthermore, we revealed that the stable binding mode of RPA enhances RPA2 phosphorylation by ATR. Our findings give insight into a new role of NSMF in ATR pathway.

### Keywords:

NSMF, RPA, ATR phosphorylation

## A Fast and Integrated Qubit Control System

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<sup>2</sup>Product Manager, Zurich Instruments

### Abstract:

Find out how the SHFQC Qubit Controller can help you speed up system tune-up and complex algorithm execution, and learn how to use the SHFQC to control, read out and perform fast feedback on up to 6 superconducting qubits with a single instrument. We also show how the SHFQC integrates into larger qubit control systems, demonstrate the instrument's performance and discuss the latest innovations characterizing the second generation of our Quantum Computing Control System.

### Keywords:

Qubit Control System, SHFQC

## Optimize the Signal Acquisition for Optics and Photonics Measurements

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### **Abstract:**

This webinar focusses on four prototypical techniques in optics and photonics: tunable diode laser absorption spectroscopy (TDLAS), pump-probe spectroscopy, in particular stimulated Raman scattering (SRS) microscopy, and carrier envelope offset (CEO) stabilisation. You will learn how to choose the most suitable measurement scheme for your experiment, e.g. a lock-in amplifier or a boxcar averager, and you will find out how to save precious measurement time and record high-quality data with the highest signal-to-noise ratio.

### **Keywords:**

Photonics, TDLAS, Raman scattering

## Readout DAQ system of a dual-readout calorimeter of Test Beam 2022 for future e+e- collider

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### Abstract:

To explore the origin of mass and its correlation with Higgs particles, High-Energy Physics (HEP) experiments with future e+e- colliders, such as FCC-ee and CEPC, are proposed, and the primary detection system has been designed. Dual-Readout Calorimeter (DRC), which uses two different optical fibers, is one of the subsystems to measure the energy and momentum of leptonic particles and hadrons in future HEP experiments. In June-July 2022, KFC DREAM (Korea Future Collider Dual-READout Method) team will have the test beam for two weeks with the lepton and hadron beams to measure the nuclear interaction length and the operational performance of two prototype DRC modules at CERN. The prototype DRC consists of 2.5 m optical fibers (scintillation and Cerenkov), absorber (Cu), readout detectors (MCP-PMTs, PMTs, and SiPMs), and a data acquisition (DAQ) system. The readout detectors of one module are two MCP-PMTs, and 6 PMTs, and the other module has 400 SiPMs and 16 PMTs. The DAQ system has two operational modes, fast DAQ and waveform modes, with bin event mode, and to obtain an excellent position and time resolution (<50 ps), DRS (Domino Ring Sampler) chip has been used. Also, it has self- and external trigger modes. The main parts of the detector frames and readout DAQ system were delivered last December. We will present the preparation of the readout DAQ system of two copper modules for the Test Beam at CERN in June-July 2022.

### Keywords:

FCC-ee, Dual-Readout Calorimeter, Test Beam, readout DAQ system, DRS4

## Status of energy reconstruction performance study of the dual-readout calorimeter

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### Abstract:

The dual-readout calorimeter (DRC) is one of the future collider calorimeter candidate for FCC-ee and CEPC. Using both Cerenkov and Scintillation fibers, it shows excellent performance with measuring both EM and hadronic processes. Due to projective geometry of modules implemented in DRC, there exists energy loss while reconstructing the GEANT4 simulated events. In this study, we presents the energy reconstruction performance of DRC with projective shape modules using various GEANT4 simulated events.

### Keywords:

Dual-readout calorimeter, Future collider, Detector simulation

## Hadronic Tau Identification for the Dual-Readout Calorimeter using Vision Transformer with Hyperparameter optimization

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### Abstract:

Dual-Readout Calorimeter (DRC) is a calorimeter candidate for future colliders such as FCC-ee. DRC has high resolution for charged and neutral particles, so its resolution may help to identify hadronic tau decay modes. The potential of Vision Transformer (ViT) for hadronic tau identification was revealed by our previous investigations. To maximize the identification performance, we investigate the optimization of hyperparameters, which have to be chosen before the training step.

### Keywords:

Machine Learning, Calorimeter

## Reconstruction of 3D shower shape with the dual-readout calorimeter

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### Abstract:

The technique of shower shape reconstruction is rapidly evolving with modern-day calorimetry, rooted in the outstanding achievement of the particle-flow algorithm of LHC experiments. The dual-readout calorimeter is a next-generation calorimeter of the IDEA detector concept proposed for future e+e- colliders such as FCC and CEPC. We explore the possibility of 3D shower shape reconstruction and potential application to the particle-flow technique with a longitudinally unsegmented dual-readout calorimeter using signal processing on the silicon photomultipliers' timing information.

### Keywords:

Dual-readout, Particle-flow, FCC, calorimeter, signal processing

## DAQ system commission of the dual-readout calorimeter modules.

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### Abstract:

Dual-readout calorimeter(DRC) has been proposed in IDEA detector conceptual design report (CDR) for future e+e- collider.

DRC are implemented by two different types of optical fibers(Cerenkov and scintillation fibers), allowing simultaneous measurement of the energy and momentum of electromagnetic and hadronic particles.

DAQ system consists of HV power supply, discriminator(set threshold), logic unit(and, or gate), etc...

We proceed the cosmic muon and electron beam test using the DRC modules and check the scintillation and Cerenkov signals.

We present the progress of the DRC module cosmic muon and electron beam test in this presentation.

### Keywords:

dual-readout calorimeter, FCC colider, DAQ system

## Module assembly R&D of the Dual-Readout Calorimeter for future e+e- colliders

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### Abstract:

The dual-readout calorimeter (DRC), consisting of scintillating and čerenkov fibers, is one of the calorimeter candidates in future e+e- colliders. We are building 2 modules that are made up of čerenkov fibers and scintillating fibers. Module 1 is divided in 4 readout towers, one of which is equipped with two MCP-PMT. In addition, module 1 consists of different kinds of scintillating fiber. Module 2 is divided in 9 towers with the central one read out with 400 SiPMs. All other towers are equipped with PMTs. As the first step, we will present the process to assemble the modules in this talk. The process of the assembly is divided by 3 steps: preparation, assembly, and reflector. The final step after the assembly is the readout system. 3 types of photomultipliers will be installed on modules at the final step.

### Keywords:

Dual-readout Calorimeter, Future collider, Prototype

## Update of calibration and EM/jet energy resolution study with 4pi dual-readout calorimeter

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### Abstract:

The dual-readout calorimeter, which is the new technology of the calorimeter, has been proposed in the conceptual design report of both FCC-ee and CEPC projects. In this presentation, we will show the result of calibration and EM/Jet energy resolution study for the dual-readout calorimeter with GEANT4 simulation. Calibration of dual-readout calorimeter has been performed by 20 GeV electron measuring corresponding energy to a photoelectron for each component. EM and jet energy resolution of the dual-readout calorimeter is measured with various energy of electron and u quark jet on the basis of calibration constant. The anti-kt algorithm is used to reconstruct jets based on the measured energy with the calorimeter. The high quality energy resolution for jets can be achieved by measuring the electromagnetic shower fraction of hadron showers and correcting their energy event-by-event basis.

### Keywords:

Calorimeter, Energy resolution, Calibration, Jet

## Design of the compact TPC for a high-precision 3D beam diagnostic system

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### Abstract:

A compact Time Projection Chamber (TPC) is a good candidate detector for the three-dimensional (3D) beam profile measurement of electron or ion beam. Initially, simulation studies with COMSOL and Garfield++ were performed to design the beam monitor based on TPC. First off, the study using COMSOL multiphysics calculated the electric field distribution in the field cage and suggested an optimal design of the inner structure of the compact TPC. The transport properties of electrons in the Ar-based gases were simulated in Garfield++ to decide the drift length of the field cage. Finally, the electron avalanche in a single GEM has been studied by simulating the motion and amplification of electrons in the Ar-based gases using COMSOL and Garfield++. In this talk, we will present the design of the compact TPC for a high-precision 3D beam diagnostic system derived with COMSOL and Garfield++ simulations.

### Keywords:

Time Projection Chamber, GEM-TPC, Garfield++, COMSOL, beam diagnostics

## Progress Report of SND@LHC Experiment

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### Abstract:

Most of LHC experiments such as CMS, ATLAS and LHCb can only detect particles produced in the central region. But most of the cross sections are in the forward region where production angles are very small. Many energetic hadrons, neutrinos and feebly interacting particles (FIPs) can be produced in the forward direction. The SND@LHC detector can detect "forward moving particles" which will cover the high pseudo-rapidity region ( $7.2 < \eta < 8.6$ ). The goals of the SND@LHC experiment is to detect directly collider neutrinos at TeV energies for the first time and to search for FIPs in an unexplored domain. The SND means "Scattering and Neutrino Detector" including Nuclear emulsion targets. It can detect scattering of neutrinos and that of light dark matter. The detector is installed in TI18 tunnel, 480m away from ATLAS IP and positioned slightly off the beam axis on the opposite side of FASER experiment. Data taking is expected to begin from LHC Run 3 in 2022. In this talk, we will report the progress of the experiment.

### Keywords:

SND@LHC, LHC Neutrino, Nuclear Emulsion

# Dark gauge boson production from neutron stars vis nucleon-nucleon bremsstrahlung

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## Abstract:

We discuss the dark gauge boson emission from neutron stars via nucleon-nucleon bremsstrahlung. Through the rigorous treatment of the effective field theory prescription and the thermal effect, we derive the relevant couplings of dark gauge bosons to hadrons in the medium. As a specific example, the  $U(1)_{B-L}$  gauge boson scenario is chosen to investigate dark gauge boson emissivities during supernovae and cooling of young neutron stars. From the stellar cooling argument, we obtain the constraints on the  $B-L$  gauge coupling for given gauge boson masses in two observations: the duration of the supernova neutrino signal of SN1987A, and the inferred x-ray luminosity of the compact object in the remnant of SN1987A (NS1987A). In particular, the constraint from SN1987A on the  $U(1)_{B-L}$  gauge boson scenario is revisited. The excluded gauge coupling due to the emission of transverse polarizations is an order of magnitude enhanced compared to the previous derivation. There is also a newly excluded parameter space due to the emission of longitudinal polarizations.

## Keywords:

Beyond the Standard Model

## Models for self-resonant dark matter.

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### Abstract:

We consider a new mechanism for enhancing the scattering cross-section for dark matter without a light mediator. We find that the self-resonant mechanism can be applied to multiple components of dark matter with various spins. We discuss the possibility that self-resonant dark matter is connected to the Standard Model via dark photon or dark Higgs portals. And we show the cases that explain the current relic density while avoiding experimental bounds.

### Keywords:

Dark Matter, self-resonant

## Phenomenology of a two-component dark matter model

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### Abstract:

We study a two-component dark matter model consisting of a Dirac fermion and a complex scalar charged under new  $U(1)$  gauge group in the hidden sector. The dark fermion plays the dominant component of dark matter which explains the measured DM relic density of the Universe. It has no direct coupling to ordinary standard model particles, thus evading strong constraints from the direct DM detection experiments. The dark fermion is self-interacting through the light dark gauge boson and it would be possible to address that this model can be a resolution to the small scale structure problem of the Universe. The light dark gauge boson interacting with the standard model sector is also stable and composes the subdominant DM component. We investigate the model parameter space allowed by current experimental constraints and phenomenological bounds. We also discuss the sensitivity of future experiments such as SHiP, DUNE and ILC, for the obtained allowed parameter space.

### Keywords:

two-component dark matter, small scale structure problem, dark matter detection

## Reheating and Dark Matter Freeze-in in the Higgs-R<sup>2</sup> Inflation Model

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### Abstract:

The Higgs inflation perfectly agrees with the CMB observation, but suffers from a unitarity problem due to a large non-minimal coupling of Higgs field to the Ricci scalar. Recently, it has been shown that introducing a Ricci square term (R<sup>2</sup> term) in the Higgs inflation can solve this problem. In this talk, we discuss the post-inflationary dynamics for reheating and freeze-in dark matter in the Higgs-R<sup>2</sup> model. Taking the perturbative approach for reheating, we determine the evolution of the temperature for radiation bath produced during inflation and determine the maximum and reheating temperatures of the Universe. Also, adopting a singlet scalar dark matter, we discuss the freeze-in production of dark matter both from the non-thermal scattering during reheating and the thermal scattering after reheating.

### Keywords:

inflation, Reheating, Dark matter

## Inflation and reheating in Higgs-sigma models

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### Abstract:

There is a unitarity problem in Higgs inflation related to a large non-minimal coupling with gravity. Introducing a new scalar degree of freedom of sigma-model type, we consider a UV completion of Higgs inflation, recovering unitarity up to the Planck scale while maintaining inflationary observables in agreement with Planck data.

After inflation, a period of reheating is needed in order to transfer the energy from the inflaton condensates to the Standard Model and Dark Matter particles. Taking the perturbative approach, we determine the maximum and reheating temperatures of the Universe.

We find that the Higgs condensate dominates the reheating dynamics, determining the reheating temperature up to about  $10^{14}$  GeV.

### Keywords:

Inflation, Reheating, sigma models, Higgs Inflation

# Gravitational Waves and PBHs from Tachyonic Instability in Higgs- $R^2$ Inflation

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## Abstract:

The running of the Higgs self coupling induces numerous phenomena in early universe cosmology. In this talk I revisit Higgs- $R^2$  inflation with the running Higgs coupling. In this scenario, the Higgs running induces turns in the trajectory with tachyonic mass, leading to a temporal tachyonic growth in the curvature perturbation, ultimately resulting in a sharp peak in the curvature power spectrum. This effect induced by the Higgs leaves phenomena in the form of stochastic gravitational waves, where proposed GW observatories will be able to probe in the near future.

## Keywords:

Gravitational Waves, Cosmological Perturbations, Higgs Inflation, Inflation

## Reheating in Models with Non-minimal Coupling in metric and Palatini formalisms

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### Abstract:

We study reheating of inflationary models with general non-minimal coupling  $K(\phi)R$  with  $K(\phi) \sim \sqrt{V(\phi)}$  where  $R$  is the Ricci scalar and  $V$  is the inflaton potential. In particular, when we take the monomial potential  $K(\phi) \propto \phi^m$  with  $m \in \mathbb{Z}_+$ , we provide general analytic expressions for cosmological observables. We consider a wide range of non-minimal coupling  $\xi \in [0, \infty)$  in metric and Palatini formalisms and derive the predictions for cosmological observables and the reheating temperature taking a general equation of state parameter  $w_{\text{reh}}$ .

### Keywords:

inflation, reheating, non-minimal coupling, Palatini formalism

## Non-minimally assisted chaotic inflation

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### Abstract:

Conventional wisdom says that a chaotic inflation model with a power-law potential is ruled out by the recent Planck-BICEP/Keck results. We find, however, that the model can be assisted by a non-minimally coupled scalar field and still provides a successful inflationary model which is compatible with observationally acceptable ranges. Considering a power-law chaotic inflation model of the type  $V = M^4 \varphi^n$  with  $n = \left\{ 2, 4/3, 1, 2/3, 1/3 \right\}$ , we show that  $n = 1/3$  ( $n = \left\{ 2/3, 1/3 \right\}$ ) may be revived with the help of the quadratic (quartic) non-minimal coupling of the assistant field to gravity.

### Keywords:

Chaotic Inflation

## Analysis of test beam data for ALICE ITS3

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### Abstract:

A new silicon vertex detector (ITS3) for the ALICE experiment is planned to be installed during the LHC long shutdown 3, and it is currently under development. One main feature of the ITS3 is to use a bent chip covering a large area to significantly reduce the material budget. Various types of silicon sensors have been produced and tested with existing APLIDE chips to evaluate their performance. Currently, the test beam data is being analyzed. In this presentation, we will introduce the test beam of silicon sensors for the ITS3 and present the status of the analysis of test beam data.

### Keywords:

ALICE, ITS3, Test beam

## Development of the STARK Silicon Detector Array at CENS.

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### Abstract:

We have been developing a new barrel type silicon telescope array, STARK, to perform future studies of nuclear reactions, structures and nuclear astrophysics. The STARK is composed of 40 new double-sided silicon strip detectors named Micron X6 style, each of which has 8 resistive strips on its junction side and 4 normal strips on its ohmic side. High angular coverage and good energy and angle resolution of the array are expected to be achieved enough to scrutinize nuclear reactions. The new X6 detectors have been delivered and tested with a fission source emitting 5.7 MeV alpha particles. The full array design is completed and the supporting frame with a translation system along three-axes is manufactured so that one can align the array. PCB boards for rerouting signal lines and detector bias lines are designed and manufactured. Corresponding DAQ system has been configured with the GET (General Electronics for TPCs) in order to handle thousands of signal channels. The details about the current status of the STARK detector system development will be presented.

### Keywords:

Nuclear Astrophysics Experiments, Nuclear Structure, Nuclear Reaction, Silicon Telescope, Silicon detector system

## Development and characterization of new position-sensitive silicon strip detectors at CENS

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### Abstract:

Direct reaction experiments in inverse kinematics are one of the best suited tools to probe a broad range of nuclear properties, providing great insight into the nuclear structure of exotic nuclei and allowing the measurement of reactions relevant to many astrophysical scenarios. In order to fully exploit the RAON facility currently under construction, the CENS group has devoted a large amount of effort to develop nuclear instrumentations, such as ATOM-X Active Target TPC and STARK Silicon Telescope Array, specially designed for important direct reaction experiments. An integral part of these detector devices is the Micron X6 position-sensitive double sided silicon strip detector. This detector is segmented in 4 strips on its ohmic side and 8 resistive charge-splitting strips on its junction side enabling an excellent position measurement of charged particles with a much smaller number of signals than traditional DSSSD with similar position resolution.

Detailed specifications of the X6 detectors, optimized initial characterization methods and preliminary reports of their performance in terms of energy and position resolution will be presented. Outlook for future commissioning will also be discussed.

### Keywords:

Silicon Telescope, Silicon detector array, Nuclear Structure, Nuclear Reaction, Nuclear Astrophysics

## Active Target TPC development in CENS

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### Abstract:

Active Target Time Projection Chamber (AT-TPC) is one of the advanced charged particle detectors and it provides tracks of particles including beam and recoils. Thanks to the advantage, it is in high demand for current and future rare isotope beam experiments. The energy and position resolution of the detector can be enhanced due to the three dimensional tracking of the charged particle. A new active target TPC, so called AToM-X, is under development at the Center for Exotic Nuclear Studies (CENS) for the precise measurement of the key nuclear reactions in the nuclear astrophysical process. Details of the development status will be reported. We will also present the upgrade of the TexAT detector for upcoming reaction measurement at CRIB, RIKEN.

### Keywords:

Active Target Time Projection Chamber, charged particle detector, AToM-X, Nuclear Astrophysics, Nuclear Structure

## A New Analysis Method of the TexAT Experimental Data at High Beam Intensity

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### Abstract:

The direct measurement of  $^{14}\text{O}(\alpha,p)^{17}\text{F}$  reaction rate is proposed, using TexAT detector, which is a type of active-target time projection chamber. Due to its low estimated cross section, the high beam intensity is needed to acquire enough statistics. In order to study the performance of TexAT with the high beam rate, a commissioning experiment of  $^{14}\text{N}(\alpha,\alpha)^{14}\text{N}$  was conducted at Texas A&M University. The stable  $^{14}\text{N}$  beam with its intensity of  $3 \times 10^5$  pps was delivered to the TexAT. The TexAT successfully operated under the high beam rate condition, but several analysis difficulties were emerged from the data: a distorted pedestal due to induced negative signals and too many beam signals in an event window. Development of appropriate analysis logic to sort out a type of event is in progress. Detailed analysis processes will be discussed in the presentation.

### Keywords:

AT-TPC,  $^{14}\text{O}(\alpha,p)^{17}\text{F}$ ,  $^{14}\text{N}(\alpha,\alpha)^{14}\text{N}$

## Track Reconstruction in the Active-Target Time Projection Chamber using Machine Learning Methods

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### Abstract:

We report simulation results on the track recognition and momentum measurement in the active-target time projection chamber (AT-TPC) for stellar nucleosynthesis reaction experiments. A simulation model of the AT-TPC involves low-energy  $^{12}\text{C}+\alpha$  reactions and electromagnetic interactions in He gas. First, we generated trajectories of low-energy projectiles and recoil nuclei under 2.5 T of a superconducting magnet using Geant4 simulations. Then, we performed the track reconstruction and momentum measurement using machine learning methods. This talk will present preliminary results on the tracking performance using machine learning methods and discuss the feasibility for measuring reaction rates for  $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$  reaction at stellar energies in the COREA (Carbon Oxygen Reaction Experiment with AT-TPC) experiment.

### Keywords:

Active-target TPC, Stellar Nucleosynthesis, Geant4, Deep Learning

## Analysis Improvement of Active Target Time Projection Chamber Data Using Deep Learning Methods

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### Abstract:

Deep Learning techniques have been very popular for science data analysis. In this work, we implemented a deep learning technique to improve the data analysis of a time projection chamber, Texas Active Target. Recorded waveforms were classified into three different classes which are a particle, a noise, and a particle piled up with noise group. A plain 1D convolutional neural network was applied for this study. We achieved high performance both on the test dataset. By removing the noise signals classified by the model, we obtained the clean dataset. Improved track images and PID plots will be presented.

### Keywords:

TPC, AT-TPC, Machine Learning, Deep Learning

## Coupling between electrons and charge density wave fluctuation and its role on superconductivity

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### Abstract:

Pairing two electrons into Cooper pair is a key ingredient of superconductivity. While phonon mediates the pair in the conventional superconductivity of Bardeen-Cooper-Schrieffer (BCS) theory, the pairing glue other than the phonon is anticipated to be required for unconventional superconductivity that normally comes after the suppression of symmetry-broken phases, so-called competing behavior. Similarly, an intricate competition between the charge density wave (CDW) order and superconductivity is exhibited in numerous CDW systems, suggesting CDW-originated bosonic mode as a possible pairing glue. However, the role of the CDW-originated bosonic modes to superconductivity remains elusive.

In this talk, I will present the spectroscopic evidence of coupling between electron and CDW fluctuation, investigated by a temperature- and intercalation-dependent kink in the angle-resolved photoemission spectra of 2H-PdxTaSe<sub>2</sub>. Kinks are observed only when the CDW phase exists, regardless of whether a long- or short-range order is established. Notably, the coupling strength is enhanced upon long-range CDW suppression. Interestingly, estimation of the superconducting critical temperature by incorporating the observed coupling characteristics into McMillan's equation yields results closely resembling the known values of the superconducting dome, suggesting a compelling possibility that this new coupling mediates Cooper pairs in 2H-TaSe<sub>2</sub>.

### Keywords:

Charge density wave , superconductivity, 2H-TaSe<sub>2</sub>, angle-resolved photoemission spectroscopy

## Strong antiferromagnetic proximity coupling in a heterostructured superconductor $\text{Sr}_2\text{VO}_{3-\delta}\text{FeAs}$

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### Abstract:

We report observation of strong magnetic proximity coupling in a heterostructured superconductor  $\text{Sr}_2\text{VO}_{3-\delta}\text{FeAs}$ , determined by the upper critical fields  $H_{c2}(T)$  measurements up to 65 T. Using the resistivity and the radio-frequency measurements for both  $H // ab$  and  $H // c$ , we found a strong upward curvature of  $H_{c2}^c(T)$ , together with a steep increase of  $H_{c2}^{ab}(T)$  near  $T_c$ , yielding the anisotropic factor  $\gamma_H = H_{c2}^{ab}/H_{c2}^c$  up to  $\sim 20$ , much higher than those of other iron-based superconductors. These are attributed to the Jaccarino-Peter effect, rather than to the multiband effect, due to strong exchange interaction between itinerant Fe spins of the FeAs layers and localized V spins of Mott-insulating  $\text{SrVO}_{3-\delta}$  layers. These findings provide evidence for strong antiferromagnetic proximity coupling, comparable with the intralayer superexchange interaction of  $\text{SrVO}_{3-\delta}$  layer and sufficient to induce magnetic frustration in  $\text{Sr}_2\text{VO}_{3-\delta}\text{FeAs}$ .

## Abnormal pressure-induced quantum phase transition from superconducting to charge-density wave state in LuPd<sub>2</sub>In and LuPtPdIn

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### Abstract:

We investigate the pressure effects on the electronic structures and phonon properties of rare-earth-based cubic-heusler compound LuPd<sub>2</sub>In and LuPtPdIn, on *ab initio* density functional theory. We find the unusual phase transition from superconducting (SC) to charge-density wave (CDW) state under pressure, which is quite abnormal in the aspect that pressure usually suppresses CDW state in typical systems. The SC transition temperature ( $T_c$ ) of LuPd<sub>2</sub>In and LuPtPdIn increases first with increasing pressure up to 28 GPa and 13 GPa, above which CDW state takes place. We demonstrate that the extraordinary transition originates from phonon softening instability at  $\mathbf{q} = \mathbf{M}$  in Brillouin zone.

### Keywords:

superconductor, phonon

## Theory of superconductivity in doped quantum paraelectrics

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### Abstract:

Recent experiments on Nb-doped SrTiO<sub>3</sub> have shown that the superconducting energy gap to the transition temperature ratio maintains the Bardeen-Cooper-Schrieffer (BCS) value throughout its superconducting dome. Motivated by these and related studies, we show that the Cooper pairing mediated by a single soft transverse-optical phonon is the most natural mechanism for such a superconducting dome given experimental constraints, and present the microscopic theory for this pairing mechanism. Furthermore, we show that this mechanism is consistent with the  $T^2$  resistivity in the normal state. Lastly, we discuss what physical insights SrTiO<sub>3</sub> provides for superconductivity in other quantum paraelectrics such as KTaO<sub>3</sub>.

### Keywords:

superconductivity, ferroelectricity, odd parity phonon, phenomenological model

## Flexoelectricity in a ferromagnetic metal

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### Abstract:

Electric fields have played a key role in discovering and controlling exotic electronic states of condensed matter. However, electric fields usually do not work in metals as free carriers tend to screen electrostatic fields. While a pseudo-electric field generated by inhomogeneous lattice strain, namely a flexoelectric field, can in principle work in all classes of materials, it remains experimentally unexplored in metals. Here, using heteroepitaxy and atomic-scale imaging, we show that flexoelectric fields can polarize a metallic oxide SrRuO<sub>3</sub> with unexpectedly large Ru off-center displacements. We also observe that the flexoelectrically induced polar state of SrRuO<sub>3</sub> leads to sizable lattice expansion, similar to the electrostrictive expansion caused by ionic displacements in dielectrics under an external electric field. We further suggest that flexoelectrically driven Ru off-centering promotes strong coupling between lattice and electronic degrees of freedom, possibly enhancing the ferromagnetism of SrRuO<sub>3</sub>. Beyond conventional electric fields, flexoelectric fields may universally engender novel electronic states and their control via pure atomic displacements in a nondestructive and fast manner.

### Keywords:

flexoelectricity, strain gradient, metallic, ferromagnetism, transition metal oxide

## Magnetotransport at the interface between heavy metal and antiferromagnetic oxide

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### Abstract:

Noncollinear magnetic chromites have displayed not only a wide spectrum of antiferromagnetism but also possible multiferroic properties.  $\text{YCrO}_3$  (YCO) is one example of orthorhombic chromites possessing a complex antiferromagnetic (AFM) configuration as well as spin-lattice coupling via antisymmetric exchange interaction along Cr-O-Cr bonds. The noncollinear AFM order along with weak ferromagnetism of YCO has not been well understood in terms of strain engineering and interfacial magnetotransport. We have studied structural and magnetic properties of epitaxial YCO thin films grown on four different substrates by performing X-ray diffraction, first-principles calculation, X-ray absorption spectroscopy, and magnetic property measurement equipped with SQUID magnetometer. Furthermore, we have explored the anomalous Hall effect and unidirectional magnetoresistance at the interface between YCO and Pt in order to understand the interplay between a noncollinear antiferromagnet and a heavy metal with strong spin-orbit coupling.

### Keywords:

Transition-metal oxides, Interfacial magnetism, Magnetoresistance, Antiferromagnets

## Inhibition of atomic interdiffusion in heteroepitaxy system via a graphene interlayer

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### Abstract:

Due to the heterogeneity between the seed substrate and required materials, defect suppression and control of the interface are considered important factors in heteroepitaxy for future electronic, spintronic, and energy storage materials. However, there are critical issues in conventional heteroepitaxy for growing highly oriented single-crystalline materials such as defect density formed by lattice mismatch and substrate dependence. In order to overcome these limitations, remote epitaxy has been proposed as a new approach to growing various materials with low defect densities compared to the conventional epitaxy method.[1] In addition, the grown materials can be exfoliated and transferred from the rigid substrate using a graphene interlayer. Although the role of a graphene interlayer on epitaxial growth was reported by both theoretical analyses and experimental results in various crystal systems,[2] the effect of remote heteroepitaxy according to the material combination through graphene has not clearly identified yet.

Here, we directly observe the interface of epitaxial films grown on the graphene-coated substrate, wherein the graphene is formed by dry-transferred from SiC substrates using a metal stressor layer of by wet-transferred from Cu-foils to unveil the role of interfaces including transferred graphene on atomic interaction for epitaxial growth.[3] Based on these findings, GaP and InP with different thicknesses are formed onto graphene-coated GaAs substrate to identify the effect of graphene interlayer on heteroepitaxial growth. In conventional heteroepitaxy, a non-uniform interface is formed to relax the strain generated by lattice mismatch as the thickness of the film increases, and the formation of GaP in InP/GaAs system via atomic interdiffusion was also observed. However, single-crystalline monolayer graphene in remote heteroepitaxy effectively prevents the atomic interdiffusion, as well as suppresses the formation of defects through a fully relaxed interface. These findings show that the growth of heterogeneous materials on graphene provides a uniform interface by controlling interatomic diffusion, and freestanding single crystals with controlled defect density through graphene can be utilized in various fields.

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[2] Polarity governs atomic interaction through two-dimensional materials. *Nature Materials*, **17**(11), 999-1004 (2018).

[3] Role of transferred graphene on atomic interaction of GaAs for remote epitaxy. *Journal of Applied Physics*, **130**(17), 174901 (2021).

### Keywords:

remote epitaxy, heteroepitaxy, interdiffusion, graphene

## Microspectroscopy Study of Atomically Thin Optical Materials

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### **Abstract:**

Atomically thin materials are a promising candidate for applications in electronic and optical devices with their unique physical properties. Metal-organic Chemical Vapor Deposition (MOCVD) can be used to controllably grow atomically thin materials with desired functionality. Microspectroscopy has become a versatile tool to characterize atomically thin materials. By choosing appropriate optical configurations, various techniques can be used to investigate atomically thin materials with micron-scale spatial resolution. In this presentation, I will present an optical spectroscopic study of the MOCVD grown atomically thin materials, toward emerging optical functionalities.

### **Keywords:**

Optical spectroscopy, Atomically thin materials

## Direct observation of interfacial charge trapping in SrRuO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures through noise spectroscopy

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### Abstract:

Charge transport in conductive oxides is predominantly determined by electron-phonon scattering or - defect scattering. However, when the thickness of the oxide decreases, the charge trapping by point defects starts to influence the electronic properties of the oxide thin film. In this study, we report the interfacial charge trapping phenomena in an atomically thin SrRuO<sub>3</sub> /SrTiO<sub>3</sub> (SRO/STO) heterostructure observed by noise spectroscopy. We demonstrate that the oxygen vacancy point defects in the STO substrates cause the interfacial charge trapping and result in strong low-frequency noise. We verify that the electron transport characteristics of the ultrathin SRO film is dominated not by the conventional electron mobility fluctuation but by the number fluctuation, originated from the interfacial charge trapping. In addition, we appeal that the noise spectroscopy technique can be a simple but powerful method to explore the interfacial charge trapping phenomena in oxide thin film heterostructures.

### Keywords:

Noise Spectroscopy, Interfacial Charge Trapping, SrRuO<sub>3</sub>, SrTiO<sub>3</sub>, Thin Films

## Correlated study of physical properties and atomic structures in 2D materials with Atomic Electron Tomography

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### Abstract:

The field of research in two-dimensional (2D) materials has experienced extraordinary growth during the past decade. To understand the structure-property relationship of 2D materials and heterostructures at the fundamental level, we must know their 3D atomic structure with high precision and correlate their physical properties with their atomic structure [1].

In this talk, I will show the recently-developed scanning atomic electron tomography (sAET) to localize the 3D atomic coordinates in 2D materials and heterostructures with picometer precision [2] [3]. Using Re-doped MoS<sub>2</sub> monolayer and MoS<sub>2</sub>-WSe<sub>2</sub> lateral heterostructure as model systems, I will show the correlated study of 2D materials structures and band engineering properties at the atomic level. We identified many fundamental 3D atomic structures associated with the sample, such as dopants, vacancies and atomic-scale ripples and measured the 3D atomic displacement and the full strain tensor of the 2D material. Furthermore, the experimental 3D atomic coordinates were used as direct input to DFT to correlate crystal defects with the electronic band structure at the single-atom level. We observed stark differences between the band structures obtained from the experimental and relaxed atomic models. We anticipate sAET will be generally applicable to the determination of the 3D atomic coordinates of 2D materials, heterostructures and thin films.

References:

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- [2] Tian, X., et al., *Nat. Mater.* **19**, 867-873 (2020).
- [3] Tian, X., et al., *Sci. Adv.* **7**, eabi6699 (2021).

### Keywords:

scanning atomic electron tomography, 2D materials, 3D atomic structure

# Operando Transmission Electron Microscopy Investigation on Domain Dynamics in 2D Ferroelectric Materials

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## Abstract:

Control of interlayer stacking angle in two-dimensional (2-D) van der Waals (vdW) heterostructure enables one to engineer the crystal symmetry to imprint novel functionality. By stacking two layers of transition metal dichalcogenides (TMD) with designed twist angle, one can break the inversion symmetry and thereby develop vertical electric polarization. The direction of the electric polarization can be switched electrically, suggesting that the twisted bilayer TMD can host ferroelectricity. Such ferroelectricity reported in twisted bilayer vdW system is distinguished from conventional ferroelectrics in that the lateral sliding of the constituent layers induces vertical electric polarizations. Due to the reduced dimension, the ferroelectric domains do not require forward growth along the third dimension, suggesting unconventional 2-D domain dynamics under an applied electric field. Here we employ *operando* transmission electron microscopy (TEM) to investigate the domain dynamics in 2-D vdW ferroelectrics. *Operando* TEM technique enables one to examine the structural change in the environment that mimics the device operating condition. On a thin SiN based TEM compatible platform, we fabricated double capacitor structure on 2D vdW ferroelectrics. Electrical gating in double capacitor structure and real time observation of structural change in a simultaneous manner provides an insight onto the switching mechanism of the 2-D vdW ferroelectrics.

## Keywords:

ferroelectricity, transmission electron microscopy, 2D van der Waals interface

## Surface inhomogeneity examined by spatially-resolved ARPES

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### Abstract:

Angle-resolved photoemission spectroscopy (ARPES) has been considered one of the most powerful tools in modern materials science because it allows us to directly observe the electronic states related to the macroscopic physical properties of materials. Accordingly, the ARPES technique has been continuously developed to improve resolution and further implement additional functions to resolve spin, time, or spatial domain [1]. Among the latest advanced ARPES techniques, spatially-resolved ARPES has recently attracted growing interest because of its capability to obtain local electronic information at the micro- or nano-metric length scales by condensing an incident light [2-4]. In this talk, we will introduce recent progress on spatially-resolved ARPES [4] and then present its capability to investigate the surface inhomogeneity in Y-based high- $T_c$  cuprates [5, 6]. In addition, we will present machine-learning-based analysis methods for automatically classifying a large amount of spatial mapping ARPES data by spectral features [7].

### References

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### Keywords:

ARPES, Spatially-resolved ARPES, Surface inhomogeneity, machine learning

## Probing catalytic reactions of single molecules on TiO<sub>2</sub> surface with STM

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### Abstract:

The scanning tunneling microscopy (STM) is a unique technology that can resolve the atomic-scale structure and electronic structure of surfaces and single molecules. STM studies on model catalyst systems have enabled us to understand a lot of fundamental and important questions by direct observation of the relevant systems. I will introduce our recent STM studies on TiO<sub>2</sub> catalysts.

Among various applications of well-known photocatalyst TiO<sub>2</sub>, advanced oxidation process (AOP) is the technology that generally uses the hydroxyl radicals (•OH), the strong oxidants for degradation of organic contaminants in wastewater. We can produce •OH with the help of primary oxidants such as H<sub>2</sub>O<sub>2</sub> and catalysts. When H<sub>2</sub>O<sub>2</sub> and TiO<sub>2</sub> is used together, the concentration of the •OH generated becomes much higher than when used separately, even without UV light. The understanding of this synergistic reaction process would be essential for the further development of AOPs, while very little has been revealed experimentally with respect to H<sub>2</sub>O<sub>2</sub> at the single-molecule level yet. Here, we successfully elucidated the intermediate step of AOP upon adsorption of H<sub>2</sub>O<sub>2</sub> molecules. We found that Ti-O-O-Ti peroxides were formed on the surface of TiO<sub>2</sub>(110) by dissociative adsorption of aqueous H<sub>2</sub>O<sub>2</sub>.

TiO<sub>2</sub> absorbs UV light and decomposes the water molecule into •OH in aqueous condition. One of the drawbacks of using a photocatalyst for water purification is that photocatalytic efficiency is dependent on the amount of available light. We found that modification of TiO<sub>2</sub> surface could enhance the catalytic activity of TiO<sub>2</sub> surface. Due to the increased electronic hole density at the TiO<sub>2</sub> surface from modifications, water molecules were dissociated into •OH even without the irradiation of UV light. The gap states and charge transfer at the interface played an important role in enhanced catalytic performance.

### Keywords:

TiO<sub>2</sub>, STM, photocatalyst, photocatalyst, photocatalyst

## Decoherence of nitrogen-vacancy spin ensembles in a dipolar spin bath in diamond

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### Abstract:

Nitrogen-vacancy (NV) centers in diamond have been developed into essential hardware units for a wide range of solid-state-based quantum technology applications. While such applications require the long spin lifetimes of the NV centers, they are often limited due to decoherence. In this study, we theoretically investigate the decoherence of NV spin ensembles induced by nitrogen impurities (P1 centers), which are one of the most dominant and inevitable magnetic field noise sources in diamond. We combined cluster correlation expansion and density functional theory to compute the Hahn-echo spin coherence time of the NV centers for a broad range of P1 concentrations. Results indicate a clear linear dependence of  $T_2$  on P1 concentrations on a log scale with a slope of -1.06, which is in excellent agreement with previous experimental results. The interplay between the Jahn-Teller effect and the hyperfine interaction in the P1 center plays a critical role in determining the bath dynamics and the resulting NV decoherence. Our results provide a theoretical upper bound for the NV spin  $T_2$  over a wide range of P1 densities, serving as a key reference for materials optimization and spin bath characterization to develop highly coherent NV-based devices for quantum information technology.

### Keywords:

Decoherence, Nitrogen-vacancy (NV) centers

## Probing Spin Casimir Force with Scanning Tunneling Microscopy

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### Abstract:

We theoretically analyze a state-of-the-art experimental method based on a combination of electron spin resonance and scanning tunneling microscopy (ESR-STM), to directly probe the tiny force due to quantum fluctuations of spins. As an application, we consider the Kondo impurity exchange coupled to the probe spin. The ESR-STM setup probe the force by detecting the small level shifts in the probe spin induced by the spin fluctuations of the Kondo impurity. We use the open quantum system approach by regarding the probe spin as the "system" and the Kondo impurity spin as the fluctuating "bath" to evaluate the resonance line shifts in terms of the dynamic spin susceptibility of the Kondo impurity. We consider various common adatoms on surfaces as possible probe spins and estimate the corresponding level shifts. It is found that the sensitivity is most pronounced for the probe spins with transverse magnetic anisotropy.

### Keywords:

scanning tunneling microscopy, electron spin resonance, Casimir force

## A simulation tool for all-electric electron spin resonance using non-equilibrium Green's functions

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### Abstract:

Using a mixed methodology with non-equilibrium Green's functions to treat the transport processes and a reduced density matrix to treat the magnetic degrees of freedom, we have developed a simulation tool to compute the time-dependent current under a periodic or pulsed time-dependent bias in a tunneling junction with a magnetic impurity. The magnetic degrees of freedom are taken into account via a spin Hamiltonian that is rich enough to treat magnetic nanostructures of increasing complexity. The current proceeds through orbitals localized at the nanostructure that are coupled via a Hund's coupling with the rest of the spin of the nanostructure. This full Hamiltonian is rich enough to virtually represent any real experiment of electron spin resonance (ESR) with the scanning tunneling microscope. We will expound the theory, show the solution method and present some results on selected systems for both continuous-wave and pulsed ESR [1,2].

### References:

- [1] J. Reina-Gálvez, N. Lorente, F. Delgado, and L. Arrachea, Phys. Rev. B104, 245435 (2021).
- [2] J. Reina-Gálvez, C. Wolf and N. Lorente, unpublished.

### Keywords:

non-equilibrium Green's functions, reduced density matrix, scanning tunneling microscope, electron spin resonance

# Superconducting Nanoelectromechanics for Sensing and Transduction

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## Abstract:

Nanoscale mechanical systems serve as versatile physical interfaces with their ability to interact with various quantum states such as microwave and optical photons, qubits, spins, and electrons. Therefore, engineering and utilizing these interactions in nanomechanical systems are essential for a wide range of applications in sensing and quantum technology. In this context, superconducting nanoelectromechanical device is of great scientific and technological importance as this on-chip system can support strong electromechanical coupling of microwave fields (~GHz) and mechanical modes (~MHz).

My talk will focus on describing a niobium-based superconducting electromechanical device we developed at KRISS and discuss its linear and nonlinear electromechanics. We employ niobium as a base superconducting material due to its superior superconducting properties compared to those of aluminum. Our device demonstrates fundamental optomechanical effects including electromechanical cooling and amplification, and electromechanically induced reflection at 4.2K and in strong magnetic fields up to 0.8 T. Moreover, this device can be driven beyond the linear regime and presents a nonlinear effect called electromechanical frequency comb. I will discuss the dynamics behind the generation of the frequency comb and their potential applications in nanomechanical sensing. Lastly, I will conclude my talk by briefly describing our ongoing efforts to develop optoelectromechanical quantum transducers at KRISS.

## Keywords:

superconducting electromechanical device

## Twisted van der Waals Josephson junction based on high- $T_c$ superconductor

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### Abstract:

Stacking two-dimensional van der Waals (vdW) materials rotated with respect to each other shows versatility for studying exotic quantum phenomena. Especially, anisotropic layered materials have great potential for such twistrionics applications, providing high tunability. Here, we report anisotropic superconducting order parameters in twisted  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  (Bi-2212) vdW junctions with an atomically clean vdW interface, achieved using the microcleave-and-stack technique. The vdW junctions with twist angles of  $0^\circ$  and  $90^\circ$  showed the maximum Josephson coupling, comparable to that of intrinsic Josephson junctions. As the twist angle approaches  $45^\circ$ , Josephson coupling is suppressed, and eventually disappears at  $45^\circ$ . The observed twist angle dependence of the Josephson coupling can be explained quantitatively by theoretical calculation with the  $d$ -wave superconducting order parameter of Bi-2212 and finite tunneling incoherence of the junction. Our results revealed the anisotropic nature of Bi-2212 and provided a novel fabrication technique for vdW-based twistrionics platforms compatible with air-sensitive vdW materials.

### Keywords:

twistrionics, Josephson junction,  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ , high- $T_c$  superconductor, van der Waals material

## Error Mitigation for Quantum State Tomography of Fixed-frequency Superconducting Transmon Qubits

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### Abstract:

초전도 조셉슨 접합을 이용한 큐비트는 현재 유망한 양자컴퓨터 기술 중 하나이다. 특히 트랜스몬 큐비트는 조셉슨에너지 대비 전하에너지의 비율을 크게 만들어 상대적으로 전하요동에 대한 민감도를 낮춤으로써 큐비트 생존시간 및 결맞음 시간을 향상시킬 수 있어 가장 널리 사용되고 있으며, 그 특성과 응용에 관한 많은 연구가 수행되고 있다. Noisy-intermediate scale quantum (NISQ) 시대에 돌입하면서 양자회로에서 발생하는 에러를 완전히 보정하는 방식이 아니라 측정 데이터를 후 보정 처리(post-processing)를 통해 에러를 줄이는 에러완화(Quantum error mitigation) 연구 또한 활발히 수행되고 있다. 본 연구에서는 초전도 고정주파수를 갖는 초전도 큐비트를 활용하여 양자에러완화 유무에 따라 양자상태단층촬영(Quantum state tomography) 결과를 분석하였다.

### Keywords:

Superconducting Qubit, Error mitigation, Quantum state tomography

## Electrical Improvement using PtSe<sub>2</sub>/PtTe<sub>2</sub> Edge Contact Synthesized by Molecular Beam Epitaxy

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### Abstract:

One-dimensional (1D) edge contact is considered as one of the keys to reduce contact resistance between two-dimensional transition-metal dichalcogenides (TMDs) and contact metal, overcoming the problems of surface contact, such as orbital hybridization and surface damage. Although several studies have investigated edge contact, there are some problems such as inevitable etching damage and a limited area. Herein, a tellurization method is applied to a specific lateral region to fabricate PtTe<sub>2</sub>/PtSe<sub>2</sub>/PtTe<sub>2</sub> edge-contact field-effect transistors (FETs) without etching damage. X-ray photoelectron spectroscopy, Raman spectroscopy, and annular dark-field scanning transmission electron microscopy (ADF-STEM) are used to verify tellurization, which evidences the complete transformation of PtSe<sub>2</sub> to PtTe<sub>2</sub> by the substitution of Se atoms with evaporated Te atoms. Furthermore, tellurization is applied to a specific lateral region by utilizing the hexagonal boron nitride to block the detachment of Se atoms and the interdiffusion of evaporated Te atoms, which is confirmed by Raman spectroscopy and ADF-STEM. Finally, the 1D edge-contact FETs fabricated by tellurization shows a higher on-off ratio and carrier mobility than the surface-contact FET, owing to the reduction in contact resistance. Therefore, the fabrication method of the PtSe<sub>2</sub>-based 1D edge-contact device with free contact resistance can be applied to achieve various TMD-based electrical devices for a high on-off ratio and carrier mobility, which has yet to be demonstrated in large-area TMD-based electrical devices.

### Keywords:

Platinum diselenide, Molecular beam epitaxy, Edge contact, Transition metal dichalcogenides

## Deep learning potentials: Application to the h-BN growth on Pt(111)

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### Abstract:

In this study, we construct deep learning potentials for (B, N)/Pt(111) to simulate the initial process of the hexagonal boron nitride (h-BN) synthesis on the Pt(111) surface. The deep learning potential learns the training data produced by the active learning method. The MD simulations reveal that B adatoms diffuse into the substrate while N adatoms stay on the substrate. Early in the h-BN synthesis process, the B and N adatoms combine to form BN chains, and then the BN chain becomes a Y-shape structure when the B or N adatoms are attached to the side of the BN chain. The Y-shape structure becomes hexagonal as the B and N adatoms are attached more to the Y-shape BN chain. Some of the N adatoms combine to form the N<sub>2</sub> molecule. We also investigate the effect of variable B:N ratio on the h-BN formation. The present results provide deep insights for the growth of 2D materials on the metal surface and expand the versatility of neural network potentials to the growth phenomena.

### Keywords:

Machine learning, Interatomic potential, Pt(111), h-BN, Molecular dynamics

## Manipulating Optical Properties of Monolayer Tungsten Disulfide by Stoichiometry

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### Abstract:

We have studied influence of stoichiometry on the optical properties of chemically synthesized monolayer tungsten disulfide. The monolayer flakes of the tungsten disulfide have been grown by metal-organic chemical vapor deposition (MOCVD). [Nature 550, 229 (2017)] With the help of metal-organic vapor phase precursor, the stoichiometry of flakes can be controlled precisely. We have systematically investigated the optical properties of monolayer tungsten disulfide grown under different chalcogen to metal precursor ratios. This work can pave the way to grow high optical-quality synthetic monolayer crystals and manipulate their optical properties at the growth stage.

### Keywords:

2D material, WS<sub>2</sub>, Photo Luminescence

## Mechanical behaviors of graphene nano-mechanical resonator under strain in different directions

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### Abstract:

In this study, we have fabricated graphene nano-mechanical resonators under strain in different directions and studied its mechanical behaviors. We clamped suspended graphene using PMMA(Poly(methyl methacrylate)) in different shapes to observe strains in uniaxial, biaxial, and radial directions. The mechanical resonance properties of the suspended graphene structures by analyzing their vibrational modes through an optical measurement method using a laser interferometer. In addition, the strain level and direction of the graphene resonators were estimated using AFM topography and force-distance spectroscopy. Therefore, we could demonstrate the direction of residual stress generated by PMMA through the analysis of mechanical characterization of the graphene resonator.

### Keywords:

Graphene, Resonator, Graphene resonator, NEMS, Nano-Electro-Mechanical Systems

## Capacitive graphene gas sensing device and its principle of operation

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### Abstract:

Graphene is one of the promising gas sensing materials due to its unique properties, such as high surface-to-volume ratio, low electrical noise, high conductivity, and ability of gas molecules adsorption. Most research has focused on resistive gas sensing devices in graphene, on the other hand, capacitive gas sensing devices hardly have been reported.

In this presentation, we introduce a capacitive graphene gas sensing device and capacitive NO<sub>2</sub> gas sensing experimental results. We fabricated back-gated graphene field-effect transistors incorporating an aluminum back gate electrode whose surface forms a few nanometers thick oxidized aluminum. In the device, the measured capacitance is the total capacitance of the device, which is the series connection of the geometrical capacitance of the insulating layer and the quantum capacitance of graphene. Due to the characteristics of capacitive measurement, the total capacitance of the device is dominantly determined by the quantum capacitance of graphene when geometrical capacitance is comparable to the minimum quantum capacitance. The absorption of NO<sub>2</sub> molecules makes p-type graphene, which leads to the change in quantum capacitance. As a result, the measured capacitance of the graphene FET device changes depending on the amount of absorbed NO<sub>2</sub> molecules.

Changes in the capacitance were measured for various concentrations of NO<sub>2</sub> gas. The measured capacitance of the device was increased when the concentration of NO<sub>2</sub> gas increased from 1 ppm to 100 ppm. In addition, we extracted residual carrier density induced by absorbed NO<sub>2</sub> from the quantum capacitance of graphene. The extracted residual carrier density explains the operation principle of capacitive gas sensing in the proposed device. The advantage of capacitive gas sensing is that the sensitivity can be enhanced by incorporating higher geometrical capacitance.

### Keywords:

graphene, gas sensing, nitrogen dioxide

## 화학기상증착법에 의한 야누스 이차원 소재의 합성 및 기초물성 연구

KIM Keun Soo <sup>\*1</sup>, [NAM Jungtae](#)<sup>1</sup>, LEE Gil Yong<sup>1</sup>, KO Yong-il<sup>1</sup>, SHIN June Hee<sup>1</sup>, NOH Yoon Seok<sup>1</sup>

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### Abstract:

2004년 흑연으로부터 원자 한층 소재인 그래핀을 스킨치테일 방법으로 떼어내어 이론적으로만 예측되었던 우수한 물성들이 실험적으로 측정되고 응용이 되면서, 그래핀은 물론 h-BN, BP, TMD 소재와 같은 2차원 소재에 대한 연구가 폭발적으로 증가해왔다. 아울러, 한가지 2차원소재가 아닌 이종의 2차원 소재를 접목하여 새로운 물성(예: twistrionics, valleytronics 등)을 갖는 하이브리드 2차원 소재에 대한 연구가 핫이슈로 거듭나고 있다. 이러한 연구동향의 한 분야로서 비대칭적 전자구조를 갖는 야누스 이차원 소재의 합성 및 응용연구가 최근에 새롭게 조명되고 있다.

이에 본 연구에서는 화학기상증착법을 이용하여 이종의 원자층 소재를 번갈아 가며 합성하여 수직방향으로 비대칭적인 2차원 야누스 소재의 합성을 시도하였다. 다양한 이차원 소재 기판에 MoS<sub>2</sub> 소재를 합성하는 방법으로 야누스 2차원 소재의 합성양상을 탐색하고 최적화하는 연구를 수행하였다. 하단 원자층 소재 표면 종류에 따라 다른 상단 원자층 소재의 젖음 특성이 달라서 합성 양상이 달라짐을 확인하였다. 합성된 시료의 라만 분광법에 의한 맵핑 분석을 통해 이종 2차원 소재 표면에 MoS<sub>2</sub> 박막이 조건별로 균일한 두께와 품질로 나타남을 확인하였다. SEM을 이용한 표면분석과 XPS 측정을 통한 성분분석을 시도하였고, 투과전자현미경을 이용하여 비대칭적 2차원 야누스 소재의 원자구조를 확인하였다. 아울러, 전계효과 트랜지스터를 제작하여 기초적인 전기물성을 평가하였다. 야누스 이차원 소재의 합성 및 기초물성 연구결과 관련 더욱 상세한 내용은 발표에서 보고할 예정이다.

### Keywords:

야누스, 그래핀, MoS<sub>2</sub>

# Correlated normal state and topological superconductivity in $UTe_2$

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## Abstract:

$UTe_2$  poses a promising platform of the paramagnetic end member among the Uranium-based superconductor where a spin-triplet superconducting pairing superconductivity arises from ferromagnetic fluctuation. Here, we report a theoretical calculation to predict a correlation-driven large Fermi surface (FS) in  $UTe_2$ . The geometry of the FS indicates a robust non-trivial topology of the superconducting state that hosts a Majorana fermion within the weak coupling theory. We also solve linearized Eliashberg equations in the random phase approximation level and show that two pairs of odd-parity representations accidentally have degenerate eigenvalues. This degeneracy implies the possibility of the time-reversal symmetry breaking ground state, which has been suggested by a number of former experimental and theoretical studies.

## Keywords:

Topological semimetal, Ferromagnetism, Fermi arc, Surface states

## Nonvanishing anomalous Hall effect in $Mn_3Al$ - compensated ferrimagnetic Heusler compound

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### Abstract:

It has been long believed that anomalous Hall effect (AHE) requires nonzero net magnetization. Recent studies, however, revealed that some antiferromagnets can exhibit AHE. Here, we extend to compensated ferrimagnets to show AHE is robust due to nonvanishing Berry curvature. The analysis is provided using group theoretical approach employing not only space or point group but also magnetic space group. More specifically, we show the Berry curvature is prominent near  $\frac{1}{2}K\Gamma$  and L point but other contributions are not negligible.

## **Fe<sub>3</sub>GeTe<sub>2</sub> : A site-differentiated Hund metal**

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### **Abstract:**

Recently, magnetic property of van der Waals materials has been attracting a lot of attention. In this talk, I will report our recent progress in understanding a metallic ferromagnet Fe<sub>3</sub>GeTe<sub>2</sub>. In particular, I will try to argue that this representative metallic ferromagnet can be best understood as a 'site-differentiated' Hund's metal. After briefly summarizing the material properties of Fe<sub>3</sub>GeTe<sub>2</sub> and the intriguing characteristics of Hund's metals, I will present our DFT+DMFT calculation results showing that all salient features of Hund's metal physics are well identified in Fe<sub>3</sub>GeTe<sub>2</sub>. Furthermore, two different Fe sites in this material are clearly distinctive from the Hund's physics point of view. This newly suggested 'site-selective' Hund's picture provides the useful insight and information to understand the experiments including the ones that are seemingly controversial to each other.

### **Keywords:**

Hund metal, density functional theory, dynamical mean-field theory, 2D materials, Magnetism

## Coherent magnetic exciton in Ni-based van der Waals magnets

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### Abstract:

The magnetic van der Waals (vdW) materials have been intensely studied as an ideal platform for investigating fundamental properties of two-dimensional magnets and a potential element for device application. Among them, the Ni-based materials like NiPS<sub>3</sub> and NiI<sub>2</sub> have drawn much attention because of their many-body electronic character and ultra-coherent magnetic exciton [1, 2]. It has been revealed that ultra-coherent magnetic exciton, which is strongly coupled with the zigzag magnetic order, appears around 1.5 eV in NiPS<sub>3</sub> with a layered honeycomb structure [1]. Consecutive study also demonstrated that similar magnetic exciton is allowed in NiI<sub>2</sub> with a layered triangular structure. Moreover, the exciton in NiI<sub>2</sub> turned out to be assisted by the multiferroic property [2]. In this talk, we will present the electronic characteristics and excitation features in Ni-based vdW materials NiPS<sub>3</sub> and NiI<sub>2</sub>. With the help of the microscopic model incorporating local many-body correlation effects, we will identify the nature of coherent magnetic exciton in the zigzag order of NiPS<sub>3</sub> and the multiferroic order of NiI<sub>2</sub>.

[1] S. Kang *et al.*, Nature 583, **785** (2020)

[2] S. Son *et al.*, Adv. Mater. (2022)

### Keywords:

Van der Waals Magnet, Magnetic Exciton, NiPS<sub>3</sub>, NiI<sub>2</sub>

## Organic/inorganic hybrid light emitting transistors for backplane/driver-free display applications

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### **Abstract:**

Light-emitting field-effect transistors (LETs) are a new class of electro-optical devices that combine in a single structure the electrical switching functionality of a field-effect transistor (FET) and the capability of light generation from an organic light emitting diode (OLED). LETs have potential applications in simplified pixels of flat panel displays, optical communication devices, and electrically driven organic lasers. There have been a number of studies on LETs fabricated with solution processed conjugated polymers, vacuum deposited thin films of small molecules and single crystals. This talk will introduce the overall LETs that have been reported in the literature in the past several years and highlight some of key considerations to improve device performance.

### **Keywords:**

light emitting transistor, organic materials

# Ferroelectric Organic Artificial Synapses for Neuromorphic Electronics

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## **Abstract:**

Inspired by the biological neural network and cognitive functions, neuromorphic computing architecture has been envisioned as an alternative computing system. Especially, this brain-inspired computing architecture is suitable for an e-textile/wearable computing platform because of the potential to efficiently process a large amount of unstructured sensing data, including diverse and complex signals from the human body or the surrounding environment. In this talk, I am going to present recent works on diverse types of ferroelectric organic artificial synapses for neuromorphic applications, which can apply to wearable and human-interactive electronic systems. Especially, several organic synaptic device platforms will be presented with their essential synaptic characteristics and potential applications. Additionally, I will suggest a novel type of three-dimensional barristor synaptic array that utilizes a ferroelectric organic layer to create a convolutional neural network, which can efficiently learn and recognize targeted images.

## **Keywords:**

Ferroelectric organic material, artificial synapse, organic synapse, neuromorphic electronics, Artificial neural network

## A study of defect control for high performance perovskite LEDs

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### Abstract:

Organic-inorganic halide perovskite materials have been demonstrated as a promising candidate for light-emitting diodes owing to their excellent optoelectronic properties, such as high photoluminescence quantum yields (PLQYs), color tunability over a widerange by simply modulating the elemental composition, and a high color purity with a narrow full width at half-maximum emission (<20nm). At present, a high external quantum efficiencies (EQEs) of over 20% in perovskite light-emitting diodes (PeLEDs) have been achieved.

However, solution-processed perovskite films inevitably contain defect sites such as voids, pinholes, grain boundaries, and undercoordinated ions, creating a large number of undesired electronic trap sites. Basically, defect-induced electronic trap sites are a major cause of undesired phenomena in PeLEDs, such as hysteresis behavior and blinking behavior of PeLEDs, which limit their applicability and commercialization.

Here, we demonstrated the simple and effective methods such as ligand engineering, encapsulation in order to control the defects in PeLEDs.

### Keywords:

perovskite, defect, passivation, perovskite LEDs

## Resistive switching behaviour in metal-halide perovskite unipolar memory devices probed by current noise spectra

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### Abstract:

Organometal halide perovskites have emerged as potential material systems for resistive memory devices besides their outstanding optical and electrical properties. Although we have recently demonstrated the advantages of halide-perovskite resistive memory with a low voltage operation and large on/off ratio[1], random distribution in operation voltage remains a challenge in memory application. This stochastic operation characteristic is due to the random formation of conducting filaments that cause resistance fluctuations in the material. Therefore, it is essential to investigate the formation and dissolution of conducting filaments and their structure. However, direct observation of a nanoscale filamentary structure is often challenging. Moreover, detailed studies of conducting filaments in halide-perovskite materials have rarely been reported. By employing a scaling theory with a fractal structure, this study investigates the geometric structures and dynamics of conducting filaments formed in organometal halide perovskite through current noise analysis[2]. The temperature-dependent electrical properties and current noise demonstrate the role of ion migration in the formation of conducting filaments. The findings could enhance the understanding of the resistive switching phenomena of perovskite resistive memory devices in terms of percolative conducting filaments. Thus, providing a route for achieving a stable memory operation by controlling the relevant structure and dynamics of the switching processes.

### References

- [1] K. Kang, H. Ahn, T. Lee et al. *Adv. Mater.* 31, 1804841 (2019)
- [2] H. Ahn, K. Kang, T. Lee et al. *Adv. Funct. Mater.* 32, 2107727 (2021)

### Keywords:

Perovskite, Resistive memory, Current noise spectra

## Vacancies in growing habitats promote the evolution of cooperation

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### Abstract:

We study evolutionary game dynamics in a growing habitat with vacancies. Fitness is determined by the global effect of the environment and a local prisoner's dilemma among neighbors. We study population growth and analyze how the environment affects evolutionary competition. As the environment becomes harsh, an absorbing phase transition from growing populations to extinction occurs. The transition point depends on which strategies are present in the population. In particular, we find a 'cooperative window' in parameter space, where only cooperators can survive. A mutant defector in a cooperative community might briefly proliferate, but over time naturally occurring vacancies separate cooperators from defectors, thereby driving defectors to extinction. Our model reveals that vacancies provide a strong boost for cooperation by spatial selection.

### Keywords:

Evolution of cooperation, Prisoner's dilemma, Eco-evolutionary dynamics, Absorbing transition

## Effect of The Adult-Born Immature Granule Cells on The Winner-Take-All Competition in The Hippocampal Dentate Gyrus

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### Abstract:

Adult neurogenesis occurs in the hippocampal dentate gyrus (DG) throughout life. Thus, young immature granule cells (imGCs) appear in adulthood. In comparison to mature GCs (mGCs) (born during development), young adult-born imGCs exhibit two competing distinct properties such as high excitability (causing high activation) and low excitatory innervation (reducing activation). We develop a spiking neural network for the DG, incorporating the imGCs, and investigate their effect on the winner-take-all (WTA) competition. When considering the high excitability of imGCs, the imGCs become very highly active, while the mGCs exhibit very sparse firing activity because of strongly increased feedback inhibition from the BCs and the HIPP cells (caused by the high activation of the imGCs). Thus, the whole population of all the GCs become a very heterogeneous one, composed of a (major) subpopulation of mGCs (exhibiting strengthened WTA competition) and a (minor) subpopulation of imGCs (showing weakened WTA competition). Next, we consider the low excitatory innervation of the imGCs (resulting in sparse firing), which could counteract the effect of high excitability. As excitatory innervation of the imGCs is decreased, the activation degree of the imGCs decreased so rapidly (i.e., their WTA competition increased), while the activation degree of the mGCs increased (i.e., their WTA competition decreased). As the effect of the imGCs is decreased, the heterogeneity degree in the whole population became reduced.

### Keywords:

Hippocampal dentate gyrus, Winner-take-all competition, Adult neurogenesis, Immature granule cells (GCs), Mature GCs

## Critical-to-Insulator Transitions and Fractality Edges in Perturbed Flatbands

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### Abstract:

We add weak quasiperiodic perturbations to one dimensional two-band ladders with both bands flat. An additional projection onto a single flatband Hilbert space allows to study the properties of the eigenstates upon variation of the control parameters of the all-bands-flat ladder. We observe localized insulating states, and an entire parameter range hosting critical states. These critical states have multifractal behavior and support subdiffusive transport. The Critical-to-Insulator transition turns energy dependent upon increasing the strength of the quasiperiodic perturbations. We therefore discover fractality edges - energy dependent transitions between an insulator and criticality.

### Keywords:

Flatbands, Quasiperiodic, Critical states, Localization

## Flat Band Induced Metal-Insulator Transitions for Weak Magnetic Flux and Spin-Orbit Coupling Disorder

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### Abstract:

We consider tunable all-band flat(ABF) lattices with  $d = 1, 2, 3$  dimensions with a angle parameter  $\theta$ . We study the transport properties of eigenstates in the presence of weak magnetic flux disorder and weak spin-orbit disorder. We show that weakly disordered ABF lattices are effectively described by a scale free model where the disorder strength is scaled out. We perform exact diagonalization on the scale free model of disordered ABF lattices to obtain the energy spectrum and eigenstates. Finite size scaling analysis of the scaling exponent of the participation number and mean level spacing statistics are used to identify whether the system is metallic or insulating. For weak magnetic flux disorder we observe unusual subexponential localization at the flatband energy for  $d = 1$  which differs from usual Anderson localization. For weak spin-orbit disorder and  $d = 2$  we identify a tunable metal-insulator transition with mobility edges. We also consider the case of mixed spin-orbit and diagonal disorder and obtain the metal-insulator transition driven by  $\theta$ .

### Keywords:

Metal-insulator transition, Anderson localization, flatband

## Optimal synchronization of Kuramoto oscillators in a growing complex network

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### Abstract:

The Kuramoto model has been widely adopted to study the synchronization phenomena of interacting units. For oscillators coupled in a complex network, the challenge is to find the network structure and/or the oscillator's frequency distribution that enhance the degree of synchronization. Previous studies have studied the optimal synchronization in a network with a fixed size through link reallocation. In the linear coupling regime, they have suggested the objective functions required to be minimized in the optimization process. Here we study the optimal synchronization in a growing network by using those objective functions. We aim to obtain the optimal intrinsic frequency of the oscillator added at each growth step when the network growing process is predetermined. By means of each objective function, we obtain the optimal frequency in terms of known parameters. The results show that the optimal condition is achieved when the average frequency including the added oscillator's frequency becomes equivalent to the linear combination of the earlier oscillators' frequencies with the normalized coefficients determined by the network structure. We verify our results numerically on the growing random network and the Barabasi-Albert network. The numerical data confirm that our results outperform naive strategies, such as random selection, local average, and global average, even when the linear approximation is weakly broken.

### Keywords:

synchronization, coupled oscillators, complex systems

## Hypergraph modeling based on international trade data

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### **Abstract:**

We analyze the international trade data in terms on hypergraph consisting of triangular hyperedges representing the exporter-importer-product relationship. We find that the bias of the exporters of low hyperdegree towards the importers of high hyperdegree and the products of low hyperdegree exists by comparing with the exponential random hypergraphs preserving the given empirical hyperdegree sequence. Such feature is not readily accessible in the pairwise networks. Our study demonstrates the usefulness of the hypergraph approach in the study of real-world complex systems and offers a theoretical framework.

### **Keywords:**

network, hypergraph, international trade

## Quantum optics with photons from warm atomic ensemble

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### Abstract:

This study reports the first ever generation of a continuous-wave (CW) four-photon polarization-entangled Greenberger–Horne–Zeilinger (GHZ) state obtained from warm atomic ensembles of 87Rb atoms. Bright, entangled multiphoton sources based on atom–photon interactions are an essential requirement for the realization of several quantum information and quantum computation schemes based on photonic quantum systems. However, it is difficult to realize high-fidelity entangled-multiphoton sources from atomic ensembles for application to practical quantum information processing. Our work is significant from the perspective of further understanding the fundamental physics underlying coherent atom–photon interactions. Moreover, it provides a practical approach to realize quantum devices in vapor cells. Additionally, the generation of such bright and stable multiphoton GHZ states from atomic media is an important step toward realizing photonic quantum computation and practical quantum networks based on atom–photon interactions.

### Keywords:

multi-photon entanglement, warm atomic ensemble, collective two-photon coherence, GHZ state

## Reconfigurable optical imaging interfaces for quantum technologies

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### **Abstract:**

Optical imaging systems become an indispensable tool for many of quantum technologies, as they provide efficient, high-resolution control interfaces for the underlying quantum systems. In this focus session, I will present reconfigurable imaging interfaces for quantum control and review their emerging applications on neutral-atom quantum computing.

### **Keywords:**

neutral-atom quantum computing, reconfigurable imaging interface

# Large-scale & low power programmable photonic circuits for quantum photonics

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## Abstract:

Even with tens of qubits, quantum computers can show quantum advantages over classical computers for several specialized tasks. On the other hand, a universal quantum computer needs thousands of qubits with tangible error-correction schemes, though these requirements are not attainable with existing architectures. So far, measurement-based quantum computing (MBQC) with integrated photonics has shown a promising route to create general-purpose programmable quantum processors. However, current thermally tuned silicon photonic circuits only have shown small-scale proofs-of-concept. Their inherent power-hungry (~mW/element) and high optical loss nature hamper scaling. In addition, the heat generated by the tuning elements prohibits their usage in cryogenic temperatures, the environment needed for operating integrated single-photon detectors.

Our team has pioneered ultra-low-power micro-electro-mechanical systems (MEMS) tunable photonic components requiring < 1nW/element. Using the MEMS-tunable elements, we have demonstrated several programmable photonic processors directly applicable to quantum photonics. This talk will show the recent progress of our MEMS-enabled platform and its applications to quantum photonics.

## Keywords:

quantum photonics, MEMS-enabled silicon photonics, ultra-low power, low loss, large-scale

## Attention neural network for analyzing electron-nuclear spin interactions with varying interaction time

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### Abstract:

We present deep learning models for analyzing dynamical decoupling signals to identify and estimate interaction strength between multiple  $^{13}\text{C}$  nuclear spins surrounding a nitrogen-vacancy(NV) center in diamond. Identifying these interactions of nuclear spins is important in realizing coherently controllable spin registers, constructing a robust base for quantum network, quantum simulation platform, or quantum memory. Experimentally, we use Carr-Purcell-Meiboom-Gill pulses to measure signals of an electron's state in the NV center with various number of  $\pi$  pulses (N) controlling interaction time with nuclear spins. By analyzing and recognizing features in concatenated signals as a function of N, our models automatically identify the number of overlapped nuclear spins and estimate interaction strengths between  $^{13}\text{C}$  nuclear spins up to 90% accuracies.

### Keywords:

NV center, CPMG, hyperfine interaction

# Single-shot time-resolved visualization of ultrafast high-intensity laser-matter

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## Abstract:

The subject of ultrafast high-intensity laser matter interactions has received significant attention recently because of its fundamental importance as well as key applications such as laser filamentation, table-top soft x-ray generation and laser-based particle accelerators. In this presentation, I will talk about two recent high-intensity laser-matter interaction experiments in which our group uses single-shot time-resolved visualization techniques to fundamentally understand the underlying dynamics. First, I will talk about taking a single-shot snapshot of optical Kerr effects, glass ionization, and plasma recombination in glass [1] using state-of-the-art frequency domain holography [2, 3] when a high-intensity laser pulse interacts with a thin flexible glass sample. Second, I will talk about the measurement of electron collision times in plasma as a function of driver wavelength using single-shot time-resolved interferometry when a driver laser pulse undergoes laser filamentation (self-guidance of a high intensity laser pulse) in glass [4]. Furthermore, I will talk about our computer simulations of laser-matter interactions to be benchmarked against experiments [5].

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[5] R. I. Grynko, G. C. Nagar, and B. Shim, *Phys. Rev. A* 98, 023844 (2018).

## Keywords:

Laser matter interactions, single-shot time-resolved visualization, plasma, laser filamentation

## Ultrafast X-ray Spectroscopy of Solvated Molecules at PAL-XFEL

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### Abstract:

The geometrical structures of molecular species during chemical reactions as well as relevant electronic configurations and spin-states are crucial information on understanding various photochemical and photobiological processes. In this presentation, our recent works on the ultrafast linkage isomerization of Ru-based photochromic complexes, which have been done at PAL-XFEL, will be given. More specifically, we have utilized Ru L<sub>3</sub>-edge and S K-edge X-ray spectroscopies to unravel details of excited state dynamics. X-ray spectra reveal the spin and valence charge of the Ru atom and provide experimental evidence that metal-centered excited states mediate isomerization. Complementary X-ray spectra of the functional ligand S atoms probe the nuclear structural rearrangements, highlighting the formation of two metal-centered states with different metal-ligand bonding. Our results address an essential open question regarding the relative roles of transient charge-transfer and metal-centered states in mediating photoisomerization.

## Attosecond photoemission dynamics from molecules, clusters and liquids

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### Abstract:

Attosecond spectroscopy has opened new windows into the shortest time scales of light-matter interaction. In this talk, I will address the extension of attosecond chronoscopy, the measurement of photoemission time delays from molecules, over molecular clusters to the liquid phase. A few years ago, our research group has reported the first measurements of photoionization delays in molecules [1]. Photoionization delays of H<sub>2</sub>O and N<sub>2</sub>O molecules were measured. Delays up to ~160 as were measured in the case of N<sub>2</sub>O and shown to reflect the lifetime of a molecular shape resonance. The much smaller delays in the case of H<sub>2</sub>O were shown to reflect the absence of resonances in the photoionization continuum of H<sub>2</sub>O. In a second step, these measurements were extended to liquid water using the liquid-microjet technique. In this case, delays of 50-70 attoseconds between the photoemission from the highest occupied valence band of liquid water and the highest-occupied molecular orbital of the isolated molecule were observed [2]. These delays were found to be dominated by the influence of the first two solvation shells in liquid water. In the third step, we developed attosecond size-resolved cluster spectroscopy and obtained a molecular-level understanding of the origin of these delays [3]. We found that photoionization delays of water clusters increase with the addition of each molecule until a size of 4-5 molecules, but do not increase further beyond this size, at least within the studied size range. Comparison with our calculations showed that the photoionization delays are proportional to the first moment of the electron-hole density, which increases as a function of size in small, highly symmetric clusters, and then saturates as a consequence of the emergence of structural disorder, a phenomenon that is closely related to Anderson localization in solids. These results offer the perspective of studying electron-hole localization dynamics in complex forms of matter with attosecond temporal resolution.

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[3] X. Gong, S. Heck, D. Jelovina, C. Perry, K. Zinchenko, H. J. Wörner, Attosecond spectroscopy of size-resolved water clusters, arxiv:2106.09459 (2021)

## Defect and interface effects in optoelectronic properties of 2D van der Waals semiconductors

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### Abstract:

Two-dimensional (2D) van der Waals semiconductors have shown diverse potential in optoelectronic applications due to their unique optical and electrical properties revealed at atomic layer thicknesses. The unique band structure and stable exciton characteristics of monolayer 2D semiconductors opened up a new field of research on characteristics of ultra-thin photovoltaic/light-emitting devices and novel valleytronics. In addition, a unique quantum transport phenomena through artificial van der Waals stacking of various 2D material libraries including semimetals and dielectrics have actively been studied. Meanwhile, these characteristics of ultra-thin 2D semiconductors are easily modulated by external factors compared to bulk materials. Herein, the author introduces research on specific optoelectronic properties and device functionalities manipulated by defects and interfaces such as intrinsic point defects and impurities, stacked interfaces, Coulomb interactions, and plasmonic hybridization, in 2D semiconductors.

### Keywords:

van der Waals, semiconductors, defect, interface, optoelectric

## 모노리식 풀컬러 질화물계 발광다이오드

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### Abstract:

최근 차세대 풀컬러 디스플레이 광원으로 청색 및 녹색은 질화물계 LED와 적색은 인화물 및 비소화물 LED가 사용되고 있는 마이크로 LED 디스플레이가 많은 관심을 받고 있다. 하지만 재료의 성장법 및 물성이 크게 다르기 때문에, 세개의 광원을 결합해야 하는데 있어서 고난이도의 소자 제작 공정이 필요하다. 이에, 하나의 재료를 이용하여 적색, 녹색 및 청색 광원을 구현할 수 있는 모노리식 풀컬러 LED를 구현하고자 하는 연구가 지속되고 있다. 본 연구에서는 고농도 In원자를 포함한 InGaN활성층의 상분리 현상을 이용하여 인듐 원자의 조성적 요동을 발생시켜 전류밀도 주입 증가 시 청색 편이 현상을 극대화하여 적색에서 청색까지의 풀컬러 광원을 동일 웨이퍼에서 구현할 수 있는 기술을 연구하였다. 특히, 고농도의 인듐을 포함하는 InGaN 다중양자우물구조 성장시 발생하는 V-형 결함을 이용하여 인듐의 조성적 요동을 제어하였으며, 이를 이용한 발광 다이오드 웨이퍼에 주입전류 밀도를 제어하기 위해 다양한 크기의 마이크로 발광 다이오드를 설계하여 적색 발광에서 청녹색 발광영역까지 파장 제어가 가능하였다. 또한, 반분극 GaN계 LED의 표면 결함을 이용한 인듐의 조성적 요동을 이용하여 역시 적색에서 청색까지 광세기를 각각 제어하여 다양한 파장의 광원을 얻을 수 있었으며, 삼색 동시 발광을 통한 백색광을 얻을 수 있었다. 이는 다양한 파장의 조명 및 풀컬러 디스플레이에 응용할 수 있는 다파장 광원을 하나의 웨이퍼에서 동시에 얻을 수 있음을 나타내며 다양한 응용분야로 확장될 수 있을 의미한다.

### Keywords:

GaN , LED, Band-filling effect, In phase separation

## **Fabrication of Transferable Metal oxide nanostructures and applications to optoelectronic devices**

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### **Abstract:**

Metal oxide nanomaterials including ZnO, SnO<sub>2</sub>, Zinc-tin-oxide (ZTO) and TiO<sub>2</sub> are very useful to be used in the versatile application fields such as light-emitting diodes (LEDs), solar cells, and photodetectors due to their easiness of fabrication and morphology control in synthesis process. Among them, ZTO and TiO<sub>2</sub> has been considered as attractive next generation optoelectronic materials due to their superior physical and chemical properties. Recently many groups reported that the various phases of ZTO including perovskite, amorphous, and spinel, effect on their optoelectronic device performances in versatile applications such as anodes of battery, active layer in transistor, photovoltaic devices, photodetector, and gas sensors based on the outstanding properties. Here, I present for the fabrication of transferable nanostructures including nano/microspheres monolayers and nanorods consisting of metal oxide spheres and nanorods, respectively, and their applications to optoelectronics such as LED and photodetectors to improve the electrical and optical device performances. In addition, I will introduce the recent research achievements in our group for the utilization of transferable metal oxide nanostructures for flexible perovskite photodetectors to enhance the surface and interfacial property modification resulting in the improvement of device performances.

### **Keywords:**

Metal oxide, Transferable nanostructures, Photodetectors, Optoelectronics, ZTO & TiO<sub>2</sub>

## 태양전지 효율향상을 위한 복사냉각구조 도입

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### Abstract:

태양전지의 효율은 쇼클리-퀘이서 한계(SQ limit)에 의해 제한되며, 흡수소재의 밴드갭에 따라 각기 다른 효율 최대치를 갖는다. 한편, 태양전지의 온도가 증가하면 SQ limit 가 낮아지며, 특히 기온이 급격하게 증가하는 상황에서는 태양전지 뿐 만 아니라 모듈에서 흡수되는 열로 인해 태양전지의 효율이 저하되는 단점이 있다. 따라서 태양전지 또는 태양광 모듈의 온도를 낮추기 위한 효과적인 방안이 제시될 필요가 있다. 물체의 온도를 낮추기 위해서는 공랭식 또는 수랭식을 통상 채택할 수 있으나, 추가적 전기를 사용한다는 측면에서 여전히 단점이 존재한다. 반면, 복사열을 제어하는 방법으로 최근 개발된 '수동 복사 냉각 (passive radiative cooling)' 방식은 적외선 복사열을 우주로 내보낼 수 있는 기술로 외부 전기를 사용하지 않는다는 측면에서 차세대 에너지 절감기술로 각광받고 있다.

본 발표에서는 태양전지의 온도를 낮추고 이를 통해 효율을 증대시키기 위한 복사냉각구조가 집적된 태양전지에 대해 논한다. 태양전지에 복사냉각구조를 도입함으로써 SQ-limit이 어느정도 개선될 수 있는지 이론적으로 보이고, 이후 마이크로구조 기반의 복사냉각구조의 제작방법 및 집적방법, 그리고 집적 이후 태양전지 효율 개선 정도에 대해 보인다.

### Keywords:

태양전지, 수동복사냉각, 마이크로구조

## LED기반 고체조명 응용을 위한 희토류족 없는 형광체 물질 합성 및 발광특성 연구

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### Abstract:

백열등 및 형광등의 기존 광원과 비교할 때 light-emitting diode (LED) 기반 백색광 광원은 고효율, 긴 수명, 높은 신뢰성, 전력 소비 감소, 비용 효율성 및 열복사 및 수은 없는 환경 친화성과 같은 장점으로 인해 일반 조명 응용 분야에 상당한 잠재력을 가지고 있다. 일반적으로 희토류족은 준비된 형광체의 host lattice 물질에서 다색광을 생성하기 위한 많은 형광체의 발광 활성제로 사용된다. 모든 희토류족 물질은 화학적 성질이 비슷하기 때문에 고가의 분리 및 정제 기술이 필요하여 대부분이 고가이다. 이러한 이유로 희토류족이 없는 소재의 설계가 절실히 필요하다. 근자외선 (near-ultraviolet) LED 칩기반의 백색LED는 청색 LED 칩기반 백색 LED의 열악한 색재현성, 낮은 연색지수 (color rendering index) 값 및 고온에서의 열 안정성 저하와 같은 여러 단점을 극복하는 데 사용할 수 있다. 최근 희토류족인  $\text{Eu}^{3+}$  이온을 대체하여  $\text{Mn}^{4+}$  이온은 적색 발광을 위한 형광체 제작을 위해 활발한 연구가 진행되고 있다. 특히, 적색 형광체는 고효율 및 높은 연색지수의 LED 조명을 위해 필요하다. 또한  $\text{Bi}^{3+}$  이온은 좋은 활성제로 작용할 수 있으며 host lattice의 crystal field 환경에 따라 결정되는 전체 가시 영역에서 다양한 빛을 방출할 수 있다. 따라서 본 발표에서는 다양한 합성법을 이용하여 LED기반 고체조명 응용을 위한 희토류족 없는 형광체 물질 합성 및 광특성에 대해 발표한다. 제작된 형광체의 구조적 특성을 연구하기 위한 X선 회절 (X-ray diffraction) 패턴 및 발광 특성은 광발광 여기 (photoluminescence excitation) 및 광발광 (photoluminescence) 스펙트럼을 통해 분석되었다. 얻어진 결과로부터, 이들 형광체는 LED기반 고체조명을 위한 유망한 후보물질로 기대될 수 있다.

### Keywords:

희토류족 없는, 형광체, 발광특성, 고체조명

## Quantum Acoustics: single-electron quantum dots moving in surface-acoustic waves minima

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### Abstract:

The long-distance quantum transfer between electron-spin qubits in semiconductors is important for realizing large-scale quantum computing circuits. Electron-spin to photon-polarisation conversion is a promising technology for achieving free-space or fiber-coupled quantum transfer. In this work, using only regular lithography techniques on a conventional 15 nm GaAs quantum well, we demonstrate the acoustically-driven generation of single photons from single electrons, without the need for a self-assembled quantum dot. In this talk, the recent SAW technique for single-electron transport with a ~GHz speed for generation of single-photon in GaAs/AlGaAs heterostructures by electrical means.

## Toward Large-Scale Production of Single Crystal 2D Materials

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### Abstract:

Two-dimensional materials (2DMs) have been intensively studied for almost two-decade since the isolation of graphene from bulk graphite into devices in 2004. Over the past few years, the utilization of 2DMs in various areas of industry has strongly intensified. However, even though considerable efforts have been spent on the development of various methods of the production of 2DMs, the efficient production of 2DMs of a guaranteed quality over a large scale remains a challenge. In this seminar, I am going to introduce our strategies to produce 2DMs via top-down and bottom-up approaches. At first, I will present a scalable growth of single-crystal graphene (SCG) on through "transplanting" uniaxially aligned graphene "seedlings" on the larger-area catalytic growth substrate [1]. By inducing homo-epitaxial growth of graphene from the edges of the seed arrays without additional nucleation, we achieved the SCG with an area four times larger than the mother graphene seed substrate. And then, I will introduce atomic spalling of the van der Waals crystals that achieve large area 2DMs (graphene, MoS<sub>2</sub>, MoSe<sub>2</sub>, and WSe<sub>2</sub>) with a controlled number of layers [2]. We found that being a layered crystal with a weak interlayer vdW force enables to control of the crack propagation depth at the scale corresponding to the single atomic thickness by adjusting interfacial toughness and the internal stress of the stressor film. The presented results show huge potential for the manufacture of layer-resolved high-quality vdW materials, which can be developed into practical functional electronic and photonic devices.

### Keywords:

2D materials, CVD, spalling, exfoliation

## Synthesis and Property Control of Nano Carbon and Its Composite Materials

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### Abstract:

Carbon nano-materials such as graphene and graphene quantum dots are most promising materials to be employed to various application owing to its unique electrical, mechanical, chemical and optical properties. However, there are still several issues to be solved to control structural-morphological characteristics, fabrication process and stability of properties what we want. Here, we have synthesized the large-scale and high-quality graphene films by chemical vapor deposition (CVD). And also, CNT fibers (CNTFs)-Cu and graphene-Cu hybrid materials for high-performance mechanical and electrical property will be discussed. The core CNTFs and GFs are synthesized by chemical vapor deposition (CVD), followed by electroplating of Cu shells, where the large surface area of CNTFs and GFs in contact with Cu maximizes the mechanical toughness of the cores-shell wires. At the same time, the unique electrical and thermal characteristics of graphene allows ~10 times higher current density limit, providing more efficient and reliable delivery of electrical energies through the GFs-Cu wires. We also report a facile one-step synthesis of nitrogen (N) doped high-crystalline graphene quantum dots (N-GQDs) using top-down and bottom-up approaches. An interesting property of nGQDs can be simply controlled by synthetic conditions with different N contents. This finding indicates that our approach could lead to low-cost and efficient processability that is scalable and environmentally friendly. We believe that the shape, size and functionality of these GQDs can be controlled using other chemical species to provide a variety opportunities for use in opto-electronics, biological applications and sensors.

### Keywords:

Graphene, CNT Fibers, Composite Materials, Graphene Quantum Dots

## Research beyond AlphaFold: Development of Artificial Intelligence for Drug Discovery and Design

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### **Abstract:**

Understanding protein-ligand interactions provides an important basis for the structure-based drug discovery. Traditional computational approaches often perform poorly on describing interaction accuracy or strength primarily due to their limited molecular representations. We are developing a series of artificial intelligence (AI) neural networks for computer-aided drug discovery (CADD) to overcome limitations in such classic computational approaches through improved molecular representations and integration of the latest deep learning (DL) techniques. In this talk, I will first overview the revolution in protein structure prediction led by Google DeepMind's AlphaFold, its impact on structure-based drug discovery, and my perspective on remaining grand challenges in the field. Then I'll share my recent works to tackle those challenges, especially focusing on building a chemistry-aware AI in order to "imagine" ligand binding motifs solely based on the physicochemical properties of receptor structure. Preliminary results on its applications to peptide drug design and drug binding site prediction will be presented.

### **Keywords:**

Drug discovery, artificial intelligence

# A Machine Learning Study on the Glass Transitions and Their Structural Order

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## Abstract:

When systems in liquid phases such as polymer melts and colloidal suspensions are supercooled rapidly, the systems may avoid crystallization and undergo a glass transition. While the structures of the systems in glassy states are not very different from those in liquid states, glasses exhibit surprisingly high viscosity, thus becoming amorphous solids. Even though such glass transition is ubiquitous and has been observed in various biological systems, there have been unanswered and challenging questions: is the glass transition a thermodynamic transition or a kinetic trap? If it is the thermodynamic transition, what may be a structural order parameter? Is there any universal structural order parameter like medium range crystalline order (MRCO)? In order to answer those questions, we perform extensive molecular dynamics simulations for two-dimensional (2D) colloidal suspensions as a model system. We obtain snapshots from the simulations and train several neural network models. We report in this talk that one can take advantage of the machine learning successfully to predict the glass states only from snapshots of 2D colloids, and also that there would be a universal (but highly correlated) structural order parameter beyond MRCO.

## Keywords:

Machine learning, glass transition

## Computational approach to discover potent neutralizing antibody against all SARS-CoV-2 variants

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### Abstract:

Computational protein design has become a powerful approach for creating valuable proteins. We have developed a computational pipeline to discover antibodies that bind to a pre-defined surface of target proteins. Our approach is showcased by discovering and developing a human neutralizing antibody that binds to the receptor-binding domain (RBD) of the SARS-CoV-2 spike glycoprotein of all currently circulating variants of the virus, including Omicron, with potent affinity (pico- to femto-molar dissociation constants, KDs). Initially, a lead antibody was computationally discovered using sequence design protocols in the Rosetta software suite and crystallographically validated to bind, albeit weakly, to a highly conserved surface of the RBD of wild-type SARS-CoV-2 (Wuhan strain). Subsequently, a tightly binding Ab (KD = 7.2 nM) was developed through experimental affinity enhancement. This then served as a template for the quick computational discovery of an antibody that binds the RBD of the Alpha variant (with the N501Y mutation) with extremely high affinity (KD < 1 pM). Consistent with its measured affinity, D27LEY exhibited a strong in vitro neutralization activity against the wild-type virus and the Alpha, Delta and Omicron variants.

### References

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2. Rosetta:MSF: a modular framework for multi-state computational protein design. *PLoS Comput Biol.* 2017 13:e1005600.
3. De novo design of modular and tunable protein biosensors. *Nature.* 2021 591:482-487

### Keywords:

Computational antibody design

## Search for leptophobic $Z'$ resonances decaying to charginos in the dilepton plus missing transverse momentum final state at the HL-LHC

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### Abstract:

The prospects of a search for a massive leptophobic  $Z'$  decaying to a pair of charginos at the High Luminosity LHC at CERN is explored in the dilepton plus missing transverse energy final state. Simulated events from proton-proton collisions at a center-of-mass energy of 14 TeV collected by the upgraded CMS detector are used. The charginos decay to leptonically decaying W boson and a neutralino. A deep neural network is used for signal extraction. The expected signal sensitivities for a  $Z'$  with narrow width are presented for an integrated luminosity of  $3\text{ab}^{-1}$  in the chargino versus  $Z'$  mass frame. The combined analysis will be able to exclude  $Z'$  masses over 4 TeV.

### Keywords:

$Z'$ , SUSY

# Observation and Measurement of the electroweak production of $Z\gamma(W\gamma)$ and two jets in pp collisions at $\sqrt{s} = 13$ TeV and constraints on anomalous gauge couplings

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## Abstract:

Vector boson scattering(VBS) process in understanding the electroweak(EW) sector is well established in hadron collider experiment. We report that the observation and measurement have been performed for EW production of a W(Z) boson, a photon and two jets through the VBS using the LHC proton-proton collision data taken at  $\sqrt{s} = 13$  TeV collected with the CMS detector. The measurement is performed selecting one lepton for W and two leptons for Z, with a photon and two high  $p_T$  jet in forward direction(VBS tagged jets). The EW contribution to the production is consistent with the standard model prediction and the exclusion limits on anomalous quartic gauge couplings in the effective field theory framework are set.

## Keywords:

diboson production, vector boson scattering, CMS, LHC

## Di-lepton pair identification with highly boosted signature in the CMS experiment

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### Abstract:

A heavy resonance such as a hypothetical  $Z'$  boson may decay into a pair of di-lepton systems indirectly when the direct coupling between the  $Z'$  boson and leptons is prohibited. If the intermediate boson is significantly lighter than the  $Z'$  boson, final state leptons in the di-lepton system can be seriously collimated, making detection of a lepton pair challenging. We introduce efforts to identify a highly boosted di-lepton system in the CMS experiment based on the Monte-Carlo study.

### Keywords:

CMS, boosted,  $Z'$ , di-lepton, merged leptons

## Search for excited leptons in $l\bar{l}\gamma$ final states at 13 TeV

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### Abstract:

A search for excited leptons (electrons and muons) is presented using 2017+2018 data collected by the CMS experiment at a center-of-mass energy of 13 TeV and corresponding to an integrated luminosity of 101 /fb. Excited leptons are predicted by various theoretical models beyond the standard model (SM) that quarks and leptons are made of unknown fundamental constituents never observed yet. Excited leptons ( $l^* = e^*, \mu^*$ ) in  $l\bar{l}\gamma$  ( $l = e, \mu$ ) final states where the excited lepton decays to a SM lepton and a photon ( $l^* \rightarrow l\gamma$ ) are studied. We select events which have two same-flavor leptons and one photon and we apply Z-veto which dilepton mass should be larger than 116 GeV due to  $Z\gamma$  process. Background is estimated directly from fits to data and signal extraction using unbinned maximum-likelihood fits on 3-body invariant mass is used. Several systematic studies including bias study are updated and preliminary limit will be presented.

### Keywords:

cms, excited leptons

# Prospect of gravity-mediated dark matter search from the dileptonic decay of $t\bar{t}$ at the high luminosity large hadron collider

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## Abstract:

A search for a gravity-mediated dark matter produced via spin-2 mediator in the dileptonic final state of  $t\bar{t}$  is presented. The high luminosity condition is planned to have an integrated luminosity of  $3.0 \text{ ab}^{-1}$  with a center of mass-energy of 14 TeV. The selection cuts based on the large missing transverse energy and transverse mass coming from undetected dark matter are set to distinguish signals against backgrounds, and the signal yields are estimated using the selected events. Finally, the yields are converted to the exclusion region on the 2-dimensional mass plane of mediator and dark matter with considering the constraint by the known relic density at the 95% confidence level.

## Keywords:

dark matter, high luminosity, LHC,  $t\bar{t}$

## Calculation of PDF + $\alpha_s$ uncertainties and the NNLO k-factor for $W'$ search at $\sqrt{s} = 14$ TeV

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### Abstract:

In heavy vector-boson  $W'$  search, It's necessary to calculate a higher-order correction, and the Parton Distribution Functions (PDF) +  $\alpha_s$  uncertainty to predict the theoretical cross-section precisely. Therefore we calculate the k-factor and the PDF +  $\alpha_s$  uncertainties for  $W'$  search in pp collision at 14 TeV center of mass-energy. The k-factor is defined as the ratio of the next-to-next-to-leading order (NNLO) to the leading order (LO) cross-section. We calculate it using FEWZ 3.2. The PDF +  $\alpha_s$  uncertainty is a major systematic in this search. We estimate PDF +  $\alpha_s$  uncertainties with the most recent PDF sets; CT18, NNPDF 4.0, MSHT20 at NNLO. These results will be applied to the Run3 data analysis.

### Keywords:

$W'$ ,  $W$  prime, PDF uncertainty, K-factor

## Search for new physics inside jets using non-isolated leptons

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### Abstract:

One of the main goal of CMS experiment is to find a new physics beyond the Standard Model(BSM). CMS experiment has been using various types of leptons to achieve it, such as isolated leptons, high transverse momentum leptons, and boosted leptons. However there is still no direct evidence for BSM physics, which may mean that we have not yet scrutinize a phase space containing BSM particles. Lepton flavour violation results at LHCb experiment show that there should exist something new in b-jets. Non-isolated leptons, which are leptons inside jets, could thus be a good candidate to find a new physics. We will present preliminary results of BSM searches using non-isolated leptons.

### Keywords:

non-isolated lepton, BSM physics, CMS experiment

## **A study of initial state radiation on the Drell-Yan events at $\sqrt{s} = 13 \text{ TeV}$**

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### **Abstract:**

We present the updated results of initial state radiation (ISR) study using the Drell-Yan (DY) events from pp collision at LHC with  $\sqrt{s} = 13 \text{ TeV}$ , 137.2 fb<sup>-1</sup> CMS data. ISR from hadron collisions plays an important role in the jet physics, which has an impact on the precision measurements and searches for new physics. We develop a systematic way to study the ISR effect using the dielectron and dimuon channel of the DY events. The truncated mean of the dilepton transverse momentum distribution is found to have a logarithmic slope as a function of dilepton invariant mass square. This logarithmic slope can be used to control ISR effect in the SM processes and new physics processes.

### **Keywords:**

CMS, Standard Model

## Measurement of Noise term in JER using random cones method at CMS detector

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### Abstract:

Jet energy resolution(JER) can be parameterized with the NSC fit for calorimeter resolutions. The noise term of JER is obtained by measuring the fluctuations in the energy deposits due to pile-up using data samples that are collected by zero bias triggers. In this analysis, the random cones method is used for these measurements. Two random cones are produced by random  $\phi$  values and within opposite  $\eta$  regions. Energy deposits in each random cone which has a 0.4 cone size are summed. Noise term can be obtained from the difference of  $p_T$  of two random cones ( $p_T^{R.C.1} - p_T^{R.C.2}$ ). Through this approach, the contribution to the resolution from the noise term due to pile-up can be directly estimated. In this talk, the extracted noise terms in random cones, based on the full 13 TeV Run 2 data samples collected by the CMS experiment, are presented.

### Keywords:

CMS, Jet Energy Resolution, Noise Term, Random cones method, LHC

## Seesaw lepton masses and muon $g-2$ from heavy vector-like leptons

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### Abstract:

We propose a model for the vector-like lepton to explain the small muon mass by a seesaw mechanism, based on lepton-specific two Higgs doublet models with a local  $U(1)'$  symmetry. There is no bare muon mass for a nonzero  $U(1)'$  charge of the leptophilic Higgs doublet, so the physical muon mass is generated due to the mixing between the vector-like lepton and the muon after the leptophilic Higgs doublet and the dark Higgs get VEVs. In this scenario, the non-decoupling effects of the vector-like lepton give rise to leading contributions to the muon  $g-2$ , thanks to the light  $Z'$  and the light dark Higgs boson. We discuss various constraints on the model from lepton flavor violation, electroweak precision and Higgs data, as well as collider searches.

### Keywords:

Muon  $g-2$ , Vector-like lepton, Dark photon, Seesaw mechanism

## Far-forward tau neutrinos at the LHC

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### Abstract:

A large number of tau neutrinos and antineutrinos are produced in the far-forward region at the Large Hadron Collider (LHC). Two new upcoming experiments, FASER $\nu$  and SND@LHC, will measure forward neutrinos during Run 3, and proposed experiments for a Forward Physics Facility are under design to operate during the high luminosity era. These experiments will probe neutrino pseudorapidities in the range of  $\eta > 6.9$  and higher, where small and large values of parton longitudinal momentum fraction  $x$  in the parton distribution functions (PDF) are important for theoretical predictions. We show the PDF associated uncertainties in the predictions of flux and events of tau neutrinos plus antineutrinos, predominantly from the decay of  $D_s^*$  meson, the production of which is evaluated in a next-to-leading order (NLO) QCD using the 40 PDF sets of the PROSA19 group. We compare results with other 3-flavor NLO PDF sets of the CT14, ABMP16 and NNPDF3.1 collaborations. The Forward Physics Facility in the high luminosity era will provide data capable of constraining NLO QCD evaluations with these PDF sets.

### Keywords:

Forward Physics, Tau neutrinos, Neutrinos from heavy flavor

## Update on the quarkonium spectral function calculation from lattice NRQCD at non-zero temperature

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### **Abstract:**

Quarkonium melting is expected to play a role of thermometer in Quark-Gluon Plasma (QGP) environment and lattice NRQCD allows us to understand its physics based on first principles of quantum field theory. However, obtaining realistic/quantitative knowledge is hampered by the difficulty associated with reconstructing quarkonium spectral function at non-zero temperature. We discuss recent efforts by FASTSUM collaboration on the spectral function reconstruction.

### **Keywords:**

Lattice QCD, bottomonium, spectral function, numerical method, quark-gluon plasma

## Comprehensive study of the light charged Higgs boson in the type-I two-Higgs-doublet model

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### Abstract:

Even though there are many experimental and theoretical constraints, It is possible to exist charged Higgs boson lighter than top quark in type I 2HDM. We scan the parameter space with theoretical, experimental constraints. We found that masses of neutral scalar(pseudoscalar)  $m_H(m_A)$  must be less than 580 GeV, and the two are related. Additionally, We figure out that the decay mode of charged Higgs changed depending on whether the  $m_A$  was lighter or heavier than charged Higgs mass. We do the signal background analysis for the three decay modes.  $[\tau\nu][\tau\nu]$  mode and  $[\tau\nu][\tau\nu]WW$  mode target heavy A, and  $[bbW][bbW]$  channel target light A. The first mode has a high potential to discover the light charged Higgs, and the third mode is challenging in LHC.

### Keywords:

charged higgs, 2HDM

## Phenomenology of unusual top partners in composite Higgs models

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### Abstract:

We consider a particular composite Higgs model which contains SU(3) color octet top partners besides the usually considered triplet representations. Moreover, color singlet top partners are present as well which can in principle serve as dark matter candidates. We investigate the LHC phenomenology of these unusual top partners. Some of these states could be confused with gluinos predicted in supersymmetric models at first glance.

### Keywords:

LHC, BSM, composite Higgs, phenomenology

## Portraying Double Higgs at the Large Hadron Collider

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### Abstract:

The Higgs potential is vital to understand the electroweak symmetry breaking mechanism, and probing the Higgs self-interaction is arguably one of the most important physics targets at current and upcoming collider experiments. In particular, the triple Higgs coupling may be accessible at the HL-LHC by combining results in multiple channels, which motivates to study all possible decay modes the double Higgs production. In this paper, we revisit the double Higgs production at the HL-LHC in the final state with two b-tagged jets, two leptons and missing transverse momentum. We focus on performance of various neural network architectures with different types of input features: low-level (four momenta), high-level (kinematic variables) and image-based. We find it possible to bring a modest increase in the signal sensitivity over existing results via careful optimization of machine learning algorithms making full use of novel kinematic variables,

### Keywords:

LHC, Triple Higgs Self-Coupling, Double Higgs Production, Machine Learning

## Status of preparation of dual-readout calorimeter module for 2022 test beam

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### Abstract:

Calorimeters has been the important role in high energy physics experiments since they allow four-vector of both neutral and charged particles. Future lepton collider experiments (FCC-ee and CEPC) are proposed for the higgs factory to understand the property of higgs (origin of mass and its relation to the Higgs mechanism). High-quality energy measurements for these experiments are essential to study couplings between Higgs and all decay products. The dual read calorimeter (DRC) is considered a good option to allow this requirement. The KFC-DREAM (Korea Future Collider Dual-REAdout Method calorimeter) collaboration has a plan of test beam with two copper-fiber calorimeters at CERN in June and July 2022. The main programs measure the nuclear interaction lengths and study the performance of the copper-fiber calorimeters. And our main goal is to build two modules which have different configurations for DRC. In this talk, we will present our status of preparation of two modules for upcoming test beam.

### Keywords:

Dual read calorimeter, Calorimeter, FCC-ee, CEPC

## Quasielastic Charged-Current Neutrino-Nucleus Scattering with Non-Relativistic Nuclear Energy Density Functionals

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### Abstract:

Charged-current neutrino-nucleus scattering is considered in the quasielastic region with the KIDS (Korea-IBS-Daegu-SKKU) nuclear energy density functional. We focus on the uncertainties stemming from the axial mass and the in-medium effective mass of the nucleon inside nucleus. Comparing the result of theory to the state-of-the-art data from MiniBooNE, T2K, and MINERvA, we constrain the ranges of the axial mass and the effective mass that are compatible with the data. We find that the total cross section is insensitive to the effective mass, so the axial mass could be determined independently of the uncertainty in the effective mass. Differential cross sections at different kinematics are, on the other hand, dependent on the effective mass as well as the axial mass. Within the uncertainty of the axial mass constrained from the total cross section, the ambiguity of the effective mass is investigated. We obtain the ranges of the axial mass and the effective mass consistent with the values in the literature.

### Keywords:

Neutrino-nucleus scattering, Density functional theory

## Neutrino reactions on $^{12}\text{C}$ by KDAR neutrino

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### Abstract:

We studied neutrino reactions on  $^{12}\text{C}$  by the kaon decay at rest (KDAR) at JPARC. This neutrino beam is unique in that we have a mono-energy muon neutrino beam and the expected 235 MeV energy is located between the inelastic scattering region and QE region. Moreover the neutrino beam is feasible near future at JPARC.

Theoretical calculations are performed by two independent nuclear models. One is the QRPA and the other approach is the DWBA. The former is the so called two-step process through the formation of the compound nuclei by the neutrino interaction, while the latter is one-step process. We compared both results and discussed their physical meanings in the neutrino physics and related fields.

### Keywords:

Neutrino-induced reactions, KDAR neutrino

## Monoenergetic neutrons from the ${}^9\text{Be}(p,n){}^9\text{B}$ reaction induced by 35, 40 and 45 MeV protons

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### Abstract:

The development of accelerator driven systems, spallation neutron sources and other nuclear technologies require cross section data of neutron-induced reactions above 20 MeV. But the cross section data for neutron energies above 30 MeV are not so abundant in EXFOR, mainly due to the difficulties in obtaining monoenergetic neutron sources. Therefore, the need of developing a quasi-monoenergetic neutron production system. Quasi-monoenergetic or continuous-energy neutrons above 20 MeV have been produced by inducing reactions such as  ${}^7\text{Li}(p,n){}^7\text{Be}$ ,  ${}^9\text{Be}(p,n){}^9\text{B}$ ,  ${}^6\text{Li}(d,n){}^7\text{Be}$  and  ${}^9\text{Be}(d,n){}^{10}\text{B}$ . The work reported in the literature show that the beryllium target has so far been used for producing only such quasi-monoenergetic neutrons with a finite width in energy, and has not been used to produce monoenergetic neutron beams. The PHITS code which combines incorporating the intra-nuclear cascade (INC) model with the Distorted Wave Born Approximation (DWBA) method, was developed for the simulation of the neutron yields of the  ${}^7\text{Li}(p, n){}^7\text{Be}$  and  ${}^9\text{Be}(p, n){}^9\text{B}$  reactions over the energy range of 10 to 50 MeV.

In the present work, it is observed that by bombarding 0.25 mm thick beryllium with protons, produce two monoenergetic neutron peaks are produced due to the  ${}^9\text{Be}(p,n){}^9\text{B}$  reaction in the PHITS simulation. For 35, 40 and 45 MeV protons, respectively, two peaks of neutrons for each proton energy appear at the neutron energies of (i) 29.4 and 31.8 MeV, (ii) 34.5 and 36.8 MeV, and (iii) 39.7 and 42.0 MeV. For validation of the simulated monoenergetic neutron peaks was done by inducing nuclear reactions with 'effective' threshold energies in-between the two peaks of monoenergetic neutrons. In validating the monoenergetic neutron peak due to the ground state of  ${}^9\text{B}$ , samples of  ${}^{93}\text{Nb}$ ,  ${}^{63}\text{Cu}$  and  ${}^{209}\text{Bi}$  were irradiated with neutrons from the  ${}^9\text{Be}(p,n){}^9\text{B}$  reaction with 35, 40 and 45 MeV protons. The induced activity of  ${}^{90}\text{Nb}$ ,  ${}^{60}\text{Cu}$  and  ${}^{204}\text{Bi}$  radioisotopes observed in gamma ray spectrum provided evidence that  ${}^{93}\text{Nb}(n,4n){}^{90}\text{Nb}$ ,  ${}^{63}\text{Cu}(n,4n){}^{60}\text{Cu}$  and  ${}^{209}\text{Bi}(n,6n){}^{204}\text{Bi}$  reactions were induced, respectively, by the neutrons of higher energies. These neutron energies are just above the 'effective' threshold energies of the respective (n, xn) reactions. The present studies show that the simulated two peaks of monoenergetic neutrons can be experimentally validated and can be used to measure the cross sections for the neutron induced reactions and other applications.

### Keywords:

Monoenergetic neutrons; Beryllium target; (n, xn) cross section; PHITS

## Measurement of the cross sections for the $^{209}\text{Bi}(n,4n)^{206}\text{Bi}$ and $^{232}\text{Th}(n,6n)^{227}\text{Th}$ reactions by using monoenergetic neutrons generated by the $^9\text{Be}(p,n)^9\text{B}$ reaction

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### Abstract:

Neutron-induced reaction cross sections such as (n,xn) cross sections are increasingly necessary, in particular, at neutron energies above 20 MeV for the purpose of fast neutron flux measurement, improving Monte-Carlo simulation code, and design of the accelerator-driven system (ADS). On the other hand, there are no sufficient (n,xn) cross section data at energies above 20 MeV. In this work, we bombarded a 0.25 mm thick beryllium target with protons to produce monoenergetic fast neutrons. The cross sections of the  $^{209}\text{Bi}(n,4n)^{206}\text{Bi}$  reaction were measured at 29.6, 31.8, 34.5, 36.8, 39.7, and 42.0 MeV. For the measurement of  $^{232}\text{Th}(n,6n)^{227}\text{Th}$  cross section, neutrons with 39.7 and 42.0 MeV energies were used. These newly measured cross sections are close to those predicted by the EAF-2010 and TALYS. The present studies show that the simulated two peaks of monoenergetic neutrons can be experimentally validated and can be used to measure the cross sections for the neutron-induced reactions and other applications.

### Keywords:

Monoenergetic neutrons, Beryllium target, (n,xn) cross section

## Evaluations of neutron induced reaction cross sections for $^{35,36,37}\text{Cl}$

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### **Abstract:**

We have performed evaluations of cross sections for neutron induced reactions on  $^{35,36,37}\text{Cl}$  for molten salt reactors, where chloride U, Pu and/or Th are used as nuclear fuel. We have included covariances in our evaluations. Random files for our Total Monte Carlo analyses of integral quantities also will be provided.

### **Keywords:**

chlorine, neutron induced reaction, cross sections, evaluation, molten salt reactor.

## The elastic scattering of $^{10}\text{C}$ with dynamic polarization potentials

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### Abstract:

In the recently introduced elastic scattering cross section data of the  $^{10}\text{C} + ^{208}\text{Pb}$  system at energy near the Coulomb barrier [1], it can be seen that the breakup reaction effect generated from the neutron rich nuclei is quite evident. As is well known,  $^{10}\text{C}$  is one of the proton rich nuclei with the Brunnian (or super-Borromean) structure interconnected by the four nucleus,  $\alpha + \alpha + p + p$ . In contrast to  $^8\text{B}$  and  $^{17}\text{F}$  nuclei, however, it can be seen that there is a significant contribution of the breakup reaction to the total reaction. This is different from the characteristics of nuclear reactions involving the proton rich nuclei reported so far. Therefore, the goal of our present work is to examine the cause of the suppression in elastic scattering cross section between the  $^{10}\text{C}$ , which is a proton rich nuclei, and  $^{208}\text{Pb}$  target nuclei.

[1] R. Linares et al. Phys. Rev. C 103, 044613 (2021).

### Keywords:

optical model, near the Coulomb barrier, elastic scattering, breakup reaction, proton rich nuclei

## Study of alpha transfer at energies near Coulomb barrier using DNS model

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### Abstract:

The transfer of clusters between nuclei has aroused great interest for a long time. In nuclear physics it is often helpful to presume the existence of clusters in the nucleus, and the participation of these clusters in nuclear reaction. These reactions including transfer of clusters between nuclei is used as a means of synthesizing exotic nuclei for example neutron-rich, proton-rich, or superheavy nuclei. The aim of this work is to study for the phenomenon of alpha transfer mechanism at low energies near the Coulomb barrier energy.

Within the di-nuclear system (DNS) model, many of alpha transfer reactions with stable and radioactive ion beams at incident energies around the Coulomb barrier are investigated.

### Keywords:

alpha transfer reaction, Di-nuclear system (DNS) model

## Chiral nuclear force up to NNLO with vector mesons

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### **Abstract:**

We will report progress in constructing a novel nuclear force by using chiral perturbation theory including vector mesons as well as pions.

In particular, the up to next-to-next-to-leading order chiral nuclear force with vector mesons will be presented

and compared with the conventional chiral perturbation theory results.

The role of vector mesons will be discussed in terms of the convergence with respect to chiral order and the accuracy of the resulting theoretical predictions.

### **Keywords:**

nuclear force, vector meson, chiral perturbation theory

## Bound-to-continuum approach for keV-energy nucleon radiative capture reaction

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### Abstract:

The nucleon radiative capture reaction in which the nucleon is absorbed by the target nucleus, and the gamma radiation is then detected is important in applied nuclear physics and nuclear astrophysics. At very low energy as in the cores of stars, it is complicated for nuclear experiments to measure the astrophysical S factor that is a rescaling of a nuclear reaction's total cross-section. In this work, the keV-nucleon radiative capture reactions are studied using the bound-to-continuum potential model in which both scattering and bound states are treated simultaneously and based on the Skyrme Hartree-Fock approximation. The obtained results are shown to be in good agreement with the available experimental data. The extrapolation to the very low energy, including the zero energy is reliable.

### Keywords:

nuclear astrophysics, radiative capture reaction, potential model, Skyrme Hartree-Fock approximation, bound-to-continuum

## 우라늄 동위원소에 대한 중성자 입사 핵반응 단면적 평가

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### Abstract:

원자력에너지의 핵심 연료인 우라늄 동위원소에 대한 중성자 입사 핵반응 평가는 핵반응 이론의 발달과 수많은 실험데이터를 바탕으로 다른 핵종들에 비해 월등히 높은 정밀도를 나타낸다. 그럼에도 불구하고 소형원자로 및 사용후핵연료 연구 등과 관련하여 중성자 핵반응 평가에 대한 더 높은 정밀도가 요구된다. 특히 비탄성 산란 단면적, 포획 단면적, 방출 중성자 스펙트럼등에 대한 미분 실험데이터의 큰 불확도는 평가 파일의 정밀도 향상에 주된 어려움으로 작용한다. 이는 핵반응 평가 파일이 주로 미분 실험값을 이론 모델로 재생산함으로써 만들어지기 때문에 실험값의 불확도가 크면 평가 파일의 정밀도를 보장하기 어렵기 때문이다. 이를 극복하기 위해 본 연구에서는 미분 실험데이터뿐만 아니라, ICSBEP (International Criticality Safety Benchmark Evaluation Project) 에서 제공하는 적분 실험값을 고려하여, 핵반응 데이터 평가의 정밀도를 향상시키는 방법을 제시한다.

### Keywords:

핵반응, ICSBEP, 방출 스펙트럼

## Some recent progress on topological magnons

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### **Abstract:**

Inelastic neutron scattering provides detailed information about the dispersion relations of magnon bands. In this talk, I describe how this technique can provide bulk signatures of magnon band topology in the vicinity of linear touching points. The scattering intensity exhibits a characteristic winding pattern around such points that is tied to magnon spin-momentum locking. This has recently been observed in CoTiO<sub>3</sub> and in elemental gadolinium. In addition, when magnon decay is dynamically and kinematically allowed, the lineshape too exhibit signatures characteristic of the presence of exceptional structures in the non-Hermitian bands. I also highlight the importance of spin-space symmetries in many cases of magnon band topology.

### **Keywords:**

topology, magnons, spin waves, quantum magnetism

# Topological Dirac magnons in Cr-based honeycomb ferromagnets: Dzyaloshinskii-Moriya versus Kitaev exchanges

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## Abstract:

The magnon band structures of ferromagnets on honeycomb lattices are analogous to the electronic band structure of graphene, which exhibits crossings between two modes with linear energy-momentum relations at the so-called Dirac wave vectors  $Q_K = (\pm 1/3, \pm 1/3)$ . The linearly dispersive magnons near the Dirac wave vectors are thus called Dirac magnons with references to the Dirac fermions in the graphene [1]. In the graphene's band structure, spin-orbit couplings across the next nearest neighbor bonds break the time reversal symmetry and open small energy gaps at the Dirac wave vectors causing the Dirac fermions to become massive in the bulk bands. Spin-orbit-coupled topological gap openings were also predicted in magnons of honeycomb ferromagnets, and eventually observed in a series of Cr-based van der Waals magnets. In this talk, we will review the recent experimental works on observing Dirac magnons and topological gap openings in  $\text{CrX}_3$  ( $X = \text{Br}, \text{Cr}, \text{I}$ ) and  $\text{Cr}_2\text{Z}_2\text{Te}_6$  ( $Z = \text{Si}, \text{Ge}$ ) using inelastic neutron scattering [2-5]. We will discuss how the spin-orbit couplings, either as antisymmetric Dzyaloshinskii-Moriya or bond-directional Kitaev exchanges, can reproduce the observed magnon bands involving the gap openings at the Dirac wave vectors. Finally, we will see how the in-plane magnetic field dependence of the magnons rules out the Kitaev exchange and leaves the Dzyaloshinskii-Moriya exchange to be the only possible candidate [2].

[1] J. Fransson *et al.*, Phys. Rev. B **94**, 075401 (2016)

[2] L. Chen *et al.*, Phys. Rev. X **8**, 041028 (2018); L. Chen, et al., *ibid* **11**, 031047 (2021)

[3] L. Chen *et al.*, 2D Materials **9**, 015006 (2022)

[4] Z. Cai et al., Phys. Rev. B **104**, L020402 (2021)

[5] F. Zhu et al., Sci. Adv. **7**, eabi7532 (2021)

## Keywords:

topological magnons, Dirac magnons, honeycomb ferromagnets, inelastic neutron scattering

## Thermal Hall effect of Kitaev quantum spin liquid candidate materials

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### Abstract:

$\alpha$ -RuCl<sub>3</sub> represents one of the most intriguing quantum materials of the past years. Numerous evidence for a significant Kitaev interaction between the  $j=1/2$  moments which are located at the vertices of a honeycomb lattice has nourished hope to find fingerprints of the celebrated Kitaev model in this compound. Indeed, reports of a half-quantized thermal Hall effect in this compound seem to match perfectly with the predicted thermal transport due to an emergent Majorana edge mode of the Kitaev quantum spin liquid (QSL). On the other hand, we have demonstrated that the longitudinal thermal transport of  $\alpha$ -RuCl<sub>3</sub> is due to phonons and is determined by a strong phonon-spin scattering. Interestingly, its temperature dependence is very similar to that of the thermal Hall conductivity which suggests the possibility of an alternative phononic scenario for the thermal Hall effect.

Recently, Na<sub>2</sub>Co<sub>2</sub>TeO<sub>6</sub> emerged as a new and interesting candidate material for a Kitaev QSL. Our data for the longitudinal thermal conductivity reveal a striking similarity to that of  $\alpha$ -RuCl<sub>3</sub>, as well as a large thermal Hall effect. Thus, with these two materials at hand, one can hope to obtain fresh information as to whether the thermal Hall effect in the Kitaev QSL compounds is due to genuine Majorana heat transport or due to phonons.

### Keywords:

Thermal Hall effect, Kitaev model, topological quantum spin liquid

## New Kitaev spin liquid candidate materials; ruthenium trihalides $\text{RuX}_3$ ( $X = \text{Br}, \text{I}$ )

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### Abstract:

$\alpha\text{-RuCl}_3$  has been attracting intensive attention as the most probable candidate material for the Kitaev quantum spin liquid. Despite a naive expectation for the spin liquid state from the Kitaev model,  $\alpha\text{-RuCl}_3$  shows a zigzag-type antiferromagnetic order at  $T_N \sim 7\text{-}15$  K due to non Kitaev-type interactions. On the other hand, when the magnetic order is suppressed by applying a magnetic field, the half-integer quantization, which is a characteristic behavior in Kitaev spin liquids, has been reported in thermal Hall effect measurements[1]. This indicates that  $\alpha\text{-RuCl}_3$  is located in the vicinity of the ferromagnetic Kitaev limit, which we are focusing on ruthenium trihalides as a platform for exploring novel electronic states. In this talk, we will present the successful synthesis of two new Kitaev spin liquid candidate materials,  $\text{RuBr}_3$ [2] and  $\text{RuI}_3$ [3,4], via the high-pressure method.  $\text{RuBr}_3$  possesses an ideal honeycomb lattice of  $\text{Ru}^{3+}$  with  $R\text{-}3$  symmetry and shows the antiferromagnetic order with zigzag-type magnetic structure at  $T_N = 34$  K. The moment angle from honeycomb plane in  $\text{RuBr}_3$  is larger than that in  $\alpha\text{-RuCl}_3$ , suggesting larger Kitaev interactions in  $\text{RuBr}_3$  compared to  $\alpha\text{-RuCl}_3$ . On the other hand, there are two kinds of polymorph in  $\text{RuI}_3$  with the honeycomb lattice;  $R\text{-}3$  and  $P\text{-}31c$ .  $\text{RuI}_3$  with the honeycomb structure shows a semi-metallic feature in the electrical resistivity and no magnetic order down to the lowest measurement temperature. Metal-insulator transition occurs by an introduction of iodine for halogen site  $X$  in  $\text{RuX}_3$ . In our presentation, we will show an electronic phase diagram of  $\text{RuX}_3$  and discuss the effect of bandwidth control in Ruthenium trihalides.

[1] Y. Kasahara *et al.*, Nature 559, 227 (2018).

[2] Y. Imai *et al.*, Phys. Rev. B 105, L041112 (2022).

[3] K. Nawa, Y. Imai *et al.*, J. Phys. Soc. Jpn. 90, 123703 (2021).

[4] D. Ni *et al.*, Adv. Mater. 34, 2106831 (2022).

### Keywords:

two-dimensional honeycomb lattices, Kitaev interaction, high-pressure synthesis, semi-metal

## Nanoscale Probing and Utilizing Surface Plasmon-driven Hot Carriers

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### Abstract:

The detection of hot electrons and understanding the correlation between hot electron generation and surface phenomena are challenging questions in the surface science and catalysis community. Hot electron flow generated on a gold thin film by photon absorption (or internal photoemission) appears to be correlated with localized surface plasmon resonance. It has been found that the hot electron flux generated under photon absorption and exothermic chemical reaction is the major mediator of energy conversion process [1-3]. In this talk, I introduce the research direction to attempt to detect the surface plasmon driven hot carrier at the nanometer scale by using scanning probe microscopy. To detect and utilize the hot electron flows at the macroscale level, the metal-semiconductor nanodiodes were constructed. At the nanometer scale, we utilized photoconductive atomic force microscopy to observe photoinduced hot electrons on a triangular Au nanoprism on TiO<sub>2</sub> under incident light. This is the direct proof of the intrinsic relation between hot electrons and localized surface plasmon resonance. We observed surface plasmon induced hot hole by using the system of Au nanoprism on p-type GaN. I will discuss the impact of hot carriers in the photocatalytic activity under photoelectrochemical water splitting by using Au-based plasmonic nanostructures.

[1] J. Y. Park et al. Chemical Reviews 115, 2781-2817 (2015).

[2] J. Y. Park et al. Accounts of Chemical Research 48, 2475-2483 (2015).

[3] S. W. Lee et al. Surface Science Reports 76 100532 (2021).

### Keywords:

hot electron, surface plasmon, photoconductive atomic force microscopy

## An efficient numerical method for finding a common supercell between two similar crystalline surfaces

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### Abstract:

Fundamental properties of two-dimensional (2D) heterostructures are mainly determined by interface geometries. Here, we propose a new numerical method for efficiently finding a common supercell between two similar crystalline surfaces such as square-square and rhombus-rhombus lattices. Using the complex plane, we can regard the 2D lattice as the 2D complex vector. Then, the relationship between two surfaces becomes the eigenvector-eigenvalue relationship where an operator corresponds to a transformation matrix. We show that this transformation matrix between two surfaces can be determined by its eigenvalue which is obtained by two given 2D lattice parameters and its rotational angle. Taken together, we are able to directly find the transformation matrix and common supercell between two similar crystalline surfaces with  $O(\log N)$  time complexity once we have their lattice parameters, where  $N$  is the maximum index of the transformation matrix. This is much faster than the conventional algorithm ( $\sim O(N^4)$ ).

### Keywords:

Interface, Heterostructure, Complex plane

## Ab Initio Simulations of Water/Metal Interfaces and Perspective on Electric Double Layer Modeling

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### Abstract:

Water/metal interfaces play a crucial role in electrochemical energy conversion/storage, photoconversion, sensors, and corrosion, just to name a few. Electrochemical interfaces are typically associated with forming an electric double layer whose theoretical modeling requires an appropriate description of the polarization of both the electrode and the electrolyte. In principle, ab initio molecular dynamics simulations are the natural choice as they reliably treat the competing water–water and water–metal interactions and explicitly consider the electronic degrees of freedom. However, this approach is computationally still very demanding and only allows simulations of relatively small canonical ensembles for limited simulation times. Thus, there is a computationally less demanding but still reliable approach for the electric double layer. We will first review the recent progress in ab initio simulations of water/metal interfaces, starting from static systems such as adsorbed ice-like layers, followed by a discussion of studies concerned with the structural and electronic properties of thin water films at metal surfaces. Then, we will briefly address the variation of the interface properties by adding explicit ion species into the water film. Finally, by comparing a continuum method based on a grand canonical scheme with ab initio approaches, we will provide an outlook on possible future directions in the atomistic modeling of electric double layers.

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### Keywords:

Ab initio molecular dynamics, Water/metal interfaces, Electric double layer

## Formation of stable PdO films on alloys for oxidation catalysis

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### Abstract:

Methane based fuels such as natural gas and biogas are increasingly used to increase the sustainability of transports and energy conversion processes [1]. Methane is, however, a strong greenhouse gas with a global warming potential about 70 times higher than that for CO<sub>2</sub> over a 20 years period. Hence it is of crucial importance to clean the exhausts from any unburned methane as well as CO originating from incomplete combustion of methane. For both of these reactions, a thin bulk PdO film has been shown to be highly active. At conditions where this film forms, however, the oxidation will continue until a thicker inactive oxide is formed and the catalyst becomes inactive. This so-called oxygen poisoning constitutes a major issue in oxidation catalysis, especially for inert reactants such as methane.

To stabilize the active PdO phase, we are studying methane oxidation over thin films of alloys of Pd and Au. The hypothesis is that the limited amount of Pd will limit the oxide thickness. The oxidation of PdAu, however, turned out more difficult than expected, and so far our results focus on the formation of PdO on PdAu, rather than catalytic reactions.

In this presentation we will report results, based on grazing incidence X-ray diffraction (GIXRD) and X-ray reflectivity (XRR), on the growth of PdO on thin PdAu thin films on sapphire in pure O<sub>2</sub>, compared with films of pure Pd. In brief, a significantly higher pressure is needed to oxidize the alloy film, but in addition, a higher temperature is needed for initiating the oxide formation, while a lower temperature is needed to make the oxide well ordered.

### Keywords:

PdAu, Oxidation, PdO, GIXRD, XRR

## New driving mechanisms for STM-ESR

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### Abstract:

During this talk we address the problem of electronic spin resonance of an individual atom on a surface driven by a scanning tunneling microscope. Several mechanisms have been proposed so far, some of them based on the modulation of exchange and crystal field associated with a piezoelectric displacement of the adatom driven by the radio frequency (RF) tip electric field. As the distance between the tip and the adatom varies in the experiment, the mechanisms involved should change. We know that, as the experiment is carried out, the driven mechanisms involved will have signatures of exchange interaction, magnetic dipole interaction, modulation of the adatom's crystal field and even some signature of the modulation of the gyromagnetic factor.

We discuss thoroughly the cases of hydrogenated Ti ( $S= 1/2$ ) and Fe ( $S= 2$ ) on MgO, relevant for recent experiments. We model the system using two approaches. First, we performed calculations by direct diagonalization of a many electron Hamiltonian considering the electrons in the d shell of the ad-atom. All the microscopic models are constructed using density functional theory (DFT) calculations. Second, we obtain some pseudoanalytical results using an effective spin model which helps us to understand some fundamental aspects. Both, microscopic model and effective Hamiltonian, are constructed taking into account the exchange and magnetic dipolar interaction between the ad-atom and the spin polarized tip.

At the end of this talk we will sketch a model to account for the driving of ESR-STM via modulation of exchange between a probe spin and a nearby surface spin. We also consider the exchange modulation between the tip and the probe spin. We work out the case of Ti-H dimer and Fe as a nearby surface spin. We also analyze the effect of the tip electric field on the piezoelectric displacement of both atoms, by means of DFT calculation.

### Keywords:

spin dynamics, scanning tunneling microscope (STM), Electron spin resonance (ESR), Modelling

## Understanding the magnetic behavior of molecules with spin functionalities deposited on Superconductors

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### Abstract:

Single Molecule Magnets (SMMs) are molecules with remarkable magnetic properties as extremely long magnetization relaxation time and magnetic hysteresis at the single molecule level at low temperatures.[1]

Being able to join magnetic memory and quantum features, they represent suitable building blocks for novel technologies at the nanoscale, such as spintronic applications. Both the electronic and magnetic properties of SMMs are particularly sensitive to the interaction with substrates, and the signature of this interaction has been observed on a wide range of metallic and non-metallic substrates either at the single molecule level or at the larger scale of molecular films.[2–4]

The evidence of the strong interactions occurring at the surface/molecule interface are found in the magnetic hysteresis loop of SMMs films, which is quenched when molecules interact directly with conducting substrates but preserved - or even boosted - by the use of decoupling layers. Here I will present a route for controlling the magnetism and quantum features of diverse SMM systems by engineering the substrate with decoupling layers or superconducting materials. The investigation of magnetic molecules on substrates here presented will be discussed based on a multi-techniques approach involving scanning tunnelling microscopy, photoemissions techniques and synchrotron experiments. In particular, I will focus on the role of the superconductors in influencing magnetic molecules and how these hybrid systems hold potentials for spintronics and quantum technologies. [5,6]

Indeed the transition of the substrate to the superconducting state affects the magnetization of the SMMs that locally switch from a blocked magnetization state to a resonant quantum tunneling regime. Exploiting the different nature of SMM systems interaction with the substrate, the sensitivity to the spatial magnetic field variation on the superconductor is resolved. This innovative approach opens interesting perspectives for controlling single molecule magnets in spintronic devices as well as for their use as local probes for superconducting materials.

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- [6] Serrano, G. et al., *Nat. Mater.*, 19, 546 (2020)

### Keywords:

spin dynamics, superconductors, molecular spins, molecules

## Electron Spin Resonance of Individual Atomic and Molecular Spins on Surfaces

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### Abstract:

In this talk, I will introduce electron spin resonance scanning tunneling microscopy (ESR-STM) as a new architecture for coherent control of spins on surfaces [1,2]. This technique allows to address single atoms and molecules on surfaces with unprecedented energy resolution. Thus, it can be used for instance to sense the magnetic coupling between spin centers on the nanoscale [3], including their spin dynamics [4,5]. The high energy resolution also grants access to the hyperfine interaction between the electron and nuclear spin of different atomic species [6]. I want in particular highlight in this talk, that we could extend this technique also recently to individual molecules [7], which allowed us to study their magnetic interaction and spin states. It also permitted us to probe their coherent properties in single-spin Rabi and Hahn echo schemes [8]. This opens up a path towards quantum information processing and quantum sensing using atomic building blocks, including atoms and molecules.

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### Keywords:

spin dynamics, scanning tunneling microscope (STM), Electron spin resonance (ESR), Molecular Magnets

## Electron-electron double resonance in an ESR-STM

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### Abstract:

The combination of electron-spin resonance (ESR) and the scanning tunneling microscope (STM) has enabled the study of electronic states at the single atom level. So far, this method has been used successfully to study single atoms and molecules either by continuous wave (CW) or pulsed radio-frequency driving. [1,2]

A strong limitations of currently available techniques is the single-frequency driving, which only allows the control of a single spin at a time. In our recent work, we developed a technique that allows to simultaneously drive two (and conceptually more) spins whilst using a conventional ESR-STM setup. In this talk, I will present an update of our findings, including CW and pulsed driving of two coupled  $S=1/2$  Titanium atoms on thin insulating layers as well as open quantum systems simulations which give further insights into the physics.[3]

References:

- 1 Kai Yang *et al.*, Science 336, 509-512 (2019)
- 2 Xue Zhang *et al.*, Nature Chemistry, 14, 59-65 (2022)
- 3 Soo-hyon Phark *et al.*, arXiv:2108.09880 (2021)

### Keywords:

double resonance, electron spin resonance (ESR), scanning tunneling microscope (STM), quantum manipulation, quantum coherence

## Interfacial Phonon Modes of Ferroelastic WO<sub>3</sub> Twin Wall

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### Abstract:

The twin wall between two different ferroelastic orientation states in WO<sub>3</sub> films has a symmetric structure originating from spontaneous strains of adjacent orientation states. Here, we present the observation of domains and walls through Angle-resolved polarized Raman scattering. Remarkably, we find that a low-energy Raman mode is largely enhanced at the twin walls, of which the width can be presumed to be ~ 25 nm from a diffusive X-ray superlattice peak. The interfacial effect on the enhancement of Raman signal per unit area is estimated to be three times larger than the contribution of domains. This phenomenon is explained based on the fact that the Raman scattering tensor is slightly modified by a compatibility between the ferroelastic spontaneous strains. The finding provides a new avenue into the lattice dynamics of ferroelastic twin wall.

### Keywords:

ferroelastic twin wall, Raman scattering, phonon, spontaneous strain, prototypic phase

## Rotation-induced metastable polar structures in perovskite $\text{CaSnO}_3$ : a first-principles study

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### Abstract:

We present a first-principles density-functional-theory study on the relation between octahedral rotation patterns and polar instability for perovskite oxides. As oxygen octahedron rotation patterns are one of the important parameters that can change the phase of the material in many perovskite oxides, we investigate rotation-pattern-dependent polar metastable phases of  $\text{CaSnO}_3$ . Based on the rotation patterns commonly observed in perovskite oxides, we systematically investigate the phonon dispersions and identify the unstable polar modes for each of the rotation patterns, until the metastable polar structures are obtained. We find that materials with  $a^+a^+a^+$ ,  $a^-a^-a^-$ , and  $a^+a^+c^-$  rotational patterns have metastable polar structures in which sizable polarization comparable to the conventional ferroelectrics are present. The metastable polar structures could be stabilized in a substrate-film configuration and suitable substrate-film geometries will be presented. We believe that our study will provide a guideline for finding new functional ferroelectric perovskite thin films.

### Keywords:

first-principles calculation, ferroelectricity, dielectric properties, perovskite oxides, oxide heterostructures

## Defect-assisted phase transition near magnetic Néel temperature in La substituted BiFeO<sub>3</sub> thin films

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### Abstract:

The emergence of a phase in complex oxide systems can reveal unforeseen opportunities to explore new novel materials and device concepts [1]. Generally, various crystal defects reside in the domain walls such as anti-Frenkel defect, and oxygen vacancies are introduced to manipulate optical, magnetic, mechanical properties of parent materials [2]. However, it has not yet been explored how crystal defects in domain walls interact with other degrees of freedom and affect overall phase transitions. In this study, we have found that defect dipoles mediated by the flexoelectric effect in complex oxide materials can exert new phase transition. The existence of micron-sized polar domains with strain-driven morphotropic phase boundaries (MPBs) can play a significant role in the multiple electronic states of La-substituted BiFeO<sub>3</sub> thin films. Impedance spectroscopy reveals that ionic migration is the key factor changing the multiple electronic states. In addition, capacitance anomaly shows that migration of defects is coupled with magnetic Néel temperature. Our findings will offer valuable information on tuning electronic states correlated with ionic migration and magnetic orders.

### References

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### Keywords:

Dielectrics, Ionic diffusion, phase transition

## Ab initio study for electron-phonon coupling of Nb-doped SrTiO<sub>3</sub> with Jellium model

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### Abstract:

Doped SrTiO<sub>3</sub>(STO) is one of the most dilute bulk systems with a superconducting ground state. As such, the applicability of the BCS-Eliashberg paradigm is highly uncertain. However, there are recent experimental reports that observed the BCS pairing gap to T<sub>c</sub> ratio for the superconductivity in Nb-doped STO. Motivated by these reports, we study Nb-doped STO by density functional theory. To describe low concentration doping, we adopt the jellium model. We confirm the jellium model is in good qualitative agreement with experimental phonon data for Nb-doped STO. We obtain changes in frequency of transverse-optical phonon, which affect the superconducting state. Furthermore, we discuss the effect of the doping concentration on the electron-phonon coupling in the jellium model.

### Keywords:

SrTiO<sub>3</sub>, Superconductor, BCS theory, Density functional theory, electron-phonon coupling

## Characterization of polar-chiral magnetic material doped Ni<sub>3</sub>TeO<sub>6</sub> systems.

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### Abstract:

Orthotellurate Ni<sub>3</sub>TeO<sub>6</sub> (NTO)-type systems are both polar and chiral with various magnetic ordering, which is provided by transition metal magnetic ion.[1,2] The effect of magnetic anisotropy under chemical doping and different cation reveal various magnetic structure[3,4], however, all magnetic structure is combined on the chiral crystal structure. Here we introduce the study of characterization of doped Ni<sub>3</sub>TeO<sub>6</sub> systems. We successfully grow the Ni<sub>3</sub>TeO<sub>6</sub> type single crystals with different magnetic anisotropy, and characterize the physical properties included magneto-dielectric and linear magneto-electric effects. By x-ray natural circular dichroism at Ni edge, chiral and its enantiomer shows the opposite XNCD signals with different magnetic anisotropy.

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### Keywords:

Chiral structure, magnetoelectric, multifunctional oxides

## Dynamic Mechanical Writing of Ferroelectric Nanobubble-like Domains

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### Abstract:

Mechanical switching of ferroelectric polarization has been extensively demonstrated on various ferroelectric thin films using tips of scanning probe microscopy (SPM), in which the out-of-plane polarization can be switched from upward to downward mainly due to flexoelectric fields induced by quasi-static loading or sliding of SPM tips. Here, we for the first time demonstrate that dynamic forces of mechanical tapping and hitting of SPM tips can selectively switch the out-of-plane polarization from downward to upward as well as induce the phase transition from the tetragonal-like (T') monoclinic phase to the rhombohedral-like (R') monoclinic phase in compressively strained BiFeO<sub>3</sub> (BFO) thin films. The switched-up domains can be both electrically and mechanically switched back to the down domain and scaled down to nanobubble-like domains with long retention properties (several months), which may be achieved by the balance between the electric and elastic boundary conditions resulting in their topological feature. The up switching of polarization may be attributed to the metastable state induced by the phase transition under tapping, the ferroelastic relaxation, and the upward depolarization field, which is stronger than the downward flexoelectric field. Our study provides the observation of ferroelectric bubble structures based on comprehensive dynamic mechanical switching mechanisms and opens a new era for bidirectional mechanical switching of ferroelectric polarization for non-volatile magnetoelectric devices.

### Keywords:

High frequency dynamic force, Dynamic strain gradient, Ferroelectric nanobubble, Morphotropic phase boundary, Phase transition

## Electrocatalytic activity of BaRuO<sub>3</sub> thin films depending on the crystalline quality

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### Abstract:

The transition metal oxides (TMO) are widely used for chemical energy storage and conversion. In particular, the studies on electrocatalytic activity of the TMOs are highly necessary for the development of future energy industry. The electrocatalytic activity are strongly influenced by the crystal structure and surface electronic structure of a catalyst. Interestingly, a trade-off relation exists in terms of the crystalline quality of the catalyst. For example, whereas the crystalline perovskite Ruthenates show high electrocatalytic activities [1, 2], amorphous structures are more viable in actual applications. On the other hand, high crystallinity, which assures the translational symmetry of a lattice necessary for the application of electronic band structure, is fundamentally important for predicting its electrocatalytic reaction. [3] Because thin film system is suitable for controlling the crystallinity of a material, the TMO thin film system has been adopted as an excellent model system for examining and understanding the electrocatalytic reaction in terms of intrinsic activity.

In this study, we compared the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) activities and stabilities between the crystalline and amorphous BaRuO<sub>3</sub> thin films. We suggest that the cubic crystalline phase (3C) BaRuO<sub>3</sub> thin film would have a higher electrocatalytic activity (both OER and HER) than the amorphous BaRuO<sub>3</sub> thin film. We systematically controlled the crystallinity by varying the growth temperature ( $T_g$ ) using pulsed laser deposition and confirmed crystalline phase for  $T_g = 400 - 600$  °C and amorphous phase in room temperature to 300 °C by X-ray diffraction. Using cyclic voltammetry, we identified that the 3C BaRuO<sub>3</sub> thin film exhibits higher current density (normalized by geometric surface area at 1.4 V vs. RHE) of 1.1 mA than the amorphous thin film (0.1 mA) by about an order of magnitude in OER. Similar increase in current density was observed for HER, i.e., 2.5 mA for the 3C BaRuO<sub>3</sub> thin film and 1.6 mA for the amorphous thin film. On the other hand, the chronoamperometry measurement for OER has confirmed that amorphous BaRuO<sub>3</sub> thin film shows higher chemical stability. However, HER of BaRuO<sub>3</sub> showed good stability for both crystalline and amorphous phases. From transport and optical spectroscopic measurements, we observed enhanced Drude contribution for the 3C thin film compared to the amorphous one, providing the origin of the high electrocatalytic activity. The higher electrocatalytic activity trend in the 3C BaRuO<sub>3</sub> compared to the amorphous BaRuO<sub>3</sub> is principally owing to its higher electric conductivity.

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### Keywords:

Crystal structure, Epitaxial thin film, Electrocatalytic reaction

## Studies on the roughnesses of the color boundaries in electrocoloration in an oxide thin film

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### Abstract:

Understanding spatial and temporal behaviors of ionic migration in solids is important for various technological applications, such as solid oxide fuel cells. Our model material, a  $\text{Bi}_{0.7}\text{Ca}_{0.3}\text{FeO}_{3-\delta}$  thin film is an ionic conductor having electrochromism, which show color changes according to its oxygen stoichiometry ( $3-\delta$ ).<sup>[1]</sup> We induce topotactic transitions from as-grown phase ( $\delta = 0.15$ ) to oxygen-vacancy-poor phase ( $\delta = 0$ ) by applying voltage between coplanar electrodes.<sup>[2,3]</sup> Here, we observe kinetic roughening of boundaries between the two phases with optical microscopy. Width vs. position and width vs. time are plotted with different voltages and temperatures. Studies on unstable boundaries are quite active in various systems such as ferroic domain walls or fluid invasion in porous media.<sup>[4,5]</sup> However, those studies are lacking in the area about the topotactic transition or electrocoloration in spite of its importance in technological applications.

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### Keywords:

Ionic conduction, Kinetic roughening, Electrocoloration

## Interfacial Structure of Pt Nanoparticles and Metal oxide Supports

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### Abstract:

The metal-support interaction of heterogeneous catalysts is quite important for the stability and dispersion of the catalysts. However, the determination of buried interfacial structure, particularly, nanoparticles/supports is considerably difficult. We examined the interfacial structure of Pt nanoparticles and TiO<sub>2</sub> supports by using extended x-ray absorption fine structure (EXAFS) measurements, density functional theory (DFT) calculations, and wavelet transformed EXAFS (WT-EXAFS) analysis. For the study, Pt nanoparticles on Titania-incorporated fumed silica (Pt/Ti-FS) supports were prepared and treated with hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) at room temperature (RT). EXAFS measurements of the H<sub>2</sub>O<sub>2</sub>-Pt/Ti-FS specimen were performed at the Pt L<sub>3</sub> edge during heating up to 500°C. Quantitative analysis of Fourier transformed EXAFS analysis shows that most of the oxygen atoms bonding the Pt nanoparticles of the H<sub>2</sub>O<sub>2</sub>-Pt/Ti-FS specimen disappear for T > 250°C. However, DFT calculations suggest Pt-O bonds existing at the interfaces of Pt/TiO<sub>2</sub>. We employ the WT-EXAFS analysis which holds the structural information of k-space as well as of r-space. The WT-EXAFS analysis qualitatively shows a weak but distinct signal of oxygen atoms around Pt atoms at 250°C and RT<sup>c</sup> after being heated up to 500°C and cooled down. We will also introduce the WT-EXAFS analysis, which is useful to distinguish the different species elements occupying the same crystalline site or forming the same short-range ordering.

### Keywords:

Interfacial structure, Wavelet Transform, EXAFS, DFT, Pt catalysts

## Avalanche multiplication in ambipolar WSe<sub>2</sub> field-effect transistors analyzed through channel length modulation

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### Abstract:

Recently, there have been various reports of utilizing avalanche multiplication in two-dimensional (2D) materials-based devices applications such as avalanche photodetectors and transistors [1]. Previous studies have mainly focused on developing high-performance devices with unipolar semiconductor as the active material. However, fundamental analysis of the multiplication process in ambipolar materials is required to push the performances further, as well as establish novel architectures. Although ambipolar 2D materials have the advantage of simple carrier type tuning through electrostatic gating, allowing both carrier types in a single channel poses an inherent difficulty in analyzing their individual contributions to avalanche multiplication. In ambipolar WSe<sub>2</sub> field-effect transistors (FETs), two phenomena of ambipolar transport and avalanche multiplication can occur, and both exhibit secondary rise of output current at high lateral voltage. We distinguished between these two competing phenomena using the method of channel length modulation. In long-channel devices, minority charge carriers are accumulated near the drain side of the channel, and the critical voltage is modulated in equal amounts as the gate voltage. In contrast, short-channel devices undergo carrier multiplication at high lateral voltages, and the breakdown voltage is insensitive to change in the gate voltage. Furthermore, we extracted multiplication characteristics from both electron- and hole-induced avalanche multiplication in WSe<sub>2</sub> and compared the results with conventional semiconductors. Our study provides a simple and robust method to examine carrier multiplication in ambipolar materials and will foster the development of high-performance atomically thin electronic devices utilizing avalanche multiplication.

[1] A. Gao et al., Nat. Nanotechnol. 14, 217 (2019).

### Keywords:

TMDC, Avalanche Multiplication, Ambipolar Transport

## Visualization of stacking angle distribution in twisted bilayer WS<sub>2</sub>

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### Abstract:

We present the Raman imaging method to visualize spatial distribution of stacking angle ( $\theta$ ) in twisted bilayer WS<sub>2</sub>. We have performed Raman measurements on twisted bilayer WS<sub>2</sub> with  $\theta$  range from 0 to 60°. For small twist angles ( $\theta < 6^\circ$  and  $\theta > 54^\circ$ ), we have observed that the interlayer phonon modes shifted sensitively as a function of the twist angle. In the mid-range ( $6^\circ < \theta < 54^\circ$ ), some folded phonon modes with prominent angle-dependence have been observed while they are absent in 2H- or 3R-stacked bilayer WS<sub>2</sub>. These Raman signatures can be explained by the modification of phonon dispersion due to the strong phonon-phonon interaction, lattice reconstruction, and moiré zone-folding effect, respectively. [1, 2] By utilizing such angle-dependent Raman signatures, we can visualize the angle disorder presented in the van der Waals heterostructures nondestructively.

[1] Quan, J., Linhart, L., L., ML. et al., Nat. Mater. 20, 1100-1105 (2021)

[2] Lin, M.-L. et al., ACS Nano, 12, 8, 8770-8780 (2018)

### Keywords:

twisted bilayer WS<sub>2</sub>, Raman spectroscopy

## Exciton-Polaritons in Exfoliated WS<sub>2</sub> Multilayer Flakes

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### Abstract:

Atomically thin crystals of transition metal dichalcogenides (TMDs) have attracted growing research attention due to their intriguing electrical and optical properties. In particular, the excitons in TMDs have large binding energies, which enables the observation of exciton-polaritons (EPs) at room temperature. Without fabrication of cavity structures, TMD multilayers on reflective substrates exhibit Fabry-Perot (FP) resonance for themselves, since they have very large refractive indices. Thus, exfoliated TMD flakes provide us a platform for investigating rich physics of EPs, which has not only scientific significance but also impacts on novel device applications. In this work, we studied the influences of EPs on the optical reflectance spectra of WS<sub>2</sub> multilayer flakes. EP-related reflectance dips appear in addition to the exciton modes of WS<sub>2</sub>. FP cavity mode couples to the exciton mode, resulting in EP modes with upper and lower EP branches. The thickness dependence of the two branches is very distinct, depending on the underlying materials – SiO<sub>2</sub>/Si wafers and Au thin films. To prepare ultraflat Au surface, evaporated Au thin films on SiO<sub>2</sub>/Si wafers were peeled off using UV-curable epoxy. To clarify the physical origin of the substrate dependence, numerical simulations as well as analytic calculations were performed. This work will help us to propose novel TMD-based optoelectronic devices.

### Keywords:

transition metal dichalcogenide, exciton-polariton, Fabry-Perot

## Electrically controllable neuromodulation emulated by 2D weight-tunable memristor for neuromorphic application

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### Abstract:

Two-dimensional (2D) semiconductors have emerged as a promising material for low-power and high-performance electronics because of the intrinsic atomic thickness and the exceptional properties maintaining even with ultimate scaling. Besides, the competitive ability to electrostatically control the electrochemical potential allows us to design band-modulated 2D heterostructures for implementing a variety of gate-tunable electronic devices. Such a unique capability of 2D materials can also offer great potential for realizing an energy-efficient artificial synapse with high controllability. Nevertheless, the artificial synapse utilizing functionally unique properties has rarely been demonstrated, as appropriate materials and structures with robust memristive switching characteristics and an adequately integrated device architecture are not available.

Here, we report a functionally advanced artificial synaptic architecture, a three-terminal device consisting of a defect-controlled molybdenum disulfide (MoS<sub>2</sub>) memristor on hexagonal boron nitride (h-BN), termed as a 'weight tunable memristor'. Through the precise defect control of MoS<sub>2</sub> channel, the device exhibits low power switching phenomena even without applying gate voltages, which cannot be implemented in previously reported memtransistors utilizing gate dielectric as a pre-synaptic component. One more step, owing to the electrostatically controlled space charge limited current in the ultrathin channel, the device exhibits gate-controlled memristive switching characteristics. The device can implement essential synaptic characteristics, such as short-term plasticity and long-term plasticity. Notably, by electrostatic tuning with a gate terminal, we can additionally regulate the degree and tuning rate of the synaptic weight independent of the programming impulses from source and drain terminals, with sub-1 fJ pulse input. Moreover, the changed states are within stable region for 1500 consecutive pulses. These capabilities eventually enable the accelerated consolidation and conversion of synaptic plasticity, functionally analogous to the synapse with an additional neuromodulator in biological neural networks. Furthermore, such acceleration improves the recognizing accuracy (~91 %) and reduces learning step in MNIST pattern recognition, with considerable power-saving benefits. Our demonstration represents an important step toward highly networked and energy-efficient neuromorphic electronics.

### Keywords:

2D Materials, Neuromorphic Application, memristor

## Effects of Ultrathin Interlayer on Magnetotransports in Graphene-based Heterostructure

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### Abstract:

In this work, we focus on studying the interplay of interfacial effect between graphene (Gr) and Pt layer by introducing an ultrathin ( $x = 0.05$  nm) metal ( $M$ ) interlayer ( $M = \text{Co}, \text{Mn}, \text{or Ir}$ ). The wafer-scale Gr multilayers (MLs) were prepared by CVD method on unetched Si wafers, while 3-nm-thick Pt and  $M$  films were grown using the UHV-Molecular Beam Epitaxy (MBE) system. To observe the spin transport behaviors driven by the interlayer effects of different metals, Pt-Hall bar devices were also provided using the *in-situ* shadow mask patterning technique.

The strong interlayer-dependent magnetoresistance (MR) effects were observed at 77 K in the out-of-plane geometry of the magnetic fields, which shows the appearance of the weak localization (WL)-weak antilocalization (WAL) crossover in these samples with Co, Mn, and Ir ultrathin interlayers. Particularly, the most substantial effect has been remarked for the sample 0.05-nm-thick Ir. To understand the magnetotransport phenomena for our samples, careful analysis of the MR curves was performed using the modified Hikami-Larkin-Nagaoka (HLN) equation.<sup>1</sup> The surface (interface) characterizations of  $M/\text{Gr}$  interface were carried out using the atomic force microscope (AFM), high-resolution (HR)-TEM.

Our work highlights the feasibility of defect engineering of 2D-material to develop highly effective spintronic devices.

### Reference:

[1]. Shinobu Hikami, Anatoly I. Larkin and Yosuke Nagaoka. Spin-Orbit Interaction and Magnetoresistance in the Two Dimensional Random System. *Prog Theor Phys* **63**, 707-710 (1980).

### Keywords:

Graphene, Two-dimensional material, Quantum transport

## The correlation between the composition of the Cu-doped $\text{In}_2\text{Se}_3$ thin films and their optical properties

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### Abstract:

Cu-doped  $\text{In}_2\text{Se}_3$  thin films were synthesized using a two-step process via e-beam evaporator and selenization process. Cu atoms were intentionally doped to the  $\text{In}_2\text{Se}_3$  thin film at different [Cu]:[In] ratios ([Cu]:[In] = 0, 0.27, 0.33, 0.43, and 0.57). The local electronic structure and chemical composition of Cu-doped  $\text{In}_2\text{Se}_3$  thin films were examined using x-ray absorption spectroscopy (XAS), x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD), and FE-SEM. The results show a uniform  $\text{CuInSe}_2$  phase with the existence of Cu-defects, which is thermodynamically favorable and more stable than the formation of binary phases, such as  $\text{CuInSe}_2 + \text{In}_2\text{Se}_3$  or  $\text{Cu}_2\text{Se} + \text{In}_2\text{Se}_3$ . UV/Vis/NIR absorption spectral recorded for Cu-doped  $\text{In}_2\text{Se}_3$  thin films reveal that the optical transition at lower energy is strongly dependent on the [Cu]:[In] ratio and its contribution becomes more significant upon increasing the concentration of copper. The  $\text{Cu}^{1+}$ -CB transition is expected to lead to an intragap absorption feature, which would contribute to the absorption band edge. Studying the local electronic structure and chemical composition changes of the Cu-doped  $\text{In}_2\text{Se}_3$  thin films allow us to have a better understanding of the origin of the optical transitions, as well as, better utilization of ternary semiconductor thin films in photovoltaic devices.

### Keywords:

$\text{CuInSe}_2$ , Thin Film, X-ray Spectroscopy, Optical Properties, Photovoltaic

## 게이트 전압으로 제어 가능한 광 검출기 및 양극성 트랜지스터

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### Abstract:

Next-generation electronic and optoelectronic devices require a high-quality channel layer. Graphene is a good candidate owing to its high carrier mobility and unique ambipolar transport characteristics. However, the on/off ratio and photoresponsivity of graphene are typically low. Transition metal dichalcogenides (e.g. MoSe<sub>2</sub>) are semiconductors with high photoresponsivity but lower mobility than graphene. Here we propose a graphene/MoSe<sub>2</sub> barristor with a high-k ion-gel gate dielectric. It shows the highest carrier mobility ( $\sim 247$  cm<sup>2</sup>/V·s) among reported MoSe<sub>2</sub> devices, high on/off ratio ( $3.3 \times 10^4$ ), and ambipolar behavior that is controlled by an external bias. The barristor exhibits very high external quantum efficiency (EQE, 66.3%) and photoresponsivity (285.0 mA/W). We demonstrate that an electric field applied to the gate electrode can significantly modulate the photocurrent of the barristor resulting in high gate tuning ratio (1.50  $\mu$ A/V). Therefore, this barristor shows potential for use as an ambipolar transistor with high mobility and on/off ratio and a gate-tunable photodetector with high EQE and responsivity.

### Keywords:

Ion-gel, transistor, graphene, barristor, Mose<sub>2</sub>

# Giant Nonlinearity and On/Off Ratio in HfO<sub>2</sub>-based Ferroelectric Tunnel Junction

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## Abstract:

Owing to the recent advances in oxide growth technology, ferroelectricity can exist even in a few nm-thick films, which makes it possible to develop ultrathin oxides-based ferroelectric tunneling junctions (FTJs) useful for the next generation switchable diode. Among various ferroelectric oxides, hafnium oxide is the most promising material for FTJ devices since it is compatible with complementary metal-oxide-semiconductor process and provides a feasible and synergistic concept. Despite the numerous advantages, low nonlinearity and On/Off ratio have hindered their applications to electronic devices. Here, combining density functional theory calculations and numerical tunneling current simulations, we demonstrate that the antiferroelectric-like head-to-head and tail-to-tail polarizations significantly enhance the non-linearity ( $\sim 10^2$ ) and on/off ratio ( $\sim 10^4$ ) at the same time, which will be an essential guideline to design high density and low power consumption electronics applications.

## Keywords:

head-to-head polarization, ferroelectric tunneling junctions, Nonlinearity, hafnium oxide, density functional theory calculations

# Ferroelectricity-driven phonon Berry curvature and nonlinear phonon transports

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## Abstract:

Berry curvature (BC) manifests its importance by governing topological phases of matter and generating anomalous transports. In this talk, we show that polar lattice distortion gives rise to phonon BC that induces a nonlinear phonon Hall effect. In group-IV monochalcogenide monolayers, ferroelectric distortion induces the phonon Rashba effect that opens a mass-gap in tilted Weyl phonon modes, resulting in a large phonon BC dipole. Our *ab-initio* molecular dynamics simulations reveal that the nonlinear phonon Hall transports occur in a controllable manner via ferroelectric switching.

## Keywords:

ferroelectricity, phonon Berry curvature, nonlinear phonon Hall effect

## Atomic-level insights into ferroelectric switching and preferred orientation of ultrathin hafnia

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### Abstract:

Over the past decade there has been a resurgence of interest in ferroelectric (FE) devices in the semiconductor device community. This interest was sparked by the discovery of ferroelectricity in a simple binary oxide, hafnia. Unlike conventional FE perovskite, FE hafnia exhibits ultra-scalable ferroelectricity compatible with Si electronics, providing an unprecedented opportunity for the use of FEs in advanced memory and logic devices. Many proof-of-concept devices based on FE hafnia are indeed showing some promise. However, their practical engineering is still largely relying on laborious trial-and-error process that lacks a clear theoretical guidance, and it remains challenging to rationally design the FE devices for targeted applications. Thus, the community is now calling for more fundamental investigations on the physics of ferroelectricity in hafnia.

In this presentation, we briefly review the status of the field and provide our new understanding on FE switching and surface stability of hafnia. We will first introduce an ultralow FE switching mechanism that can enable rapid growth of the FE domains in hafnia [1]. We also establish a new class of topological domain walls in  $\text{HfO}_2$ , which can help understand complex domain structures often present in FE hafnia samples. Next, we present our systematic study of surface-functionalized FE hafnia [2]. We show that their remnant polarization ( $P_r$ ) and coercive field ( $E_c$ ) can strongly depend on the surface treatments, providing a possible explanation for the enhancement of  $P_r$  in ultrathin hafnia with preferred orientation [3,4]. We believe our study represents an important step towards bridging the gap between practical engineering and the first-principles simulations in the field of FE hafnia.

[1] D.-H. Choe et al., *Mater. Today* **50**, 8 (2021).

[2] D.-H. Choe et al., *IEDM* (2021).

[3] S. S. Cheema et. al., *Nature* **580**, 478 (2020)

[4] H. Lee<sup>†</sup>, D.-H. Choe<sup>†</sup>, S. Jo<sup>†</sup> et. al., *ACS Appl. Mater. Interfaces* **13**, 36499 (2021).

### Keywords:

HfO<sub>2</sub>, Ferroelectrics, Hafnia, Polarization switching, Domain walls

## Molecular-scale photo-responsive heterojunction device with two-dimensional semiconductor

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### Abstract:

Until now, a specifically designed functional molecular species has been recognized as an absolute necessity for realizing the functional behavior in molecular electronic photodiodes.<sup>[1-4]</sup> Here, we demonstrate a new type of molecular-scale photodiode implemented by molecular heterostructure<sup>[5]</sup> composed of standard molecules and 2D semiconductor. Two non-functionalized molecular species that have opposite direction in their dipole moment (i.e., 1-octanethiol (denoted as C8) and tridecafluoro-1-octanethiol (F6H2)) were used herein. As a 2D semiconductor, a four-layered (4<sub>L</sub>)-WSe<sub>2</sub> was used to form a heterojunction with the SAMs. Depending on the direction of molecular dipole moments, the interfacial band alignment at 4<sub>L</sub>-WSe<sub>2</sub>/molecules interfaces are differently shifted, resulting in change of the photocurrent direction and rectifying direction. Especially, in the case of the F6H2/4<sub>L</sub>-WSe<sub>2</sub> junction, the current response at zero bias under the light illumination ( $\lambda = 532$  nm, 9  $\mu$ W) is higher than 4 orders of magnitude as compared with under the dark condition. In addition, the constant value of photocurrent over a chopper frequency of 5-900 Hz was observed, achieving the photo-response time of  $\sim 100$   $\mu$ s that is faster as compared to other molecular photodiodes. This study suggests a new concept of molecular-scale photodiode where can engineer the photo-current direction depending on the molecular dipole moments.

[1] Yasutomi, S. *et al.* A molecular photodiode system that can switch photocurrent direction *Science* **304**, 1944-1947 (2004).

[2] Wieghold, S. *et al.* Photoresponse of supramolecular self-assembled networks on graphene-diamond interfaces *Nat. Commun.* **7**, 10700 (2016).

[3] Najarian, A. M. *et al.* Orbital control of photocurrents in large area all-carbon molecular junctions *J. Am. Chem. Soc.* **140**, 1900-1909 (2018).

[4] Najarian, A. M. & McCreery, R. L. Long-range activationless photostimulated charge transport in symmetric molecular junctions *ACS Nano* **13**, 867-877 (2019).

[5] Shin, J. *et al.* Tunable rectification in a molecular heterojunction with two-dimensional semiconductors *Nat. Commun.* **11**, 1412 (2020).

### Keywords:

Molecular-scale device, Photo-responsive device, Molecular photodiode

## Tailoring the interfacial band offset by the molecular dipole orientation for a molecular heterojunction selector

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### Abstract:

Molecular functional devices have been investigated through the study of molecular structure and its corresponding discrete orbital states since it determines the transport behaviors. [1,2] In contrast to the conventional strategy, we recently demonstrated a novel strategy and design rule for realizing molecular-scale diode features based on the energy band engineering between simple alkanethiol or conjugated molecules and two-dimensional (2D) semiconductors.[3] Likewise, understanding and designing interfacial band alignment in a molecular heterojunction provides a foundation for realizing its desirable electronic functionality. In this study, we implemented the opposite direction of the molecular dipole moment in the molecular heterojunction with 2D semiconductors ( $1_L$ -MoS<sub>2</sub> or  $1_L$ -WSe<sub>2</sub>). The direction of the band bending of the 2D semiconductors were determined by the molecular dipole moment which could control the rectification direction. Notably, it widely adjusts the degree of the current increase and the nonlinearity of the rectification characteristics that it could be suggests as the tailored molecular-scale heterojunction selector that can prevent sneak current flow in a crossbar array structure. It was significantly affected by the molecular dipole moment direction, type of two-dimensional semiconductor, and metal work function. According to the choice of these heterojunction constituents, the nonlinearity is widely tuned from  $1.0 \times 10^1$  to  $3.6 \times 10^4$  for the reading voltage scheme and  $1.0 \times 10^1$  to  $3.6 \times 10^4$  for the half-voltage reading scheme, which could be scaled up to an ~482 Gbit crossbar array. In addition, based on understanding the molecular heterojunction system, we develop the study to other various molecular heterojunction devices with 2D semiconductors, such as molecular synapse.

[1] L. A. Bumm, J. J. Arnold, M. T. Cygan, T. D. Dunbar, T. P. Burgin, L. Jones, D. L. Allara, J. M. Tour, P. S. Weiss, *Science* 271, 1705 (1996),.

[2] H. Song, Y. Kim, Y. H. Jang, H. Jeong, M. A. Reed, T. Lee, *Nature* 462, 1039 (2009).

[3] J. Shin, S. Yang, Y. Jang, J. S. Eo, T.-W. Kim, T. Lee, C.-H. Lee, G. Wang, *Nat. Commun.* 11, 1 (2020).

### Keywords:

Molecular heterojunction, 2D semiconductor, molecular selector, molecular dipole moment

## Improvement of interface carrier recombination in band gap graded Cu(In,Ga)Se<sub>2</sub> thin film solar cells

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### Abstract:

Cu(In,Ga)Se<sub>2</sub> (CIGS) based thin film solar cells are attracting attention as commercialize photovoltaic devices and numbers of research have been done to maximize its performance. To fabricate the highly efficient devices, efficient carrier transport at the interfaces is crucial. In this study, three CIGS thin film solar cell samples with various Ga-graded were prepared to examine its effects on interface properties, and the high band gap graded sample showed the highest efficiency. Especially, the samples were mechanically etched to reveal its layer structure. Formation of band gap grading in CIGS by tuning the Ga composition was observed via secondary ion mass spectrometry (SIMS). The greater band gap grading sample have higher ratio of remaining Ga on surface of CIGS absorber than lower band gap grading sample, while Cu/(Ga+In) ratio was kept in same. Admittance spectroscopy (AS) results showed that the high band gap graded devices has the largest activation energy. To investigate the electrical and optical properties at absorber/buffer interface, Kelvin probe force microscopy (KPFM) and micro-photoluminescence (PL) spectroscopy were used. Work function at the CIGS/CdS interface was obtained by KPFM and high band gap graded sample showed the smallest work function difference. Small band gap graded samples showed the large work function difference which can cause recombination of carriers. Electron-defect interaction at interface was observed in high band gap sample through PL results indicating that origin of high activation energy is interface defects. In conclusion, improved interface recombination in high band gap graded devices enhanced the device efficiency even though high band gap grading cause interface defects.

### Keywords:

Cu(In,Ga)Se<sub>2</sub> thin film solar cells, Kelvin probe force microscopy, Interface carrier transport, Interface band offset

## Deposit patterns from coffee and milk

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### **Abstract:**

As a potential bioinks, modern bioprinting technology demands polymer-free soft materials. The creation of a biocompatible, well-printable material remains a key issue in this research. Final printability is determined by mechanical qualities and the shape of the final deposition. We use latte droplets containing coffee and milk as a model system to investigate drying-mediated patterns, especially crack development and prevention in droplet deposit patterns following evaporation. In the presence of milk, we find that intermolecular interactions and the surfactant-like nature of milk are responsible for achieving a crack-free uniform deposition pattern of coffee solution. This discovery might be valuable in the development of bioinks or biomaterial-based inks that are both biocompatible and printable.

### **Keywords:**

deposition pattern; crack; biofluid-droplet evaporation; milk; latte

## Fluorescent spectroscopy and Doppler imaging of Yb atomic gas via 399nm

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### Abstract:

Ion trap-based Quantum system has been one of the leading architectures toward building a scalable and practical quantum computer. Among various atomic species, we use Yb as a qubit since it has a hyperfine clock structure and excellent qubit properties. In order to trap Yb ions in space, conditions such as laser frequency, beam overlap, oven temperature, and Doppler effect must be considered. In particular, finding out resonant frequencies of the Yb isotopes is important for selectively ionizing and trapping a specific isotope. In this work, we observed the relative frequency differences between Yb isotopes and we can calibrate an optical wavemeter via comparing previous literatures. In addition, we obtain the spatial map of the Yb fluorescence and its Doppler effect through frequency scanning of 399nm laser using CCD camera. Finally, we obtain characteristic properties of the atomic oven such as gas' velocity and density distribution with different oven temperature. Our experiment may provide a useful information of optimizing trap condition and the trap design.

### Keywords:

Spectroscopy, Doppler effect, Ion trap

## Multimodal imaging system for quantifying optical properties of biological tissue via structured illumination

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### **Abstract:**

Structured illumination techniques have been widely used for measuring optical properties such as scattering and absorption coefficients and enhancing optical resolution. By adjusting the spatial frequency of the structured illumination patterns, the optical properties of a target could be retrieved in a label-free manner, which allows the discrimination of the healthy and abnormal tissue. The structured illumination technique's accuracy mainly relies on the illumination pattern; however, it is challenging to implement a precise structured-illumination system due to distortions. This presentation will introduce a multimodal imaging system that combines a structured illumination technique with a spectral imaging method. Moreover, a new method for correcting distortions in illumination patterns is also discussed. The proposed imaging system could measure optical properties of biological tissue over a spectral domain, which provides significant information for accurate disease diagnosis.

### **Keywords:**

multimodal imaging, structured illumination, biomedical optics, clinical applications, synthetic pattern

## Keratin-based sustainable electronics

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### Abstract:

In the last few decades, structural proteins have been studied for a broad variety of biomedical applications, from the delivery of drugs, to the fabrication of scaffold for tissue engineering and regenerative medicine. In recent years, proteins have been studied from a material science point of view, being regarded as biological and biodegradable alternatives to polymers in technological applications. Because of their renewability and biodegradability, upcycling proteins waste biomass can provide a more sustainable solution to conventional plastics. With this concept, we aimed at developing a "wastetronics" device, in which keratin proteins, extracted from discarded biomass, were transformed into the basic elements of a passive analog electronic device: resistor, capacitor, inductance. These elements were then combined together to make a fully protein-based high pass filter. These results could be a first step into the development of more sustainable protein-based electronic devices.

### Keywords:

keratin, passive electronics, sustainability, cell interaction

## 실크 단백질에 기반한 광학, 전자소자 연구

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### **Abstract:**

Silk, a natural protein extracted from cocoons, has been attractive for biomedical and bio-optical applications due to its biocompatibility, optical transparency, and robust mechanical properties. Here I introduce high technological reinvents of silk. Silk can be used as a base material for the demonstration of fully biocompatible optical devices and give functionalities by doping biofunctional molecules. This approach offers much fascinating potential applications such as *in vivo* monitoring and a super-sensitive biosensor.

### **Keywords:**

실크 단백질, 바이오, 광학소자, 전자소자

# First-principles theory of extending the spin qubit coherence time in hexagonal boron nitride

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## Abstract:

Negatively charged boron vacancies ( $V_B^-$ ) in hexagonal boron nitride (h-BN) are a rapidly developing qubit platform in two-dimensional materials for solid-state quantum applications. However, their spin coherence time ( $T_2$ ) is very short, limited to a few microseconds owing to the inherently dense nuclear spin bath of the h-BN host. As the coherence time is one of the most fundamental properties of spin qubits, the short  $T_2$  time of  $V_B^-$  significantly limits its potential as a promising spin qubit candidate. In this study, we theoretically proposed two materials engineering methods, which can substantially extend the  $T_2$  time of the  $V_B^-$  spin by four times more than its intrinsic  $T_2$ . We performed quantum many-body computations by combining density functional theory and cluster correlation expansion and showed that replacing all the boron atoms in h-BN with the  $^{10}\text{B}$  isotope leads to the coherence enhancement of the  $V_B^-$  spin by a factor of three. In addition, the  $T_2$  time of the  $V_B^-$  can be further enhanced by inducing a curvature around  $V_B^-$ . Herein, we elucidate that the curvature-induced inhomogeneous strain creates spatially varying quadrupole nuclear interactions, which effectively suppress the nuclear spin flip-flop dynamics in the bath. We show that the combination of isotopic enrichment and strain engineering can maximize the  $V_B^- T_2$ , yielding 207.2 and 102.6  $\mu\text{s}$  for single- and multi-layer h- $^{10}\text{BN}$ , respectively. Furthermore, our results can be applied to any spin qubit in h-BN, strengthening their potential as material platforms to realize high-precision quantum sensors, quantum spin registers, and atomically thin quantum magnets.

## Keywords:

hexagonal boron nitride, spin qubits, decoherence

## Semiconductor spin-based training of optical microscopes

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### **Abstract:**

Diamond spins are excellent quantum sensors for a wide range of applications, including NMR spectroscopy, spintronics, and condensed-matter physics. In this talk, I will introduce that the diamond spins can be used as a reference beacon of optical microscopes that can extend today's capabilities of optical imaging. I will conclude this talk by discussing the implicit remarks and perspectives of this spin-based training of optical microscopes.

### **Keywords:**

NV centers, wavefront shaping, quantum sensor

## Single photon emission from defects in GaN and AlN

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### **Abstract:**

Solid-state single-photon emitters are central building blocks in photonic-based quantum information. So far, single photon emitters in diamond and silicon carbide, as well as semiconductor quantum dots, have emerged as excellent solid-state single photon emitters. Although these single photon emitters in diamond and SiC have superior properties amongst solid-state emitters, there is a lack of active photonic components and wafer-scale thin film single-crystal diamond or SiC on low-index insulator, which limit the scalability of monolithic quantum information processing architectures in these materials. In this talk, I will introduce new single-photon emitters and discuss their optical properties and photonic applications. GaN and AlN defects emitting single photons at room temperature, and two-dimensional material-based single-photon emitters with controllable position and polarization will be discussed.

### **Keywords:**

single photon emitter, quantum photonics, GaN, AlN

# Nanofabrication of single-crystal diamond for quantum information technology

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## **Abstract:**

Diamond is a host material for a few promising quantum information processing platforms such as nitrogen-vacancy (NV) and silicon-vacancy (SiV) color centers. Innate feature of solid-state platform that can trap atom-scale system at a fixed position offers a great scalability but it comes at a price.

For example, optical index contrast between the diamond and vacuum makes it difficult to extract photons from color centers. Also, inhomogeneous environment for each color centers is an obstacle must be overcome when they are linked together towards a large-scale system.

These challenges can be partially overcome by taking advantages of nano-devices made by fabrication. Despite that diamond used to be a notoriously hard-to-fabricate material, continuous efforts over the last decade have led to multiple established techniques for diverse functional devices.

In this talk, we discuss a historical development of diamond nano-fabrication and current state-of-the-art techniques. Its application to various quantum technologies will also be discussed.

## Spatially inhomogeneous operation of phase-change memory

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### Abstract:

Rapid changes in the electrical resistance depending on the phases (amorphous and crystal) are one of the most promising bases for universal memory. Phase-change region is spatially inhomogeneous during memory operation in a unit cell because Joule heat for the phase-change is generated at the interface between the metal and compounds. However, delicate optimization of the electrical and thermal properties at the interface is underexplored compared to the bulk. In this study, we modulate the electrical and thermal conductivities by incorporating oxygen in Ag-In-Sb-Te, superior memory compounds where oxygen is chosen for high accessibility and efficiency for the modulation of conductivity. We further analyze the oxidation and crystallization process at the atomic level. Based on the results, we successfully improve the memory performances such as speed, energy, signal ratio, and reliability simultaneously by inserting the oxygenated layer as an interfacial layer. Our study proves that there is considerable room to optimize memory performance at the interface.

### Keywords:

Phase-change memory, Joule heating, Inhomogeneous operation, Thermal conductivity

## Schottky Barrier Lowering Induced by Ultrathin Aluminum Oxynitride Interlayer in Metal/SiC Junctions

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### Abstract:

It is known that the electrical characteristics of SiC Schottky diode depend strongly on the interface energy barrier (Schottky barrier) and lower Schottky barriers bring essential advantages of improving the power efficiency and obtaining the fast switching. In this work, the Schottky barrier of metal/SiC junction is reported experimentally to be reduced significantly with an ultra-thin (down to ~1.0 nm) aluminum oxynitride (AlON) interlayer inserted at the junction interface. It was also found that the junction resistance decreased with the AlON interlayer. The barrier height was lowered by up to 0.8 eV and the reduction was similar for three types of metal with different work function (Pt: 5.65 eV, Ni: 5.01 eV, Cu: 4.33 eV). The adjustment of Schottky barrier with an interlayer is generally considered to be due to the potential change driven by fixed charges in the interlayer or Fermi-level depinning associated with the suppression of metal-induced gap states. In our case, the Fermi-level pinning factor remained almost unchanged, implying that the surface states of SiC is NOT the main factor of the observed Schottky barrier reduction. It seems most likely that the Schottky barrier reduction arises from the fixed positive charges in the AlON thin film.

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### Keywords:

Silicon Carbide, Schottky Barrier, Aluminum Oxynitride, Interlayer, Junction Resistance

## Particle Filtering for Suppressing Nuclear Spin Noise in GaAs Singlet-Triplet Spin Qubit

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### Abstract:

We propose and experimentally demonstrate a fast Hamiltonian parameter estimation protocol based on the sequential Monte-Carlo method (particle filter) for learning nuclear spin environment in semiconductor quantum dots. We show that qubit frequency estimation per shot with rms error less than 0.1 MHz can be achieved. Using a field-programmable gate array (FPGA), we demonstrate prolonging the coherence time of singlet-triplet qubits in GaAs gate-defined quantum dot by more than two orders of magnitude compared with bare evolution, with a short estimation latency of 50us including single-shot measurement and parallel computation time. Reducing the time required for precise parameter estimation down to one single-shot measurement time, the method is directly applicable to various quantum control protocols including fast detection of non-Markovian spin dynamics and multi-qubit Hamiltonian learning.

### Keywords:

sequential monte-carlo, particle filter, overhauser field, nuclear spin noise, semiconductor qubit

## Approaching ideal visibility in singlet-triplet qubit operations using energy-selective tunneling-based Hamiltonian estimation

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### Abstract:

We report energy-selective tunneling readout-based Hamiltonian parameter estimation of a two-electron spin qubit in a GaAs quantum dot array. Optimization of readout fidelity enables a single-shot measurement time of 16  $\mu\text{s}$  on average, with adaptive initialization and unambiguous qubit frequency estimation based on real-time Bayesian inference. Triggering the operation sequence conditional on the frequency detected in the probe step, we observed a 40-fold increase in coherence time without resorting to dynamic nuclear polarization. We also demonstrated quantum oscillation visibility, single-shot measurement fidelity, and state initialization fidelity of 97.7%, 99%, and over 99.9%, respectively. By pushing the sensitivity of the energy-selective tunneling-based spin-to-charge conversion to the limit, the technique is useful for advanced quantum control protocols such as error mitigation schemes, where fast qubit parameter calibration with a large signal-to-noise ratio is crucial.

### Keywords:

Spin qubit, GaAs quantum dot, Energy-selective tunneling readout

## Exciton complexes in gate-tuned transition metal dichalcogenides

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### Abstract:

The excitons in transition metal dichalcogenides have attracted enormous attention due to the large binding energy and the valley-contrasting properties, which make these materials promising in studying exciton physics and realizing novel photonic devices. Their extremely large binding energy allows us not only to observe them even at room temperature but also to study exciton complexes such as trions, biexcitons, etc. Recently, some authors have argued that excitons and trions in doped-transition metal dichalcogenides can be considered as the exciton-polarons, which are the superposition states of a bare exciton and an exciton dressed with a single electron-hole pair. In this work, we fabricate the  $WS_2/hBN$  heterostructure devices for studying new quasiparticles in the doped system and present the experimental results of the exciton-polarons through gate-dependent photoluminescence and reflection measurements. We find that the oscillator strength of attractive polaron gradually increases as increasing the doping density, while that of the repulsive polarons monotonically decreases. These results contradict the three-body trion pictures which show zero oscillator strength for the trions and no dependence on carrier density.

### Keywords:

transition metal dichalcogenides, trion, exciton complexes

## Thru-hole epitaxy of GaN over stacked graphene multiple transferred onto a sapphire substrate

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### Abstract:

In contrast with conventional growth method, remote epitaxy has great advantages such as no constraints to lattice match with a substrate and readily detachable from the underlying substrate. On the other hand, remote epitaxy requires stringent conditions for growth and transfer of 2D materials in terms of the number of layers and quality. Here, we report thru-hole epitaxy, which is basically epitaxial lateral growth over multi-stacked 2D materials, graphene, as a mask. In spite of multiple stacks, AFM and TEM results revealed that inherently existing large number of small opening areas in graphene still contained thru-holes all the way down to the substrate in such a way that atomic species were allowed to go through them and nucleate on the underlying substrate. Due to the very small size of thru-holes, the grown GaN domains were readily separated from the underlying substrate by using a thermal release tape while XRD results confirmed that the grown GaN domains were crystallographically well aligned with the underlying substrate. Our results suggest that thru-hole epitaxy can be applicable to the fabrication of flexible electronic devices in a much less demanding manner in comparison with remote epitaxy.

### Keywords:

thru-hole epitaxy, graphene, GaN

## Exciton-Polaritons with MOCVD-grown GaAs Microcavity

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### Abstract:

Exciton-polaritons are composite bosonic particles that result from strong light-matter interactions in a semiconductor microcavity. Since observation of polariton condensation in GaAs-based microcavity, molecular beam epitaxy has been traditionally used due to its high-quality growth technique. Meanwhile, metalorganic chemical vapor deposition (MOCVD) has barely been focused on studying polariton condensation, although it is a highly scalable growth technique. Here, we realized that polariton condensation using MOCVD-grown GaAs-based microcavity. We measured the Rabi splitting values of  $\sim 10$  meV and the angle-resolved reflectance spectrum. We also observed condensation behaviors with the angle-resolved photoluminescence depending on the pumping laser power. With this result, we will be able to open the mass-productive way for the applications of polariton devices.

### Keywords:

Exciton-polariton, MOCVD, Light-matter interaction

## Mechanoadaptive Reorganization of Stress Fiber Subtypes in Alveolar Epithelial Cells under Cyclic Stretches

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### Abstract:

Applying cyclic stretches to cells induces the remodeling of cytoskeletons including actin stress fibers in the cytosol. However, the correlation between the reorganization of stress fiber subtypes and strain-dependent responses of the cytoplasm and nucleus has remained unclear. Here, we applied uniaxial cyclic stretches at 5%, 10%, and 15% strains to human alveolar epithelial cells (AECs) followed by the release of the mechanical stretch. The dynamic transition of stress fiber subtypes associated with the orientation and elongation of cyclically stretched AECs was observed and analyzed. Strain-dependent transition kinetics of stress fiber subtypes allowed us to propose a model for stretch-induced responses of the cytoplasm and nucleus in AECs. Moreover, the cytotoxic effect of nanoparticles on the remodeling of stress fibers in AECs was evaluated when AECs were exposed to polystyrene nanoparticles under human breath-mimicking conditions.

### Keywords:

Stress fiber subtypes, Cyclic stretches, Cell reorientation, Mechanoadaptation, Alveolar epithelial cell, Polystyrene nanoparticles

## Topology of mammalian transcription

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### Abstract:

Mammalian genome is organized into a hierarchical structure at multiple scales in a cell nucleus. At the most macroscopic scale, individual chromosomes are segregated into own separated intranuclear regions, which is so called chromosome territories. On the other hand, recent intensive studies using live-cell imaging techniques have characterized behaviors of subnuclear compartments, exemplified with transcriptional condensates and nuclear speckles. They are functionally specialized non-membrane bound organelles, mostly follow liquid properties. However, how the genome structure and subnuclear organelles are spatially organized in the nucleus has not been elucidated. We found that chromatin looping by CTCF, a chromatin architectural protein, acts as an architectural prerequisite for the assembly of phase-separated transcriptional condensates. Moreover, we observed a layered structure of transcriptional and splicing condensates near the nuclear matrix discovered by super-resolution imaging of RNA polymerase II, nuclear speckles, and Scaffold attachment factor A (SAF-A, a nuclear matrix associated proteins).

### Keywords:

Nucleus, Gene expression, Transcription, Chromatin, Transcriptional condensate, Genome organization, Super-resolution, Live cell imaging

## Characterization of invadopodia formation and maturation by mechanical activation of $\alpha 5\beta 1$ integrin

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### Abstract:

Invadopodia are protrusive actin bundle structures associated with cancer invasion and metastasis by secreting proteolytic enzymes, matrix metalloproteases (MMPs) for degradation of surrounding extracellular matrix (ECM). Integrin tension, in particular, tension applied to  $\alpha 5\beta 1$  integrin is attributed to formation and maturation of the invadopodia on metastatic cancer cells, however, the mechanical mechanism involved in the invadopodia process has been unanswered due to the lack of techniques to measure the integrin tension with single molecule precision. Here, we develop an engineered-DNA-based force sensor, termed "Tension Gauge Tether (TGT)" for the measurement of integrin tension at the single molecule level. Using a combination of the TGT assay and a live cell imaging system, the spatio-temporal analysis of the integrin tension during invadopodia development is performed. As a result, we identified that  $\alpha 5\beta 1$  integrin tension above 40 pN initiates cell adhesion as well as formation of invadopodia. In addition, mature invadopodia pull the adhesion to the substrate with forces greater than 100 pN and secret MMPs consecutively. Our results characterize the biophysical relationship between cancer metastasis and physical force applied to integrins, ultimately providing new insights for inhibition of cancer metastasis.

### Keywords:

Invadopodia, Integrin tension, Tension probe

## 일반물리학에서 현대물리를 어떻게 가르칠 것인가

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### Abstract:

대학에서 일반물리학을 강의할 때 현대물리학에 해당하는 부분은 종종 논란의 대상이 되고 있다. 강의를 하는 사람도, 듣는 사람도 만족하지 못하며, 강의에서 아예 빼 버리는 일도 드물지 않다. 여기서는 일반물리학 과목에서 현대물리학 부분을 강의하는 일이 왜 쉽지 않은가에 대해서 포괄적으로 논의하고, 현대물리 강의를 지향해야 할 방향을 생각해 본다.

### Keywords:

일반물리학, 현대물리

## <빅뱅 우주 속의 우리> 사이버 교양과목 개발 사례

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### Abstract:

블랙홀, 중력파, 빅뱅 우주 등을 포함하는 천체물리는 과학 강연의 주요 소재가 되고 있다. 하지만, 양자역학과 일반상대론에 대한 기본적인 이해를 필요로 하는 천체물리의 특성 때문에, 대학 교양과목에서는 매우 제한적으로 다루어져 왔고, 일반물리학 강의에서도 생략되거나 간략하게 소개만 되고 있는 실정이다. 이러한 현실을 감안하여 대학생을 위한 사이버 교양과목 <빅뱅 우주 속의 우리>를 2020년에 개발하였다. 이 과목에서는 양자장론, 일반상대론, 블랙홀과 정보역설, 중력파, 빅뱅 우주론 등을 다양한 멀티미디어 자료를 활용하여 수식 없이 개념적으로 설명하는 것을 주 목적으로 하였다. 이번 발표에서는 개발된 교양과목의 교수목표, 강의자료, 강의방식, 평가결과, 수강생반응 등을 소개하고자 한다. 중등교육의 문과/이과 구분이 없어지고 융합교육이 활성화되고 있는 현 시점에서, 이러한 교양과목은 일반물리학에서 다루기 어려운 천체물리를 개념적으로 소개하는 대안이 될 수 있다.

### Keywords:

천체물리, 교양과목 개발, 블랙홀, 중력파, 빅뱅 우주

## 일반물리학 실험의 지향점

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### Abstract:

코로나19 사태로 인한 비대면 수업 상황과 프로그램 및 시뮬레이션이 강조되는 시대 흐름 속에서 일반물리학 실험의 지향점을 논의하는 자리를 갖고자 합니다. 본 발표에서는 울산과학기술원 물리학과에서 일반물리학 실험을 어떤 식으로 변화, 발전 시켜나가고 있는지 예로 들어 설명드리고자 합니다.

### Keywords:

일반물리학 실험

## **New approaches in general physics lab classbased on current IT technology**

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### **Abstract:**

It needs change in the teaching of general physics especially in lab activity. New ways of enhancing the meaning and effects of lab activity is required. In this paper, some possible approaches about lab activities based on current IT technology such as using several micro-board and sensor programming and ways of introducing student generated experiment designing will be suggested

### **Keywords:**

physics lab, micro-board, sensors

## Search for heavy Majorana neutrino in Type-1 Seesaw model using dilepton events at CMS

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### Abstract:

The discovery of non-zero neutrino masses has opened a window for heavy neutrinos at the TeV scale. Models predicting Majorana neutrinos can result in striking experimental signatures such as like-sign lepton pairs (in addition of high transverse momentum jets), or events with boosted heavy neutrino decays which result in rare boosted lepton+jets objects.

We present an update on the search for heavy neutrinos in these rare signature using events containing two leptons and jets.

We consider the full LHC run 2 dataset, using proton-proton data collected between 2016 and 2018 by the CMS detector at  $\sqrt{s} = 13$  TeV.

### Keywords:

CMS, LHC, heavy neutrino

## The CMS Muon Seed Classifier with Machine Learning for the Run3

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### Abstract:

LHCb reported the interesting analysis about the Lepton Flavor Violation in b-quark sector. With regard to the report, the CMS experiment will focus on the B-physics field in Run3 which will be operated in this year. The many B-physics analyses rely on low-pt dimuon decaying from B-mesons to trigger events. However, in this low-pt region, the muon reconstruction efficiency in CMS during Run2 was relatively poor. To recover this inefficiency, we have to consider larger Region of Interest (ROI) in the pixel tracker with respect to Level-1 or Level-2 muon objects. But it requires tremendous computing consumption to be integrated in CMS high level trigger(HLT). We present a novel development of a seed classifier designed to select the high quality muon seeds to significantly reduce computing time. This algorithm exploits the machine learning techniques, and will be essential to improve the low-pt muon reconstruction performance in CMS during Run3.

### Keywords:

CMS, Run3, Muon, HLT, Machine Learning

## Search for monotop events in pp collisions at 13 TeV from CMS experiment

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### Abstract:

One of the important goals of the Large Hadron Collider (LHC) is to find the dark matter (DM) signature. Since dark matter doesn't leave a measurable signature in the detector, one way to observe DM is when it is produced in association with a visible Standard Model particle, called MET+X where MET is the missing transverse energy and X is dark matter candidate. The event of monotop related to missing transverse energy is searched for hadronic and leptonic decaying channels. We move to Ultra Legacy data samples for signal and also background mc samples. The signal and background study is processed using the Columnar Object Framework For Effective Analysis (COFFEA) tool, an array-based python tool for high-energy collider physics to reduce time-to-insight. We present the update on both channels in this presentation.

### Keywords:

CMS, MET+X

## Measurement of $|V_{ts}|$ using jet discrimination on $t\bar{t}$ dilepton final state events in pp collision at 13 TeV

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### Abstract:

In the Standard Model (SM), the flavour-changing weak interaction between quarks is described by the CKM matrix which is unitary in the SM. However, this unitarity may be broken in several of the Beyond Standard Model scenarios. Therefore, it is important to measure the elements in the matrix with various and precise methods to precisely probe nature at a fundamental level. This study proposes to measure  $|V_{ts}|$ , one of the matrix elements which has not yet been fully studied, directly using the dilepton final state of top pair production in pp collision at 13 TeV with a jet discrimination method based on a machine learning algorithm.

### Keywords:

vt<sub>s</sub>, ckm, jet discriminatio

## Measurement of CP violation in single top t-channel production at 13 TeV

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### Abstract:

CP violation is required to solve the paradox of the baryon asymmetry of the universe. A forward-backward asymmetry of an angular distribution is defined in the top quark sector that is highly-related to the CP violation. The asymmetry measurement is performed in the t-channel production of single top quarks in proton-proton collision at the LHC at center-of-mass energy of 13 TeV using data corresponding to 41.5/fb collected by the CMS detector. The preliminary results have been compared to Standard Model Monte Carlo simulation to probe new particle physics models.

### Keywords:

LHC, CMS, top quark, t-channel, CP violation

## Positive resampler using DNN for Monte Carlo events with negative weight

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### Abstract:

Monte Carlo event generators are often used in collider experiments such as LHC to produce required samples for the research. To meet the next-to-leading-order quantum corrections, these generators often assign negative weight values to the produced samples. Negative weight samples can cause problems when used in applications, such as in machine learning. In this study, we present the positive resampler which reweights such negative weight events to have positive definite weight values. Using this positive resampler, we resample CMS four top quarks samples which contain events with negative weight.

### Keywords:

CMS, Monte Carlo, Event generator, DNN, Collider

## Study of a novel approach for the identification of the additional b jets in the ttbb process

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### Abstract:

After the Higgs (H) boson discovery in 2012, from initial measurements the properties of the Higgs boson seem to be consistent with those from the H boson in the standard model of particle physics. Furthermore, from analyzing the proton collision data of the LHC the couplings of a top quark and a bottom quark in the standard model with the H boson was recently (2018) discovered in different processes. However, the confirmation that both couplings are simultaneously consistent with the predictions, is only possible by measuring the unique process where top-quark pairs are produced in association with the H boson where the H boson decays a pair of bottom-quarks (ttH(bb)). This process is yet to be discovered in the data. Therefore, the main objective of this study is to prepare and finally make this discovery. The main obstacles emerge from the overwhelming background processes of top-quark pair production in association with heavy-flavour quarks. Especially, top-quark pair production containing two bottom quarks from gluon splitting (ttbb) has the same final state with the ttH(bb) process. It is very challenging to identify those additional bottom quarks. In this study, a deep learning technique with an innovative approach of so-called "event-by-event" will be used to handle this problem. Moreover, it will lay the basis for the differential cross-section measurement of the ttbb process.

### Keywords:

top quark, deep learning, Higgs boson

# A background estimation for the charged lepton flavor violation in the top quark interaction with a muon and a tau in pp collisions at $\sqrt{s}=13\text{TeV}$

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## Abstract:

To improve the sensitivity for the study for the charged lepton flavor violation in the top quark interaction with a muon and a tau, a reliable background estimation of  $W$ +jets and QCD backgrounds is important as these processes are not modeled in the Monte Carlo simulation. In this study, we use the ABCD method, one of the most widely used data-driven methods.  $W$ +jets and QCD backgrounds are obtained from a background dominated control region and extrapolated to the signal region.

## Keywords:

Background estimation, ABCD method, CMS, Top, CLFV

## Status of COSINE-100 experiment

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### **Abstract:**

COSINE-100 is direct WIMP search experiment, which uses 106kg of thallium-doped sodium iodide [NaI(Tl)] as its target material. We have operated our detector and been collecting data since September 2016 with continuous stable operation.

The basic goal of the experiment is to test the dark matter signal from the DAMA/LIBRA experiment (DAMA). DAMA has claimed annual modulation signal of 'Dark Matter - NaI(Tl)' recoils, induced by seasonal velocity variation of dark matter according to Earth's relative motion around the Sun and the Galactic center. But no other experiment has succeeded in reproducing its result yet. So COSINE-100 aims to test DAMA's result, using same target material. In this presentation, I will summarize our dark matter search status, focused on 'model dependent WIMP signal search result'. Also, our analysis strategy for more sensitive WIMP search will be presented.

### **Keywords:**

darkmatter, WIMP, COSINE-100

## Update on dark matter searches using annual modulation in NaI crystals at COSINE-100

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### **Abstract:**

COSINE-100 is an NaI-based dark matter detection experiment with the goal of testing the long-standing but contested positive dark matter signal from experiments by the DAMA collaboration using the same target material and search method. In this talk, a summary of the most recent results from three years of data taking at COSINE-100 is presented, alongside a look towards future annual modulation searches, which will utilise increased exposure, a lowered energy threshold, and an updated fitting procedure.

### **Keywords:**

COSINE-100, NaI, Annual modulation

## **A search for dark sector particles from the Sun with the COSINE-100 detector**

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### **Abstract:**

The sun is a well-studied potential astrophysical source of new light particles that are not strongly coupled to the known Standard Model gauge forces and are referred to as "dark sector particles." Searches for dark sector particles, which may include dark matter candidates and other associated states, motivate many underground experiments. The solar Kaluza-Klein axion, the solar dark photon, and solar axion have all been proposed as dark matter candidates that would be produced in the interior of the Sun. In this talk, we will present the analysis of those scenarios through annual modulation studies with data from the COSINE-100 detector.

### **Keywords:**

COSINE-100 detector, dark sectors, dark matter particles

## Search for Bosonic Super-WIMP at COSINE-100

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### **Abstract:**

Bosonic super weakly interacting massive particles (WIMPs) have been proposed as dark matter candidates. Several experiments, including XMASS, XENON100, and MAJORANA, have searched for bosonic super-WIMPs with masses below 100 keV. Recently, experiments such as XENON1T, EDELWEISS-III, and GERDA, reported results that extended the search range to higher masses. In the experimental results to date, only absorption processes have been considered, but, as the search range is extended to higher masses, another process, Compton-like scattering processes should also be considered. The Compton-like process, which dominates the absorption process at large masses, will be presented in this talk, and the results of the bosonic super-WIMP search using COSINE-100 data will also be included.

### **Keywords:**

Bosonic super-WIMP, Dark matter, COSINE-100

## Pulse shape analysis with a phoswich detector made from organic and NaI(Tl) scintillators

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### Abstract:

A phoswich detector composed of three materials, liquid, plastic, and NaI(Tl) scintillators is constructed and data with and without radioactive sources have been collected. Light characteristics from each material are different and hence various pulse shape information is available for further studies. We report shape identification for organic scintillator pulses from those of the crystal scintillator in a single detector setup which makes external gammas identifiable. Additionally, long-term stability tests of the detector setup is presented.

### Keywords:

Phoswich, Pulse Shape Discrimination, NaI(Tl)

## **A KSVZ sensitive axion search experiment around 24.5 $\mu\text{eV}$ with an 8-cell microwave resonant cavity and a Josephson Parametric Amplifier**

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### **Abstract:**

One of the experiments at the Center for Axion and Precision Physics Research (CAPP) of the Institute for Basic Science (IBS) is searching for axion dark matter using the haloscope method sensitive to masses around 24.5  $\mu\text{eV}$ . Under an external magnetic field of 8 T and at a temperature of just below 40 mK, a unique 8-cell cavity optimizing the experimental volume is used for the first time in a search for KSVZ axions. The cryogenic section of the readout chain relies on a Josephson Parametric Amplifier implemented as the first stage of amplification with 20 dB gain, yielding a system noise temperature estimated to be mostly below 450 mK for the whole target mass range. The system is constructed to be resilient against external electromagnetic interference by employing adequate shielding practices along with custom filtering solutions. It has been in operation since the end of December aiming to cover a 100 MHz range with at least KSVZ sensitivity by the end of April 2022. In this talk, we will discuss the details of the measurement scheme and the sensitivity of the experiment.

### **Keywords:**

axion, dark matter, haloscope, josephson parametric amplifier, pizza cavity

## High-mass axion haloscope with tunable dielectric metamaterials

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### Abstract:

The axion is a well-motivated hypothetical particle which could address both the strong CP problem and dark matter mystery. Most of the high-sensitivity cavity haloscope experiments are conducted at frequencies (masses) less than 10 GHz (40  $\mu\text{eV}$ ). A novel axion haloscope design with an array of periodically deployed dielectric rods in an ordinary cavity was developed by IBS-CAPP to extend the search range above 10 GHz with high performance. Furthermore, a kirigami-inspired deformable structure, which allows 2-dimensional movement of the rods, was implemented for frequency tuning. We present the characteristics of this new cavity design and demonstrate the experimental feasibility.

### Keywords:

Axion, Metamaterial

## Background study for Korea Experiments on Magnetic Monopole

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### Abstract:

We describe the design of an experiment to search for elementary magnetic charges with mass below the electron mass ( $m_e$ ) and charge below the electron charge ( $e$ ), a mass and charge region we believe is unexplored, in  $e^+e^-$  annihilation-at-rest. The technique depends on the acceleration of pair-produced magnetic charges within a solenoidal field surrounding the positron annihilation target. Estimates of event rates, energy and time resolutions, and potential backgrounds from a detailed simulation are shown.

### Keywords:

magnetic monopole, GEANT4

## Performance of the trigger-veto detector for KAEM

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### Abstract:

Korea Experiment on Magnetic Monopole (KAEM) searches for fundamental magnetic monopoles in the low-mass and low-charge region. KAEM is configured with a thin aluminum target, sodium-22 source, two 1 Tm solenoids, 2.5 m long vacuum chamber, two electromagnetic calorimeters and the trigger-veto detector. The LYSO, CsI and CsI(Tl) crystals, which are well known and used widely, are candidates for trigger-veto and electromagnetic calorimeters. We investigated the characteristics of those crystals and the performance consistency. This study lead to decide a crystal optimized for KAEM. Also, the customized DAQ system for the trigger-veto detector is introduced and test results using the electronics and crystals are shown in this talk.

### Keywords:

KAEM

## Status of RAON

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### **Abstract:**

The Rare Isotope Science Project (RISP), launched in late of 2011 to build the Rare isotope Accelerator complex for ON-line experiment (RAON) for rare isotope science, is now at the stage of completion of Phase-I which mainly consists of SCL3 (low E superconducting linac), ISOL and experimental systems. In this spring, the RAON would be ready for the cool-down of SCL3 and the first beam commissioning of SCL3 will be performed in the second half of 2022. In this talk, overall current status and future perspective of RAON will be presented.

### **Keywords:**

RAON, RI beams, RISP, SCL

## Nuclear Astrophysics at FRIB

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### **Abstract:**

The facility for rare isotope beams (FRIB) is a new rare isotope accelerator now operating in the US. It provides fast, stopped, and reaccelerated radioactive beams as well as opportunities for harvesting long lived radioactive isotopes. All these capabilities offer opportunities to address long standing questions in nuclear astrophysics related to the origin of the elements and the properties of dense matter as probed by neutron stars. This is particularly relevant as the new capabilities in rare isotope production coincide with advances in astronomy, including gravitational wave detection and multi-messenger observations. I will discuss the major open questions that we envision to be addressed by joint efforts in FRIB experiments, nuclear theory, astrophysical modeling, and observations, highlight the connections between nuclear physics and astrophysics, and discuss some of the experimental developments that have been ongoing to take advantage of FRIB beams.

### **Keywords:**

FRIB, Nuclear Astrophysics, multi-messenger

## Unveiling new features in rare isotopes with direct reactions

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### **Abstract:**

Rare isotopes at the edges of nuclear binding are transforming our conventional rules of nuclear structure. Neutron halo is one of the most exotic phenomena that challenges our knowledge of the nuclear force. Particularly interesting are the Borromean nuclei at the edges of nuclear binding. They present unique few-body quantum systems of bound state of core and two nucleons. Their properties offer rich grounds for testing nuclear interactions and finding new information on the evolution of nuclear shells. The presentation will discuss how direct reactions at different energy scales unveil new features in Borromean nuclei. The exploration of nuclear structure through measurements of nuclear radii will be discussed. The sensitivity of the nuclear forces to properties and reactions of such nuclei will also be discussed.

### **Keywords:**

Rare isotopes, Nuclear Halo, Shell structure

## Revised magnetic structure of a frustrated 4d pyrochlore magnet $\text{Nd}_2\text{Ru}_2\text{O}_7$

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### Abstract:

Highly frustrated pyrochlore has been a subject of active research among the strongly correlated electron system to discover theoretically-proposed emerging quantum phases such as Weyl semimetal [1], where a spin-1/2 state with strong spin-orbit coupling interacts in a pyrochlore lattice. It has led to numerous works on 5d compounds such as iridates for the last decade.

A fundamental distinction between the half-integer and integer moments can imply the qualitative difference in their magnetism [2]. However, much less research has been done on the spin-1 counterpart. Here we present our neutron diffraction studies on a pyrochlore ruthenate,  $\text{Nd}_2\text{Ru}_2\text{O}_7$ , among the family of  $\text{R}_2\text{Ru}_2\text{O}_7$  ( $\text{R} = \text{Y}$  and rare-earth ions). Using high-quality powder neutron diffraction data [3], we propose magnetic structural candidates of Ru ions ( $\text{Ru}^{4+}$ ,  $S=1$ ), complemented by the systematic group theory analysis. We will discuss the implication of our results in the search for topological magnetism.

[1] W. Witczak-Krempa et al, Annu. Rev. Condens. Matter Phys. 5, 57 (2014).

[2] F.-Y. Li and G. Chen, Physical Review B 98, 045109 (2018).

[3] P. Yadav, S. Choi et al. in preparation.

### Keywords:

highly frustrated magnet, pyrochlore, ruthenate, 4d transition metal, neutron diffraction

## Colossal spin-phonon coupling and Higgs-amplitude fluctuations in $\text{Nd}_2\text{Ru}_2\text{O}_7$

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### Abstract:

Strongly correlated  $4d$  pyrochlore compounds provide exceptional platforms to realize a multitude of different states of matter, which are governed by an intimate interplay of orbital, spin, and lattice degrees of freedom [1]. Critical phenomena and dynamical fluctuations arise in the vicinity where two different states of matter meet. Recently, we succeeded in growing for the first time sizable single crystals of  $\text{Nd}_2\text{Ru}_2\text{O}_7$ , a member of the pyrochlore ruthenates. At  $T_N = 147$  K,  $\text{Nd}_2\text{Ru}_2\text{O}_7$  orders magnetically as evidenced by magnetic susceptibility and specific heat. Our temperature- and polarization-resolved Raman spectroscopic study unveils dramatic phonon anomalies associated with this transition, pointing to colossal spin-phonon coupling. In addition, a regime of significant fluctuations marked by quasi-elastic scattering exists within the ordered phase. A new low-energy mode emerges out of these fluctuations at  $T^* = 100$  K, alluding to Higgs-type amplitude fluctuations of the magnetic moment. The two-fold symmetry of this amplitude mode, incompatible with the underlying crystal structure, hints towards nematic order in  $\text{Nd}_2\text{Ru}_2\text{O}_7$ , which is corroborated by the observation of concomitant lattice instabilities.

[1] Gao, et al., Front. Phys. 15(6), 63201 (2020).

### Keywords:

Quantum Criticality, Spin-Phonon Coupling, Pyrochlore Ruthenates

## Magnetic properties of two-dimensional lead-based Halide Perovskites

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### Abstract:

Perovskite has received intense interest because of its excellent optical properties. Recently, attempts to introduce magnetism to perovskites suggest a possibility of an efficient light-controlled magnetic devices. Such suggestion has required investigation of the fundamental magnetic properties in magnetic perovskite or magnetically doped perovskite. Especially, two-dimensional (2D) halide perovskites have been rarely studied in perspective of their magnetic properties. Therefore, we tried to introduce magnetism to 2D Pb-based halide perovskite through doping magnetic ions such as cobalt, manganese, and cerium. We measured the temperature- and field-dependent magnetization and analyzed the magnetic data by using the Curie-Weiss law and Brillouin function fits. We observed the different field dependency in their paramagnetic responses depending on the doping elements. In particular, cerium-doped perovskite showed the most noticeable difference.

### Keywords:

2D halide perovskite

## Long-lived spin states of Fe atomic chains on Cu<sub>2</sub>N via Hamiltonian engineering

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### Abstract:

Understanding the dynamics of electron and nuclear spins in solid-states is crucial for their usage in information processing and storage. Measuring the spin lifetime interacting with the local environment requires high temporal and spatial resolutions. A spin-polarized scanning tunneling microscope (STM) operating at low temperature and various magnetic fields allows us to characterize the spin relaxation time of atoms on a surface with atomic precision. Here, we introduce 1D chains of Fe atoms built with a home-built STM on Cu<sub>2</sub>N/Cu (100) surfaces and the evolution of their spin lifetime depending on the length of chains and the direction and magnitude of magnetic fields. We used different schemes, such as pump-probe [1] and two state switching [2], to measure the spin lifetime ranging from sub- $\mu$ s to sub-ms. The spin lifetime is sensitively changed with the degree of mixing of the Neel states in Fe chains, which is measurable using a spin-polarized tip in STM. Our work shows a seamless measurement of the spin lifetime in a large time scale and the precise determination of spin dynamics in artificially engineered atomic structures via engineering spin Hamiltonian.

### Keywords:

STM, lifetime, Neel state, Fe atomic chains

## Chaotic nonlinear dynamics in magnetic skyrmions

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### Abstract:

Topological solitons such as magnetic vortex and skyrmion have several degrees of freedom in their dynamic motions: core in-plane translation (including gyration mode) [1] and out-of-plane oscillation (breathing mode) [2]. The combination of two or more motions of the topological solitons can be expressed as mathematical roulettes that describe differentiable curves made by a point on a rolling curve moving along a fixed curve. Orbital trajectories of celestial bodies (planets, stars, etc.) are typical examples of roulettes. Although the linear dynamic motions of skyrmions can be described using Thiele's equation [3], the nonlinear dynamic motions owing to Zeeman force [4] have not yet studied well. Since the skyrmion experiences inertial force [5], the equation of motion becomes 2<sup>nd</sup> order-nonlinear ordinary differential equation. Here we studied chaotic nonlinear dynamic motions of skyrmions including the orbit of complex roulettes. Using simulation results of nonlinear dynamic motions of skyrmions, we analyzed the chaotic movement of skyrmion's core trajectories with respect to the petal number of the roulettes, which represents the symmetry of the core orbital motion. When the field frequency was incommensurate, the petal number fluctuated sensitively depending on the initial condition of the skyrmion motions. This study provides a better understanding of the dynamic core trajectories of topological solitons in terms of mathematical roulettes. Furthermore, the skyrmion's chaotic dynamic behavior offers a guideline for the realization of skyrmion-based logic gates.

[1] Mochizuki, M. et al. Phys. Rev. Lett. **108**, 017601 (2012)

[2] Onose, Y. et al. Phys. Rev. Lett. **109**, 037603 (2012)

[3] Thiele, A. A. Phys. Rev. Lett. **30**, 230 (1973)

[4] Guslienko, K. Y. et al. Phys. Rev. B **82**, 014402 (2010)

[5] Makhfudz, I. et al. Phys. Rev. Lett. **109**, 217201 (2012)

### Keywords:

Chaos, Nonlinear dynamics, Roulette, Skyrmion

## Theory of Moire Magnets and Topological Magnons : Applications to Twisted Bilayer $\text{CrI}_3$

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### Abstract:

Moire patterns produced by misaligned two-dimensional materials gives rise to drastic modifications in the electronic structure and correlations. In this work, we construct concrete theory of twisted bilayer honeycomb magnets. Starting from the first-principles calculations of transition-metal trihalides represented by  $\text{CrI}_3$ , we firstly explore the generic spin model with full lattice mode. We discover a variety of non-collinear magnetic order that has been overlooked in the previous studies. By controlling twist angle, the collinear order undergoes the phase transitions to the simple domain wall phase and skyrmion phase. The Monte-Carlo simulation reveals the nature of phase transitions are characterized by the first-order phase transition where the critical points shows highly frustrated magnetism with non-trivial macroscopic degeneracy. Finally, we discover that the magnon excitations of the spin ground states of moire magnets are topologically non-trivial. In collinear phases, we show that the underlying magnon excitations are characterized by higher-order topological magnon phase. In the noncollinear phases with the domain, the domain wall harbors the non-trivial magnon edge mode characterized by non-trivial chern number.

### Keywords:

moire magnet, twistrionics, 2D materials

## Recent results on Kitaev interactions in Co based magnets

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### Abstract:

Kitaev quantum spin liquids (QSLs) are exotic states of matter that are predicted to host Majorana fermions and gauge flux excitations. However, so far all known Kitaev QSL candidates are known to have appreciable non-Kitaev interactions that pushes these systems far from the QSL regime. Co based magnets have been proposed to be perhaps a more ideal platform for realizing Kitaev QSLs. In this talk I will show evidence for a Kitaev interactions in both the quasi-one-dimensional ferromagnet  $\text{CoNb}_2\text{O}_6$  as well as the hexagonal magnet  $\text{BaCo}_2(\text{AsO}_4)$ . Although it is usually believed to be the best material realization of a 1D Ising chain, by combining terahertz spectroscopy and calculations we have shown that  $\text{CoNb}_2\text{O}_6$  is well described by a model with bond-dependent interactions. We call this model the 'twisted Kitaev chain', as these interactions are similar to those of the honeycomb Kitaev spin liquid. The ferromagnetic ground state of  $\text{CoNb}_2\text{O}_6$  arises from the compromise between two axes. Owing to this frustration, even at zero field domain walls have quantum motion, which is described by the celebrated Su–Schrieffer–Heeger model of polyacetylene and shows rich behavior as a function of field. Most recently, we have shown also that the honeycomb cobalt-based Kitaev QSL candidate,  $\text{BaCo}_2(\text{AsO}_4)_2$ , has dominant Kitaev interactions. Due to only small non-Kitaev terms a magnetic continuum consistent with Majorana fermions and the existence of a Kitaev QSL can be induced by a small out-of-plane-magnetic field. Our results demonstrate  $\text{BaCo}_2(\text{AsO}_4)_2$ , as a far more ideal version of Kitaev QSL compared with other candidates.

### Keywords:

THz, Kitaev, spin liquid

## Spin-orbital-entangled nature of magnetic moments and Kitaev interactions in layered Ru-halides

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### Abstract:

alpha-RuCl has been extensively studied recently because of potential bond-dependent Kitaev magnetic exchange interactions and the resulting quantum spin liquid phase that can be realized therein. It has been known that the covalency between Ru 4d- and Cl p-orbitals is crucial to induce large Kitaev interactions in this compound, therefore replacing Cl into heavier halogen elements such as Br or I can be a promising way to promote the Kitaev interaction even further. In a timely manner, there have been reports on synthesis of alpha-RuBr and alpha-RuI, which are expected to host the same spin-orbit-entangled orbitals and Kitaev exchange interactions with alpha-RuCl. Here in this work we investigate electronic structures of alpha-RuCl, RuBr, and RuI in a comparative fashion, focusing on the cooperation of the spin-orbit coupling and on-site Coulomb repulsions to realize the spin-orbit-entangled pseudospin-1/2 at Ru sites. We further estimate magnetic exchange interactions of all three compounds, showing that RuBr can be promising candidates to realize Kitaev spin liquid phases in solid-state systems. The nature of potentially correlated metallic phase in RuI<sub>3</sub> will be discussed additionally.

### Keywords:

Kitaev interaction, Ru halides, spin-orbit coupling

## Experimental Insights into Two Cobalt-Based Candidate Kitaev Magnets

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### Abstract:

Plausible materialization of Kitaev's honeycomb model for quantum spin liquids has fueled intensive research. In recent years, 3d electrons in some cobaltates have been proposed to sponsor bond-dependent Ising (or so-called Kitaev) interactions. Two-layered oxides,  $\text{Na}_2\text{Co}_2\text{TeO}_6$  and  $\text{Na}_3\text{Co}_2\text{SbO}_6$ , are at present considered promising platforms for finding spin-liquid physics. In this talk, we will present our recent experimental progress in the two materials enabled by high-quality single crystals. We find that they are markedly different and both exhibit rich phase behaviors. In  $\text{Na}_2\text{Co}_2\text{TeO}_6$ , the lowest-temperature three-dimensional (3D) magnetic order is preceded by purely 2D yet long-range order over an intermediate temperature range. Surprisingly, the order's magnetic Brillouin zone is inconsistent with a widely accepted zigzag viewpoint common to many experimental Kitaev magnets. Characteristics of the full magnetic excitation spectrum further indicate the emergence of magnetic-molecule-like clusters in the ordered state, which are connected by third-nearest-neighbor interactions.  $\text{Na}_3\text{Co}_2\text{SbO}_6$ , in contrast, exhibits very strong in-plane magnetic anisotropy, despite its apparently weak structural monoclinicity. We argue that the prominent roles of electron itinerancy and sensitivity to structural details of these cobaltates go beyond current theoretical constructions, and may contain new rich physics on their own.

### Keywords:

quantum magnetism, Kitaev honeycomb model, neutron scattering

## Gaps in Topological Magnon Spectra: Intrinsic vs. Extrinsic Effects

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### **Abstract:**

For topological magnon spectra, determining and explaining the presence or absence of a topological gap at a magnon crossing point is a central issue, and is an important step towards the realization of the magnon edge-state-based spintronics as well as for the fundamental goal of discovering a topological magnon insulator. To meet these challenges, single-crystal inelastic neutron scattering experiments play a key role. However, when the neutron intensity rapidly disperses, such as near a crossing point for a Dirac magnon, the apparent spectrum is extremely sensitive to experimental conditions including sample mosaic, resolution, and integration range. Here we study a gapless Dirac magnon candidate  $\text{CrCl}_3$  to show how the quantification of a gapless or gaped spectrum at the Dirac point is extremely sensitive to the experimental conditions. Our work provides guidelines for the examination of gaps in inelastic neutron scattering spectra to ensure that the topological gaps are not misdiagnosed or overestimated due to experimental factors.

### **Keywords:**

topological magnon, inelastic neutron scattering, Dirac magnon

## Correlated Electron States in Twisted Multilayer Graphene

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### Abstract:

Engineering moire superlattices by twisting and stacking two layers of Van der Waals materials has proved to be an effective way to promote interaction effects and induce exotic phases of matter. After discovering superconductivity and correlated insulators in magic-angle twisted bilayer graphene (MATBG), several different two-dimensional materials have been utilized to create two-layer twisted systems and various novel phases. Here, the electronic properties of van der Waals moiré superlattices can further be tuned by adjusting the interlayer coupling or the band structure of constituent layers. In this talk, we will discuss emergent electronic states observed in various twisted multilayer graphene, including twisted double bilayer graphene (TDBG), twisted trilayer graphene (TTG) with alternative twisting angles. We also fabricate n-layer twisted graphene with alternating twisted angle, where  $n \geq 4$ . In these twisted multilayer graphene systems, we also demonstrate a flat electron band that is tunable by perpendicular electric fields in a range of twist angles. Various correlated behaviors, including superconductivity and flavor polarization, will be discussed in these twisted multilayer graphene systems, seeking the relationship between broken symmetry states and superconductivity that appeared in these systems.

### Keywords:

graphene, superconductivity, moire

## The Magic of Moiré Materials

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### Abstract:

Two-dimensional crystals that are overlaid with a difference in lattice constant or a relative twist form a moiré pattern. In semiconductors and semimetals, the low-energy electronic properties of these systems are described by Hamiltonians that have the periodicity of the moiré pattern, opening up a strategy to make artificial two-dimensional crystals with lattice constants on the ten nm scale. I refer to these artificial crystals as moiré materials. Because of their large lattice constants, the band filling factors of moiré materials can be tuned over large ranges without introducing chemical dopants simply by using electrical gates. Moiré materials, can be used to flexibly simulate the physics of real atomic scale crystals, and to create new states of matter. I will overview progress that has been made in understanding the low-temperature properties of the first moiré materials - twisted graphene in which electron velocities vanish at discrete magic angle, and transition-metal dichalcogenides that simulate atomic scale Hubbard model physics, and discuss some specific opportunities to advance understanding of central issues in many-electron physics.

### Keywords:

Moiré

## Magic-Angle Twisted Graphene Family

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### Abstract:

Since the discovery of magic-angle twisted bilayer graphene (MATBG), new moiré systems have been explored to study strongly correlated and topologically nontrivial phenomena. Multiple interesting states, including but not limited to correlated insulators, quantized anomalous Hall states, ferromagnetism, and correlated Chern insulators, have been observed in various moiré materials. However, during the first few years, superconductivity was reproducibly seen only in MATBG. More recently, magic-angle twisted trilayer graphene (MATTG) has shown robust superconductivity and correlated states with an additional knob for electric displacement field tunability. Is it a coincidence? Interestingly, MATBG and MATTG, which are the only robust moiré superconductors known to date, are part of a hierarchy of magic-angle graphene systems, which exhibit a series of twist angles for different number of twisting layers. We experimentally realize magic-angle twisted 4-layer and 5-layer graphene structures, and show that they also exhibit robust superconductivity, therefore establishing alternating-twist magic-angle multilayer graphene as a family of moiré superconductors. With the application of electric displacement and magnetic fields, we find interesting similarities and differences between the members that help us understand the underlying physics behind these systems. In this talk, I will discuss the key data and our current understanding of the magic family, as well as some of our most recent progress.

### Keywords:

moiré quantum matter , magic-angle graphene , correlated electrons , superconductivity; family of superconductors

## Prediction of dual topological nature in NaZnBi

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### Abstract:

Among topological materials, topological insulators (TIs) are characterized by  $Z_2$  indices and their metallic surface states protected by time-reversal symmetry. For topological crystalline insulators (TCIs), crystal symmetry plays a key role in protecting gapless surface states. Based on first-principles density functional calculations, we report a dual topological insulator (DTI) phase in recently synthesized NaZnBi [1], which exhibit both the TI and TCI phases [2]. NaZnBi crystallizes in a PbFCl-type tetragonal structure with the  $P4/nmm$  space group and its crystal structure consists of ZnBi layers and embedded Na atoms. We find the  $Z_2$  indices  $(\nu_0; \nu_1 \nu_2 \nu_3) = (1; 000)$  and odd mirror Chern numbers  $\pm 1$  in NaZnBi. In addition, we confirm that the surface Dirac point is preserved even if either time-reversal or mirror symmetry is broken, indicating the robustness of the DTI phase. It implies that NaZnBi has the potential to be a good candidate for future device applications.

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[2] H. Lee, Y. -G. Kang, M. -C. Jung, M. J. Han, and K. J. Chang, *Robust dual topological insulator phase in NaZnBi*, NPG Asia Mater. (accepted).

### Keywords:

Dual topological insulator, Density functional theory

## Vestige of hourglass Weyl fermion and anomalous Hall effect in non-collinear antiferromagnet $\text{Co}_{1/3}\text{TaS}_2$

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### Abstract:

Combining magnetism with band topology allows for unique quantum phenomena with distinctive magnetic symmetry. Especially in a non-collinear metallic antiferromagnet, the anomalous Hall effect (AHE) can be caused by the Weyl points with broken time-reversal symmetry (TRS)<sup>1</sup>. Our first-principles calculations indicate that vortex-like magnetic ordered  $\text{Co}_{1/3}\text{TaS}_2$  exhibits a substantial AHE associated with magnetic hourglass Weyl fermions<sup>2</sup>. Hourglass dispersion has been commonly studied in non-magnetic systems, which cannot produce AHE due to TRS. However, since the hourglass Weyl point is protected by a non-symmorphic symmetry, it can be stably preserved even if the TRS is broken. We found that the vortex-like spin order can induce a magnetic hourglass Weyl dispersion. In particular, the Weyl points indirectly enforced on the  $\overline{KH}$  line can produce the AHE. Additionally, we confirmed the stability and field tunability of the AHE by spin rotating or tilting. We suggest that  $\text{Co}_{1/3}\text{TaS}_2$  is a magnetic hourglass Weyl semimetal, and also showed an AHE due to TRS broken in this material group.

<sup>1</sup>S. Nakatsuji, N. Kiyohara, & T. Higo, *Nature*, **527**, 212-215 (2015).

<sup>2</sup>P. Park, Y.-G. Kang, J. Kim, K. H. Lee, H.-J. Noh, M. J. Han, & J.-G. Park, *npj Quantum Materials*, (accepted).

### Keywords:

anomalous Hall effect, magnetic hourglass Weyl semimetal, non-collinear antiferromagnet,  $\text{Co}_{1/3}\text{TaS}_2$

## Weyl points and nodal lines in compensated ferrimagnet $Mn_3Al$

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### Abstract:

Recently, topological singularities such as Weyl points and nodal lines have been a main interest of condensed matter physics. In this work, we study Weyl points and nodal lines in compensated ferrimagnet  $Mn_3Al$  in the context of anomalous Hall effects (AHE) using first-principles calculations. After identifying Weyl points and nodal lines near the Fermi energy, its influences on AHE are investigated. The analysis shows avoided crossings are more crucial than Weyl points and nodal lines in genera.

### Keywords:

Anomalous Hall effects, Weyl points, Nodal lines

## Anomalous Hall and Nernst Effect under isotropic strain in compensated ferrimagnet Mn<sub>3</sub>Al

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### Abstract:

The role of isotropic strain on anomalous Hall (AHE) and Nernst effect (ANE) in Mn<sub>3</sub>Al, compensated ferrimagnet, is studied using first-principles calculations. Bands near the Fermi level are mostly affected by the isotropic strain. More specifically, tensile strain lowers band around  $\frac{1}{2}K\Gamma$  and  $L$  point, tensile strain moves the bands to the lower energy. On the other hand, compressive strain shifts upwards those bands. As a result, bands by strain accompanies changes in magnitude of AHC and the sign of ANE.

### Keywords:

Anomalous Hall effect, Anomalous Nernst effect, Berry curvature, Ferrimagnet

## Electronic Structure of Higher-order Ruddlesden-Popper Nickelates $R_{n+1}Ni_nO_{3n+1}$ ( $n=4-6$ )

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### Abstract:

Since the discovery of cuprates, one of the representative unconventional superconductors, the problems to understand for the pairing mechanism in the cuprates have remained. One approach to solving this problem has been to look for cuprate analogs. For that reason, people have devoted discovering nickelates superconductivity in the past 30 years. In 2019, H. Hwang and coworkers discovered nickelate superconductivity in Sr-doped NdNiO<sub>2</sub>. [1] Recently, hole-doped Pr- and La-112 superconductors have been found as well. [2-5] In 2021, the Nd-based  $n=5$  system, which is a member of the reduced layered family  $R_{n+1}Ni_nO_{2n+2}$ , was also found as a new nickelate superconductor. [6] At this moment, nickel-based superconductors open a new reclaimable land.

We are focusing on the higher-order Ruddlesden-Popper (RP) nickelates, which is the parent structure of the reduced layered family. This RP structure becomes essential because we can explore the various charge filling of Ni without cation doping. In this talk, we will address the electronic structures using first-principles calculations for the recently synthesized higher-order RP phases  $R_{n+1}Ni_nO_{3n+1}$  ( $n=4-6$ ).

Our results show hole-like large Fermi arcs of  $d_x^2-y^2$  which resembles hole-doped cuprates, and additional Fermi surfaces with  $d_z^2$  character appear to increase the number of NiO<sub>2</sub> layers indicating the RP phases go toward the 3D regime as increasing  $n$ . [7]

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### Keywords:

first-principles calculations, nickelates, higher-order Ruddlesden-Popper phases, Electronic structure, Fermi surface

## Twisted Bilayer Graphene = Topological Heavy Fermion

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### Abstract:

We show a remarkable exact mapping between twisted bilayer graphene and a topological heavy fermion problem. TBG and its many-body interacting insulating states are completely governed by the interplay between a topological semimetal and a heavy fermion band. The topological heavy fermion model solves the experimental "contradictory properties (of tbG) some associated with itinerant electrons and others associated with localized moments", and presents a unique opportunity to understand the physics of these remarkable systems.

### Keywords:

twisted bilayer graphene, electron correlation, topological phases

# Quantum Metric and Superfluid States in Twisted Bilayer Graphene Systems

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## Abstract:

The lowest energy bands of twisted bilayer systems formed by 2D crystals such as graphene can be made extremely flat by tuning the angle between layers to specific "magic angles". The flatness of the bands has two main implications: it increases the relative weight of the interactions, therefore facilitating the establishment of correlated ground states, and it enhances the contribution of the quantum metric in determining the stability and properties of such states [1]. In this talk I will show how the quantum metric affects the properties of two correlated ground states in twisted bilayer graphene systems: superconductivity, and exciton condensates. For the superconducting case I will show that the quantum metric plays a dominant role in determining the superconducting density, and the critical temperature for the Berezinskii-Kosterlitz-Thouless transition, close to the magic angle [2]. I will then compare our predictions to recent experimental results. For exciton condensates I will show that the effect of the quantum metric is even more dramatic than for the superconducting case: for experimentally relevant parameters' values the quantum metric is essential to stabilize the condensate, and in most conditions it provides the dominant contribution to the superfluid weight [3].

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## Keywords:

Quantum metric, twisted bilayer graphene, superconductivity, exciton condensate

## Geometric properties of flat band Landau levels

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### Abstract:

According to the Onsager's semiclassical quantization rule, the Landau levels of a band are bounded by bandwidth at zero magnetic field. Since dispersionless flat band has zero bandwidth, a naive semiclassical approach predicts that the Landau levels of flat band are degenerate at zero-field energy. Also, it is ambiguous how to determine the semiclassical orbits because of the large energy degeneracy of flat band. In this talk, we show that isolated flat bands have anomalous Landau level spreading that appears outside the zero-field energy bounds. Such Landau level spreading of isolated flat bands are governed by the cross-gap Berry connection or fidelity tensor that measure the wave-function geometry of multi bands. Also, we find that symmetry puts strong constraints on the Landau level spreading. Our results demonstrate that an isolated flat band is an ideal system for studying the role of wave-function geometry in describing magnetic responses of solids.

### Keywords:

Flat band, Landau level, Band geometry, Berry connection

## Evidence for Flat Band Dirac Superfluid originating from Quantum Geometry

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### Abstract:

The group velocity  $v_F$  of the electrons in a flat band superconductor is extremely slow, resulting in quenched kinetic energy. Superconductivity thus appears impossible, as conventional BCS theory implies a vanishing superfluid stiffness, coherence length, and critical current. Using twisted bilayer graphene (tBLG) [1, 2], we explore the profound effect very small  $v_F$  in a superconducting Dirac flat band system [3-7]. Non-linear transport studies [8], we measure  $v_F$  via the Schwinger effect, yielding an extremely slow  $v_F \sim 1000$  m/s for filling fraction  $n$  between  $-1/2$  and  $-3/4$  of the moiré superlattice. This same velocity yields a new limiting mechanism for the superconducting critical current, with analogies to a relativistic superfluid. We estimate the superfluid stiffness, which determines the electrodynamic response of the superconductor, showing that it is not dominated by the kinetic energy, but by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions [3-7]. We study the BCS to Bose-Einstein condensation (BEC) crossover [9] via coherence length measurements, finding an unprecedented ratio of the superconducting transition temperature to the Fermi temperature exceeding unity, illustrating how this can arise for very strong coupling superconductivity in ultra-flat Dirac bands.

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### Keywords:

Quantum geometry, Band topology, Twisted bilayer graphene, Flat bands, Superconductivity

## Relations between quantum metric and topology in geometrically flat Chern insulators

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### Abstract:

Topology of two-dimensional insulators without any symmetry is characterized by Chern numbers. While Chern numbers reveal the global, topological, feature of Bloch states in the Brillouin zone, Berry curvature tells the local, geometrical, feature of Bloch states around a given momentum. Since the integral of the Berry curvature yields the Chern number, geometry and topology are closely related. Besides Berry curvature, another geometrical property called the quantum metric is naturally defined in momentum space from the structure of the Bloch states. As the name suggests, quantum metric introduces a metric structure in the tangent space of the Brillouin zone. Although Berry curvature and the quantum metric are two distinct geometrical properties, there in fact are relations between the two [1,2]. From these relations, one can derive an inequality between the Chern number and the area of the Brillouin zone measured with respect to the quantum metric. We study various aspects of this inequality both from physical [3] and mathematical [4] perspectives. We find that we can infer topological properties just by examining properties of the quantum metric in many cases. In particular, when models approach the Landau level limit in an appropriate sense, the inequality tends to saturate and approach an equality. On a more mathematical side, the condition of the inequality becoming equality is found to be related to the holomorphic nature of the Bloch states. We find that, when the equality holds, momentum space inherits the Kähler manifold structure from the complex projective space, which is a space of states in which Bloch states live. We also propose a way to construct a geometrically flat Chern insulators obeying the equality, using holomorphic functions defined in momentum space [5]. Here, by geometrically flat, we mean that Berry curvature and the quantum metric are uniform in momentum space. Such a geometrically flat Chern insulators with holomorphic structures are known to be useful in obtaining fractional Chern insulators using analogy from the fractional quantum Hall states.

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### Keywords:

Topological insulator, quantum metric, geometrically flat band, Kähler geometry

## Understanding the space charge effect of SnO<sub>2</sub>-based perovskite solar cells

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### Abstract:

Perovskite solar cells (PSCs) have exceeded power conversion efficiency of 25% [1]. In the perovskite solar cell structure, tin oxide (SnO<sub>2</sub>) is a widely used electron transport layer (ETL) due to its low-temperature process, high mobility, wide bandgap, deep conduction band, and so on. Although SnO<sub>2</sub> possesses several advantages when used as an ETL, issues at the interface have not been clearly solved. Numerous groups have focused on modifying the interface between SnO<sub>2</sub> and perovskite [2-5], but rarely on understanding the nature of charge transport. Recently, few groups showed interest in modifying the electrode/SnO<sub>2</sub> interface. However, these reports focus on the full coverage of ITO or FTO and not on the physical properties at the interface, which is necessary for understanding PSCs. In the perspective of understanding charge transport properties, the effect of a space charge region formed between two materials (interface) is important as carrier concentration alters at this region. To study the interface effect between ITO and SnO<sub>2</sub>, we prepared two groups of SnO<sub>2</sub> thin films by their thicknesses – thin group (8.58, 11.22, and 17.05 nm) and thick group (28.49 and 51 nm) – which was controlled by SnO<sub>2</sub> solution concentration. The optical and electrical properties of SnO<sub>2</sub> films were investigated and the space charge region was identified by conductive atomic force microscopy and transfer length measurements. On the basis of experiments, negatively formed space charge region induces a depletion layer which affects the electrical property of the thin SnO<sub>2</sub> group while the unaffected thick SnO<sub>2</sub> group shows low light transmittance, indicating that a threshold thickness exists for best PSC performance. Our work will provide a novel view for understanding interfaces in perovskite solar cells.

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### Keywords:

space charge region, SnO<sub>2</sub>, ITO, interface, lead halide perovskite solar cell

## Conversion between Schottky and Ohmic contact of Zinc oxide microwire based device

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### Abstract:

In this study, electromechanical responses of individual ZnO microwires were observed under optical microscopes. Zinc oxide (ZnO) microwires were transferred from their growth substrate to an electrical lead attached to a homemade micromanipulator. A simple method for making electrical contact of manipulators to ZnO microwires will be reported. By the lowering and increasing of energy barrier height via introducing of piezoelectric potential when a mechanical deformation was applied to the MW, the metal-semiconductor local contact can be transformed from Schottky to Ohmic or from Ohmic to Schottky. This study describes a principle to explaining and controlling electrical properties of ZnO nanowires, which could be potentially useful for fabricating piezotronics devices, Ohmic/Schottky-based sensors.

### Keywords:

microwire, ZnO, piezoelectric potential

## Heteroepitaxial growth of $\gamma$ -GeSe crystals

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### Abstract:

The chalcogenides, including group IV chalcogenides, are known to display various polymorphic configurations, ranging from amorphous to different crystalline phases. Therefore, the controlled synthesis of a targeted polymorphic configuration will be of great utility for fundamental studies as well as applications. We recently reported the synthesis of the first hexagonal polymorph, so-called  $\gamma$ -phase GeSe. However, the previous reported synthesis method has limitation in product yield and polymorph selectivity for  $\gamma$ -phase GeSe. Here, we report the heteroepitaxial growth of  $\gamma$ -phase GeSe on graphene and h-BN. Using the template effect of graphene and h-BN, we significantly improve the yield and selectivity of synthesized  $\gamma$ -GeSe. Moreover, we observe the strong azimuthal correlation between synthesized  $\gamma$ -phase GeSe and underlying 2D substrate. The observed growth modes and products on different target substrates allow us to investigate the growth mechanism of  $\gamma$ -GeSe.

### Keywords:

Germanium Selenide, GeSe, CVD, Chemical vapor deposition, VLS

## Augmented sub-bandgap photoresponse in MoS<sub>2</sub> for intermediate band solar cell

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### Abstract:

Intermediate-band solar cell aims to widen the absorption spectrum by collecting sub-bandgap photons, which allows highly efficient singlet junction solar cells beyond the Shockley-Queisser limit. Although nanostructures and dopants have been employed in intermediate-band solar cells, both high absorption and sub-bandgap current from intermediate-bands are yet challenging. Here, we propose the enhancement of sub-bandgap light absorption in two-dimensional van der Waals layered materials via interface engineering. This is achieved by forming a hybridized interface layer in multilayer MoS<sub>2</sub>/Au film heterostructures, which results in about 60% of absorption intensity. By changing the thickness of MoS<sub>2</sub>, the energy of intermediate band can be modulated which at the same time preserve the absorption intensity. Under 905 nm light illumination, we demonstrate sub-bandgap photocurrent in the device comprised of MoS<sub>2</sub>/Au heterostructure, yielding a 420 pA at zero bias applied. The sub-bandgap photoresponse in the MoS<sub>2</sub>/Au heterostructure can be attributed to two combined mechanisms; absorption in hybridized interface layer, and the Fabry-Perot like cavity induced absorption enhancement. Our result is expected to have potential use in two-dimensional material-based near-infrared photodetection and light harvesting applications.

### Keywords:

2D material, MoS<sub>2</sub>/Au heterostructure, sub-bandgap absorption, intermediate band solar cell

## Terahertz conductivity of high-quality indium film by low temperature deposition

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### Abstract:

Here, we compared the morphology of indium film using a scanning electron microscope and confirmed the tendency of terahertz conductivity by using terahertz time-domain spectroscopy. The indium film was fabricated using thermal evaporation with substrate cooling ( $\sim 100$  K) methods for highly uniform surface morphology. As a result, while the indium film deposited at room temperature showed the morphology of nano-island with low terahertz conductivity, the indium film deposited by using substrate cooling methods showed an interconnected film form that performs metallic characteristics at above  $\sim 30$  nm thickness. This work suggests that the substrate cooling method is promising for the fabrication of high-quality metal film and metal contact applications for providing the van der Waals interface. This work suggests van der Waals interface from high-quality metal film and metal contact applications.

### Keywords:

Terahertz conductivity, indium

## Droplet evaporation and absorption in porous materials

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### Abstract:

Droplet evaporation and absorption are complicated dynamics that occur in porous materials at the same time, and they may be found in nature and in a variety of industrial processes. Due to capillary forces, the spontaneous movement of liquid droplets through the porous substrate, along with spreading, would result in a variation in the droplet contact radius, affecting the surface area susceptible to evaporation. Using X-ray microscopy and optical imaging methods, we investigate droplet dynamics on porous materials. We provide a detailed physical model for the development of the wetted surface over time and its influence on total droplet volume loss. We also show that evaporation is accelerated owing to the increased wetted surface area caused by spreading and absorption on porous surfaces, both experimentally and theoretically. The suggested approach provides a framework for comprehending evaporation in porous materials and applying it to recent problems like face masks.

### Keywords:

droplet evaporation, porous materials, absorption, spreading

## Electrical properties and Raman spectroscopy of aligned and suspended carbon nanotubes

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### Abstract:

We have studied electrical properties of suspended and horizontally aligned carbon nanotubes (CNTs). Aligned CNTs were synthesized by chemical vapor deposition on the ST cut single crystal quartz substrate and transferred on the electrode with trench structures. A light emission due to the joule heat occurs when a current flows through the suspended CNTs. Also, physical properties such as Raman, optical and electrical properties are investigated during Joule heating process. Details of device fabrication and physical properties will be suggested in this presentation.

### Keywords:

CNT, Carbon nanotube, Electrical property, Raman Spectroscopy

# Visualizing Antiferromagnets using Advanced Hard X-ray Scattering Techniques

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## Abstract:

Antiferromagnet-based spintronics have been intensively investigated due to their scientific and technical interests. Many researchers have tried to search for new materials and insights for the breakthrough. However, understanding of the physical properties of some model systems is yet incomplete due to experimental limitations, specifically hard X-ray-based scattering techniques.

Here, we introduce our experimental approach, e.g., Coherent Bragg Rod Analysis (COBRA) and resonant magnetic x-ray diffraction combined with full-field microscopy. Using the advanced X-ray techniques, we will systematically investigate emergent properties of quantum materials, e.g., ruthenate and iridate. Our studies also offer a comprehensive understanding based on the theoretical calculations combined with advanced hard x-ray scattering techniques. Moreover, we were able to visualize structural and (anti)ferromagnetic domains of thin films and single crystals. We propose that the techniques combined with high pressure and electric field can explore and create new phases and emergent physical properties.

## Keywords:

XRIM, COBRA

## Tailoring the magnetic-skyrmion-phase-induced topological Hall effect in oxide superlattices

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### Abstract:

Investigating the effects of the complex magnetic interactions on the formation of nontrivial magnetic phases enables a better understanding of magnetic materials. An effective method to systematically control those interactions and phases could be extensively utilized in spintronic devices. Superlattice systems function as a suitable material system to investigate the complex magnetic interactions and resultant formation of topological magnetic skyrmions, as they possess systematically tunable and well-defined material properties.

In this work, we have discovered an oxide superlattice system in which two distinct topological magnetic domain phases, namely the Bloch- and Neel-type skyrmions, exist. We first demonstrate the existence of a magnetic-skyrmion-phase-induced topological Hall effect in atomically-designed SrRuO<sub>3</sub>/SrTiO<sub>3</sub> superlattices. Importantly, we discover the nontrivial repetition number (z)-dependence of the topological Hall effect in this superlattice system. The nonmonotonic z-dependence of the topological Hall effect was understood using micromagnetic simulations: the different z-dependent evolution of two magnetic interactions (the magnetic dipole-dipole interaction and the Dzyaloshinskii-Moriya interaction) leads to the realization of two distinct magnetic domain phases (Bloch- and Neel-type skyrmions). This study demonstrates the possibility in systematic tuning of the complex magnetic interactions, magnetic domain phases, and the associated electrodynamic properties, using an artificial heterostructuring approach.

### Keywords:

magnetic skyrmion, topological Hall effect, oxide superlattice

# Tunable Pure Spin Supercurrents and the Demonstration of Their Gateability in a Spin-Wave Device

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## Abstract:

Superconducting spin currents are key to the development of superconducting spintronics [1-2] and involve the transfer of spin angular momentum via proximity-induced equal-spin triplet states in a singlet superconductor (SC) [3-5]. Our recent ferromagnetic resonance experiments [3,4] and theory [5] of Pt/Nb/Ni<sub>8</sub>Fe<sub>2</sub> proximity-coupled structures strongly suggest that spin-orbit coupling (SOC) in Pt in conjunction with a magnetic exchange field in Ni<sub>8</sub>Fe<sub>2</sub> are the essential ingredients to generate a pure spin supercurrent channel (without accompanying net charge supercurrent) in Nb. In this invited talk, I would like to describe our recent progress on tunable pure spin currents and the demonstration of a superconducting spin-wave (SW) device [6]:

- 1) By substituting Pt for a perpendicularly magnetized Pt/Co/Pt spin-sink, we were able to demonstrate the role of SOC, and show that pure spin supercurrent pumping efficiency across Nb (singlet SC) is tunable by controlling the magnetization direction of Co.
- 2) By inserting a Cu spacer with weak SOC between Nb and Pt/(Co/Pt) spin-sink, we also proved that Rashba-type SOC is key for forming and transmitting pure spin supercurrents across Nb.
- 3) Finally, by engineering these properties within a single multilayer structure, we demonstrated a prototype superconducting SW device in which lateral SW propagation is gateable via the opening or closing of a vertical pure spin supercurrent channel in Nb.

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## Keywords:

superconducting spintronics, pure spin supercurrents, Rashba-type SOC, superconducting SW device

## Strong bulk spin-orbit torques in the van der Waals ferromagnet $\text{Fe}_3\text{GeTe}_2$

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### Abstract:

The recent emergence of magnetic van der Waals materials allows for the investigation of current induced magnetization manipulation in two dimensional materials. Uniquely,  $\text{Fe}_3\text{GeTe}_2$  has a crystalline structure that allows for the presence of bulk spin-orbit torques (SOTs), that we quantify in a  $\text{Fe}_3\text{GeTe}_2$  flake. From the symmetry of the measured torques, we identify the current induced effective fields using harmonic analysis and find dominant bulk SOTs, which arise from the symmetry in the crystal structure. Our results show that  $\text{Fe}_3\text{GeTe}_2$  uniquely can exhibit bulk SOTs in addition to the conventional interfacial SOTs enabling magnetization modification even in thick single layers without the need for complex multilayer engineering.

### Keywords:

2D ferromagnet, Van der Waals, spin orbit torque

## Frontier to the spin manipulation utilizing the orbital angular momentum

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### Abstract:

The orbital and spin angular momenta are elementary electron degrees of freedom. So far, the spin angular momentum has been an indispensable element for a novel spin-based computation mechanism. For this, efficient spin manipulation is one of the most crucial issues. Recently, a novel spin manipulation mechanism has been proposed utilizing the orbital angular momentum (OAM). In contrast to the spin alignment, the alignment of the OAM occurs even in material systems composed of light elements, e.g., the Cu/Al<sub>2</sub>O<sub>3</sub> interface. Also, the utilization of the OAM for spin manipulation is favorable for power consumption compared to other mechanisms. This talk will present the efficient OAM-induced spin manipulation in several material systems.

### Keywords:

Spin manipulation, Orbital angular momentum, Spin torque

## Floquet chains and the stability of their edge modes

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### Abstract:

Floquet or periodically driven systems show topological phases that are qualitatively different from their static counterparts. In this talk I will first introduce the new kinds of topological phases that can be realized in free-fermion Floquet systems. I will then show that the edge modes encountered in certain free fermion Floquet systems are remarkably robust to adding interactions, even in disorder-free systems where generic bulk quantities can heat to infinite temperatures due to the periodic driving. This robustness of the edge modes to heating can be understood in the language of strong modes for free fermion chains, and almost strong modes for interacting chains. I will then outline a tunneling calculation for extracting the long lifetimes of these edge modes by mapping the Heisenberg time-evolution of the edge operator to dynamics of a single particle in Krylov subspace.

### Keywords:

Topological systems, Floquet systems, Spin chains

# Laser induced Geometric Effects in Quantum Materials

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## Abstract:

Geometry and topology play a prominent role in modern condensed matter physics. Exotic quantum phenomena such as the quantum Hall effect occur due to a non-trivial topology of the electronic states. However, in nonequilibrium physics, the role of geometry and topology is still not fully understood. This talk explains two geometric effects in quantum materials driven by strong coherent laser fields. 1. Floquet engineering of quantum materials [1]: Quantum systems excited by periodic driving are governed by Floquet states, and it is possible to control them using appropriate laser fields. I will give an overview of this topic with some recent updates. 2. Geometric effects in Landau-Zener tunneling [2]: Geometric effects play an essential role in nonadiabatic tunneling, as was pointed out by M. V. Berry [3]. We extend his theory to higher orders and show that it provides a basis to understand "nonadiabatic" nonlinear optics in quantum materials.

## References:

- [1] T. Oka, and S. Kitamura, *Annu. Rev. Condens. Matter Phys.* 10, 387 (2019).
- [2] S. Takayoshi, J. Wu, and T. Oka, *SciPost Phys.* 11, 075 (2021).
- [3] M. V. Berry, *Proc. R. Soc. Lond. A* 430, 405 (1990).

## Keywords:

Floquet engineering, Twisted Landau Zener tunnelling, nonlinear topological optics

# Ultrafast dynamics of phase, topology, and decoherence of graphene

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## Abstract:

We make theoretical investigations of nonequilibrium dynamical nature of graphene under the optical pumping. Phase oscillation of the Fano resonance at the doubled pump frequency on the Floquet Dirac cone is disclosed in the transient absorption. Emergences of topological order in graphene or graphene heterostructure are explored in time-resolved dichroic photoemission. Finally, the theoretical model to directly determine the quantum decoherence time  $T_2$ , belonging to the subfemtosecond range, in high harmonic generation is proposed. These findings give novel scientific insights to nonequilibrium dynamics of Dirac semiconductors.

## Keywords:

nonequilibrium dynamical nature, phase oscillation, topological order, quantum decoherence, Dirac semiconductors

## Defense strategies against cascading failures in networks: “Too-big-to-fail” and “too-small-to-fail”

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### Abstract:

“Too-big-to-fail (TBTF)” is a controversial approach to reducing the risk of cascading failures in the financial systems. In the TBTF defense strategy, most financial supports are provided to very big companies in order to avoid the complete breakdown of the entire system. We also consider “too-small-to-fail (TSTF)” as a comparative defense strategy, in which financial supports are more focused on small companies instead. We use two types of model network and a real network based on inter-industry Input-Output Table as underlying structures for cascading failures, and examine the validity of both defense strategies with two types of bailout policy, indirect (node capacity is increased) and direct (node load is decreased). We evaluate and compare the performances of TBTF and TSTF strategies in preventing cascading failures, and demonstrate that TSTF performs better when the node capacity is increased whereas TBTF works better when the node load is decreased.

### Keywords:

Cascading failure, Complex network, Too big to fail, Too small to fail

## Prediction and mitigation of cascading failures using graph neural networks

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### Abstract:

A small, localized disturbance can lead to a catastrophic global failure in the entire network. Therefore, cascading failures in infrastructure networks is a subject with great practical implications. We study the avalanche dynamics and avalanche mitigation strategy of cascading failures in electrical grids. We define avalanche centrality, which can be implemented for the effective containment of avalanches in electrical grids. Furthermore, we show that a graph neural network (GNN) trained with the avalanche centrality of small networks can successfully predict the ranking of avalanche centrality in much larger networks and real-world electrical grids that are not used to train GNN. Avalanche centrality predicted by GNN also leads to effective avalanche mitigation. This framework can be implemented in other complex processes that require heavy computational costs for simulation in large networks.

### Keywords:

Machine learning, Graph neural network, Cascading failure, Avalanche mitigation, Power grid

## Exploitation can help target searches in complex networks

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### Abstract:

Why is exploitation ubiquitous in diverse decision-making situations?

Does exploitation help achieve quick target search?

The intuitive answer is no, meaning that exploiting previously visited places squanders time in wrong places, thereby degrading search performance.

Counterintuitively, using a non-Markovian random walk model, we show here that exploitation can in fact help target search in complex networks. Our random walk process is performed by randomly deciding to either explore any neighbor of the current node or exploit a previously visited node. We analytically reveal that exploitation benefits target search in lollipop-like but not clique-like networks.

Demonstrating the improved results of our model with real-world networks, this work provides a clue in answering why many organisms frequently exploit their known areas and suggests a new direction in the development of efficient searching algorithms that can be applied in diverse fields such as computer science, sociology, etc.

### Keywords:

Random walk, Complex networks, First-passage time, Cover time, non-Markovian model

## Effects of higher-order components in hypergraphs

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### Abstract:

We investigate the higher-order components that ubiquitously exist in the real-world hypergraphs but have not received much attention, and we propose a solvable random hypergraph model having the higher-order components. We define the  $m$ -th-order connectivities and components using the number of nodes  $m$  shared between hyperedges, and we confirm that the existence of the giant higher-order components in real-world hypergraphs could not be explained simply by their degree and size distribution. Our model reproduces giant higher-order components by introducing the concept of subgroups of nodes that act together with probability  $p$  during a hypergraph formation process, and the emergence of the giant higher-order component could be solved analytically. We applied the SIS-based simple contagion model to our hypergraph model to understand the effect of the higher-order connectivity on dynamics. In this model, the rate  $\beta_n$  at which all nodes in a hyperedge will be infected is determined according to the number of infected nodes  $n$  in the hyperedge, and all infected nodes become susceptible at the rate  $\mu$ . We confirmed that the extensive presence of the higher-order connectivities smoothed the phase transition in an SIS-based simple contagion model. We anticipate that this model could provide a framework for exploring the higher-order architectures in hypergraphs.

### Keywords:

Hypergraph, Higher-order component, Percolation, Contagion

## 청정 에너지 주식시장의 성숙도 및 발전 가능성: 가격 공정성과 정보 흐름 측면

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### Abstract:

본 연구는 청정 에너지 주식(Clean energy stock; ECO)과 주식시장 인덱스(S&P 500)의 시장 효율성 비교 및 시장 간 정보 흐름 분석을 통해, 청정 에너지 주식의 성숙도 및 발전 가능성에 대해 고찰한다. 분산 비검정 및 전이 엔트로피를 적용하여 분석한 결과, ECO는 S&P 500와는 달리 약형 효율적 시장이었으며, 두 시장 간에는 대칭적 정보 흐름이 확인되었다. 추가 분석에서는 두 시장의 단기 통합, 지속가능성에 대한 투자 규모 확대, COVID-19 팬데믹 이후에도 유지되는 두 시장 간 대칭적 정보 흐름을 확인할 수 있었고, 이는 가격 공정성 측면에서 청정 에너지 주식시장 성숙도와 발전 가능성을 보여준다. 궁극적으로 본 연구 결과는 관련 시장참여자와 정책 당국에게 친환경 에너지 정책에 대한 다양한 이해당사자의 반응을 모니터링하는 수단으로 청정 에너지 주식 가격 정보가 활용 가능함을 시사한다.

### Keywords:

ESG, 청정 에너지, 시장 효율성, 전이 엔트로피

## 팜오일 시장의 효율성 분석

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### Abstract:

본 연구는 바이오 연료인 팜오일 선물시장의 시장 효율성에 대해 서부 텍사스 중질유(WTI) 선물시장을 벤치마크로 하여 유동성과 투기적 거래 측면에서 고찰한다. 분산 비 검정을 통해, 두 시장의 유동성 차이에도 불구하고 모두 약형 효율시장임이 확인된다. 로그 수익률 분포 꼬리의 멱지수를 통해 양 시장의 투기적 거래 수준을 비교함으로써, 상대적으로 낮은 유동성을 가진 팜오일 선물시장이 WTI 선물 시장과 효율성 측면에서 큰 차이가 없음을 설명할 수 있다. 전이 엔트로피를 통해 두 시장이 서로 비슷한 양의 정보를 주고받는 것을 확인했으며, 이는 두 시장에서 모두 약형 효율시장 가설이 성립하는 것과 일맥상통한다. 추가로 코로나 바이러스 팬데믹 전후를 비교하여, 두 시장에서 나타나는 투기적 거래 수준과 정보 흐름 간의 음의 상관관계를 재확인하였다. 이러한 결과로부터, 팜오일 선물시장의 투자자는 WTI 선물을 헤징 수단으로 활용할 수 있고, 정책 당국은 규제 차익 기회를 배제하기 위해 새로운 정책 수립 시 주의해야 한다.

### Keywords:

팜오일, 시장 효율성, 유동성, 투기거래, 정보 흐름

## 리츠 인덱스 기반 현물과 선물 시장에서의 가격 발견

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### Abstract:

리츠 시장은 부동산 거래의 유동성을 높이기 위해 도입되었으나, 리츠 시장은 여전히 충분히 효율적이지 못하다는 의견이 있다. 일반적으로 어떤 금융 상품에 대해 선물 거래를 도입하면 선물 상품에 미래의 정보가 더 효율적으로 반영되고 이 정보가 현물 시장에 전달되어 현물 시장의 정보 효율성이 개선된다고 알려져 있다. 우리는 이러한 관계가 리츠 시장에서도 보이는지 확인하고자 리츠 인덱스 기반 현물 및 선물 시장의 가격 발견 역할을 확인했다. 리츠 시장의 일별 수익률 데이터를 기반으로 효과적인 전이 엔트로피를 확인했을 때, 현물에서 선물로의 비대칭적인 정보흐름이 나타났다. 다음으로 시장 미시 구조에서의 현물과 선물의 가격 발견 역할을 확인하기 위해 1분 수익률 데이터를 기반으로 현, 선물의 가격 리더십을 비교했다. 그 결과 일별 수익률 데이터의 경우와 마찬가지로 현물이 선물보다 더 강한 정보 리더십을 가지고 있으며, 이러한 관계는 선물 시장의 거래가 활발해질수록 오히려 더 강해졌다. 이러한 결과를 바탕으로, 리츠 시장의 투자자는 투자 전략에 대해 점검 수 있으며, 리츠 시장의 규제당국은 선물 상품 도입의 의의에 대해 재검토하여 정책 결정에 반영할 수 있다.

### Keywords:

REITs, High-frequency data, Price discovery, Information flow

## Bitcoin Forks네트워크의 선호 이질성

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### Abstract:

본 연구는 Bitcoin과 6개의 Forks 간 정보 확산의 전송 채널에 대해 실증분석 하였다. 분석결과, (i) Bitcoin 시장은 큰 시장규모와 높은 유동성 기반의 중심적 권위를 가지는 것으로 나타났고, (ii) Bitcoin Gold와 Bitcoin Diamond 시장은 작은 시장규모와 낮은 유동성에도 불구하고, 협력을 통해 정보 확산 및 중개 역할에 기여하는 것으로 나타났다. 특히, 두 시장은 각각 낮은 근접 중심성과 높은 매개 중심성을 보였다. 본 연구는 Scaling 지수와 Hurst 지수를 활용하여 Bitcoin Forks 네트워크 상의 Bitcoin, Bitcoin Gold, Bitcoin Diamond의 역할에 대해 논증하였다. 잠재적 네트워크 외부성은 유동성이 큰 시장으로부터 **창발**하여, 가격공정성 측면에서 효율적 시장을 통해 확산되었으며, 시장 내 상당한 수준의 정보 공유에 기여하였다. 이러한 결과는 Bitcoin Forks 네트워크가 시장리더십을 지닌 단일 개체 중심의 중앙집중형 네트워크를 형성하기 보다는, 선호 이질성을 보존하는 방향으로 진화함을 시사한다.

### Keywords:

Bitcoin, Hard fork, Network analysis, Information flow

## **A second-order perturbation theory for the continuous model of indirect reciprocity**

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### **Abstract:**

Reputation is one of key mechanisms to maintain human cooperation, but its analysis gets complicated if we consider the possibility that reputation does not reach consensus because of erroneous assessment or the existence of another competing norm. The difficulty is alleviated if we assume that reputation and cooperation do not take binary values but have continuous spectra so that disagreement over reputation can be analyzed through a perturbation theory.

In this work, we carry out the analysis by expanding the dynamics of reputation to the second order of perturbation under the assumption that everyone initially cooperates with good reputation. The second-order theory clarifies the difference between Image Scoring and Simple Standing in that justified punishment for defection against a well-reputed player is indeed helpful for maintaining cooperation. Moreover, comparison among the leading eight shows that the stabilizing effect of justified punishment weakens if cooperation between two ill-reputed players is regarded as bad. Our analysis thus explains how Simple Standing achieves a high level of stability by permitting justified punishment and also by disregarding irrelevant information in assessing cooperation. This observation suggests which factors affect the stability of a social norm when reputation can be perturbed by noise or a variant of the existing norm.

### **Keywords:**

Indirect reciprocity, Prisoner's dilemma, Evolution of cooperation, Perturbation theory

## Numerical study of resonantly growing long beam instability in over-dense plasma

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### Abstract:

Depending on the electron beam parameters there can appear three beam-plasma instabilities which might be critical in beam-driven plasma wakefield accelerators. Those three instabilities are self-modulation instability (SMI), hose instability (HI), and current filamentation instability or for a long beam, oblique two-stream instability, respectively. In majority of the cases, the classification of these instabilities is not clear unless any seed for an instability is given. As an experimental design, we suggest a simple switching method among the three instabilities by sweeping beam transverse emittances and radial sizes. Particularly, we investigate the mixed mode of SMI and HI. We discuss its resonance condition and generated plasma wakefield in an over-dense plasma.

### Keywords:

beam-plasma instability, plasma wakefield accelerator, self-modulation instability, hose instability

# A Non-Destructive Correlated Energy Spread Monitor Using Stripline Beam Position Monitor for X-ray Free Electron Lasers

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## Abstract:

A non-destructive monitoring of correlated energy spread using stripline electrodes is investigated with a computer simulation for an electron beam of X-ray free electron laser. The correlated energy spread gives rise to a quadrupole moment in the transverse beam distribution at the dispersive section. In the linear accelerator of XFEL, the dispersion is provided at a magnetic-chicane bunch compressor. Thus, the correlated energy spread can be non-destructively monitored from a detection of quadrupole moment at the bunch compressor. With the beam dynamics simulation program ELEGANT, for the electron beam of PAL-XFEL, the quadrupole moment is numerically estimated as  $>0.2 \text{ mm}^2$  where the lower limit is given at the third bunch compressor when the correlated energy spread is  $\sim 0.2\%$ . The quadrupole moment affects the striplines as a variation in the signal response. A simulation carried out by CST Particle Studio estimates it as  $\sim 10 \text{ mV}$  with the quadrupole moment of  $0.2 \text{ mm}^2$  when a charge is  $200 \text{ pC}$  and a bunch length is  $10 \text{ mm}$ . Such signal level would be sufficiently high to be measured with the micro-TCA based digitizer. In conclusion, we argue that this type of non-destructive correlated energy spread monitor is applicable to the electron beam of XFEL and it could be possibly used to control a quality of generated photon beam such as X-ray spectrum.

## Keywords:

Stripline, correlated energy spread

## Generation of two-color hard X-ray pulses at PAL-XFEL

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### **Abstract:**

PAL-XFEL has been operating successfully with SASE and self-seeding mode. To expand the available operation mode of PAL-XFEL, the generation of two-color XFEL pulses has been studied. By utilizing variable gap undulator and dipole magnet located at self-seeding section, two-color XFEL pulses for pump-probe experiment can be available with single electron bunch. For lasing pump XFEL pulse, 8 undulators which are located at the upstream of the self-seeding section are used and 13 undulators in the downstream of the self-seeding section are used for lasing probe XFEL pulse. Time delay between pump and probe XFEL pulses can be controlled by changing the current of the dipole magnet. In this presentation, preliminary experimental results for two-color XFEL pulses are shown.

### **Keywords:**

Two-color XFEL, PAL-XFEL

## Two Color FEL Using Phase Shifters at Undulator Line

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### Abstract:

Phase shifters at undulator line are usually used for optimizing FEL intensity by setting 'in-phase' to match the FEL and electrons phases. Since  $\pi$  offset so called 'out-phase' suppresses FEL intensity at the resonant frequency, the 'out-phase' condition is an unwanted state. However, this 'out-phase' setting can arise side band spectrums. The spontaneous radiation or low-gain FEL theory expects that these side band spectrums have two peak spectrums and the spectrum difference is determined by the number of undulator period. This presentation shows the out-phase setting of the phase shifters can amplify two-colored spectrum seeded by the spontaneous spectrum feature. Results of FEL simulations and experiments performed at PAL-XFEL shows the two-colored spectrum FEL grows exponentially along the number of undulator segments and reaches the saturation resulting in hundreds  $\mu\text{J}$  energy.

### Keywords:

two color FEL, phase shifter

## Generation of 1 mJ/pulse self-seeded hard x-ray free electron laser and its applications

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### Abstract:

The X-ray free electron laser (XFEL) can produce an x-ray beam with ultra-intense peak brightness, and femtosecond scale pulse duration based on Self-Amplified Spontaneous Emission (SASE). However, because the radiation starts from the electron beam shot noise in SASE mode, this x-ray pulse has noisy spikes in time and spectrum. Using self-seeding method with the forward Bragg-diffraction (FBD) monochromator, we produced almost fully coherent hard X-ray self-seeded (HXRSS) free-electron laser (FEL) pulses with an unprecedented peak-brightness and a narrow spectrum from 3.5 keV to 14.6 keV.

Especially, for 9.7keV, the bandwidth of self-seeded FEL mode is 0.2eV which is 1/70 as wide compared to the spontaneous self-amplified emission (SASE) mode, and the peak brightness is  $3.2 \times 10^{35}$  photons/(s·mm<sup>2</sup>·mrad<sup>2</sup>·0.1%BW) which is the highest to date, respectively.

Recently, we enhanced the seeded FEL energy up to mJ-level with FWHM bandwidth of 0.2~0.5 eV over 5 keV to 11 keV. For various experimental applications such as resonant inelastic X-ray scattering (RIXS), nuclear resonance scattering, X-ray Raman spectroscopy, we developed x-ray energy scanning spectroscopy with the help of double crystal monochromator (DCM) which results in improved spectral impurity and fully calibrated energy scale. We will present recent experimental results of characteristics of hard X-ray self-seeded FEL and test experiments using it at PAL-XFEL.

### Keywords:

hard x-ray , free-electron laser, self-seeded free electron laser

## Helical Topological Polaritons

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### Abstract:

Topological photonics, inspired by the role of topology in identifying and designing states of condensed matter, has rapidly emerged as an important sub-field of optics to explore new photonic phases and to design optical devices that are robust against disorder and defects. Extending these ideas to strongly coupled light-matter systems can further open the possibility for studying new optical phenomena as well as pave the way for fabricating actively controllable topological devices. Owing to the increasing appreciation of the role of topology in both electronic and photonic systems, polaritons, that are half-light-half-matter quasiparticles resulting from the strong hybridization between excitons and photons, can emerge as an important platform for exploring new topological phases of matter. Topological polaritons with non-trivial topology have been proposed in polaritonic lattices with engineered symmetries to demonstrate robust chiral propagation, but their experimental realization had been at cryogenic temperatures and under strong magnetic fields, which makes their potential applications challenging. We will discuss our efforts towards generating helical topological polaritons in monolayer WS<sub>2</sub> excitons coupled to a topologically non-trivial photonic crystal protected by pseudo time-reversal symmetry. Helical topological polaritons were observed up to 200K without external magnetic field and verified in both the real and momentum space where polaritons corresponding to opposite helicities were transported to opposite directions along the topological interface. Topological helical polaritons are promising for exploring tunable polaritonic spintronic devices for robust classical and quantum information processing applications. The talk will conclude with our vision towards developing a chiral photonics platform that can generate, transmit and sense information encoded in spin and angular momentum modes of light that are promising for the development of integrated photonic systems with extremely large data processing capabilities.

### Keywords:

Topology, Polariton, Chirality

## Excitons and Polaritons in van der Waals Hetero-bilayers

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### Abstract:

Van der Waals semiconductors provide a platform for creating two-dimensional crystals layer-by-layer and engineering excitonic states therein with exceptional properties. As moiré lattice form in a heterobilayer, carriers can tunnel between closely-aligned bands in the two neighboring monolayers, leading to hybrid states that combine a large oscillator strength similar to intra-layer excitons and tunability of inter-layer ones. Such hybrid states are manifestations of the formation of moiré lattices. When coupled to cavities, the quantum confined nature of excitons in each moiré cell manifests as strong polariton nonlinearity, providing a potentially highly tunable system for ultra-low-power optoelectronics and quantum polaritonics.

[1] L. Zhang, Z. Zhang, F. Wu, D. Wang, R. Gogna, S. Hou, K. Watanabe, T. Taniguchi, K. Kulkarni, T. Kuo, S. R. Forrest, and H. Deng, *Nature Communications* 11, 1 (2020).

[2] L. Zhang, F. Wu, S. Hou, Z. Zhang, Y.-H. Chou, K. Watanabe, T. Taniguchi, S. R. Forrest, and H. Deng, *Nature* 591, 7848 (2021).

### Keywords:

2D materials, moiré superlattice, exciton polaritons

## Exciton-Polaritons in Phase-changing Lead Halide Perovskites

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### Abstract:

Lead halide perovskites are emerging platforms for exciton-polaritons due to their high oscillator strength and large binding energy of excitons. In this work, we have studied the coupling strengths in  $\text{CH}_3\text{NH}_3\text{PbBr}_3$  perovskite microcavities, in which the perovskites exhibit three crystalline phases of orthorhombic, tetragonal, and cubic structures for varying temperatures. The results show that the coupling strength is minimized in the tetragonal phase, and this is strongly correlated with the ferroelectricity that appears only in the tetragonal phase.

### Keywords:

Exciton-Polaritons, Lead Halide Perovskites, Phase Change

## Guided exciton polariton in multilayered WS<sub>2</sub>

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### Abstract:

The emergence of transition metal dichalcogenides (TMD) layers has sparked significant research interest because of their outstanding optical property and optically assessable new internal degrees of freedom called valley pseudospins. Despite its strong exciton resonance strength, the interaction between light and a TMD layer is intrinsically weak due to the huge mismatch between wavelength and the layer thickness (400~1500 nm vs. <1 nm). It is generally believed that additional photonic structures such as external cavities are necessary to increase light-matter coupling in a TMD layer. However, these additional structures easily spoil valley pseudospin information making it difficult to exploit the full potential of TMD layers. Recently, the possibility of light guiding in 2D TMD layers without a cavity, like the surface plasmon polariton in 2D graphene, has been demonstrated. Because the light-guiding is attributed to the high permittivity of 2D TMD layers near the exciton resonance, this mode is called exciton polaritons. In this talk, experimental observation of the guided exciton polariton in multilayered WS<sub>2</sub> will be discussed. By utilizing the near-field coupling method, we directly observed the anti-crossing behavior of exciton and photon dispersion curves, indicating exciton polariton dispersion. The dispersion of the guided polaritons can be easily tuned by controlling the thickness of the layer or the excitation power of the laser. More importantly, we found that the guided polariton mode can exhibit valley polarization under circularly polarized excitation. Using a resonant excitation, we also confirmed that the valley polarization of the guided polariton does not vary as a function of propagation distance, implying the possibility of valley transport using the polariton. These results pave the way for exploiting a valley pseudospin in integrated valleytronics devices using nanophotonics structures.

### Keywords:

exciton polariton, transition metal dichalcogenides

## Electromechanical systems enabled by interfacial slip in 2D material heterostructures

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### Abstract:

Understanding the mechanical deformability of nanomaterials is critical to realizing a host of next generation technologies like stretchable electronics, reconfigurable quantum states, three dimensional multifunctional surfaces, and nanoscale machines. Due to their unparalleled mechanical strength and stability, two-dimensional (2D) materials like graphene and MoS<sub>2</sub> represent the ultimate limit in size of both mechanical atomic membranes and molecular electronics. One of the most exciting research directions is on how to integrate the outstanding mechanical properties and electronic functionality of 2D materials together. For example, misaligning the layers in multilayer 2D material heterostructures generates moire superlattices which host correlated electronic states, while strain gradients spatially tune the electronic structure. In this presentation, we will: (1) Discuss strategies for designing strain, strain gradients and interfacial slip in 2D materials through nanoscale bends, microscale wrinkling, and deposited stressor layers; (2) Explore the interplay between interfacial friction and slip, mechanical deformability, material strain, and resulting optoelectronic properties; (3) Demonstrate 2D material based stretchable electronics and nanoelectromechanical systems which leverage the electromechanical coupling and interfacial structure to enhance reconfigurability. Taken together, these experiments show that interfacial slip strongly affects the mechanics and electronics of 2D material heterostructures and leads to membranes which are orders of magnitude more deformable than conventional 3D materials.

### Keywords:

2D materials, optoelectronic properties, stretchable electronics, heterostructures

# Wafer-scale heterogeneous integration of atomically thin electronic materials on arbitrary substrates toward mechanically reconfigurable devices

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## Abstract:

Advances of modern electronics have demanded to incorporate a diverse set of additional functionalities into device platforms such as high mechanical deformability and improved material/process sustainability. Traditional silicon (Si) wafers-based device manufacturing is intrinsically limited in realizing such novel aspects owing to their rigid/bulky nature as well as complex and unsustainable process schemes. Two-dimensional (2D) transition metal dichalcogenide (TMD) semiconductors are highly promising owing to their extremely large mechanical flexibility and near atom thickness coupled with van der Waals (vdW) attraction-enabled relaxed assembly requirement. Major challenges for realizing such opportunities for emerging electronics have been associated with a lack of reliable manufacturing methods to precisely separate 2D TMD layers from original growth wafers and integrate them on desired functional substrates in a controllable, scalable, and sustainable manner. In this talk, I will discuss recent efforts in my group on exploring viable manufacturing strategies to assemble wafer-scale 2D TMD layers of heterogeneously tailored components on arbitrary substrates. Specifically, we grew various 2D TMD layers of controlled layer orientation – i.e. horizontal or vertical layer alignments – on a large wafer scale via a chemical vapor deposition. We, then, precisely peeled off the wafer-scale 2D TMD layers from their original growth wafers using water preserving their intrinsic structural/chemical integrity and heterogeneously integrated them onto substrates of virtually unrestricted kinds and shapes. A range of novel applications benefiting from these atomically thin wafer-scale materials on unconventional substrates were demonstrated, including multi-dimensionally stretchable photodetectors and electro-mechanical soft actuators. The underlying principle for the successful delamination of the 2D TMD layers will be discussed in the framework of thermodynamic interfacial energy and water-driven capillary force mechanisms.

## Keywords:

2D TMD, wafer-scale, stretchable electronics, thermodynamic interfacial energy

## Chemical short-range order in SiGeSn medium-entropy alloys for optoelectronics

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### Abstract:

Si-Ge-Sn alloys has been long conceived as random solid solutions. Such a perception underlies the understanding, interpretation, and prediction of alloy's properties. However, as the race to create scalable and tunable device materials for mid-infrared technology based on Si-Ge-Sn enters a composition domain that is far beyond alloy's equilibrium solubility, a fundamental question emerges as to how random these alloys truly are. In this talk I will show, through an extensive ab initio-based Monte Carlo sampling study, that Si-Ge-Sn alloy system exhibits complex structures that are far from being a random solid solution. The deviation from random distribution of atoms in the lattice is reflected through diverse forms of chemical short-range order (SRO) of alloy atoms. I will discuss the complex characters and thermodynamic origins of SRO in SiGeSn and show how the presence of SRO substantially modifies the electronic structure and presents a new route for band engineering.

### Keywords:

Si-Ge-Sn alloys, optoelectronics, ab initio-based Monte Carlo, short-range order

## Stochasticity generates spontaneous polarity on the membrane whose degree of lateral confinement differs in different parts

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### Abstract:

Signaling molecules distribute unevenly on the cell membrane and establish cell polarity for various cellular functions. The polarizations are typically thought to involve symmetry breaking in fine-tuned reaction-diffusion kinetics. However, such explanation has rarely been identified as the mechanism behind known cell polarizations, and strict kinetic conditions required in the models further question their applicability. Here we show an alternative mechanism for cell polarity establishment enabled by stochastic reactions that interplay with the shape of the membrane. We found that phosphatidylinositol phosphate (PIP) lipid kinase and phosphatase simultaneously acting on a glass-supported membrane *in vitro* can polarize the membrane's PIP lipid (PIP1 and PIP2) distribution depending on the membrane's two-dimensional shape. The polarity direction developed near-deterministically and could be changed by engineering the phosphatase's kinetic features, which are behaviors our stochastic model also exhibits when simulated on laterally confined geometries following the experiments. Cellular extracts also show polarizing activity on cell-shaped two-dimensional PIP membranes when kinase is added. We also found that a completely different enzyme pair, Ras guanine nucleotide exchange factor (GEF) and GTPase activating protein (GAP), also polarize Ras-functionalized supported membrane *in vitro* dependent on geometry. Because both stochasticity and geometric constraints are often the given conditions in a cellular environment, it is expected that any pair of opposing interfacial enzymatic reactions will carry this influence. Our work presents a direct test on how such influence may establish near-deterministic polarity on the membrane.

### Keywords:

cell polarity, stochastic reaction, membrane geometry, supported membrane, pattern formation

## Cisplatin fixes chromatin irreversibly even at a high chloride concentration

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### Abstract:

The hallmark of cancerous cells is their perpetual cell division and deadly invasion into normal tissues. Chemotherapeutic agents have been developed to fight against cancers by generating severe damages in genetic material and thus inducing apoptosis in the affected proliferative cancer cells. Cisplatin is one of the most potent chemotherapeutic drugs developed so far. The well-known effect of cisplatin upon DNA binding is that it directly binds to and kinks DNA. Recent studies suggested several intriguing roles of histones in cisplatin's anti-cancer effect and thus, the physical effect of nucleosome formation on cisplatin activity should be considered to give a better account of the anti-cancer effect of cisplatin. Here we studied this important issue with single-molecule measurements. Surprisingly, the reduced activity of cisplatin under  $[\text{NaCl}] = 180 \text{ mM}$ , corresponding to the concentration of cellular ionic species, is still effective to impair the integrity of a nucleosome by fastening its condensed structure, even against severe mechanical and chemical disturbances. Our finding suggests that such cisplatin-induced fastening of chromatin can inhibit nucleosome remodeling required for normal biological functions. Furthermore, our in vitro chromatin transcription assay indeed revealed that the transcription activity was effectively suppressed in the presence of cisplatin. Our direct physical measurements on cisplatin-nucleosome adducts suggest that the formation of such adducts be the target of the anti-cancer drug cisplatin.

### Keywords:

cisplatin, chromatin, magnetic tweezers

## Extracting single fibril information from amyloid- $\beta$ 42 aggregates via single-molecule fluorescence imaging and deep learning

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### Abstract:

Polymorphism in the structure of amyloid fibrils suggests the existence of many different assembly pathways. Characterization of this heterogeneity is the key to understanding the aggregation mechanism and toxicity, but in practice it is extremely difficult to probe individual aggregation pathways in a mixture. Here, we present development of a method combining single-molecule fluorescence lifetime imaging and deep learning for monitoring individual fibril formation in real time and their high-throughput analysis. A deep neural network (FNet) separates an image of highly overlapping fibrils into single fibril images, which allows for tracking the growth and changes in characteristics of individual fibrils. Using this method, we investigated aggregation of the 42-residue amyloid- $\beta$  peptide (A $\beta$ 42). We demonstrate that highly heterogeneous fibril formation can be quantitatively characterized in terms of the number of cross- $\beta$  subunits, elongation speed, growth polarity and conformation of fibrils. Tracking individual fibril formation and growth also leads to the discovery of a new general nucleation mechanism (termed heterogeneous secondary nucleation), where a fibril is formed on the surface of an oligomer with a different structure. Our development will be broadly applicable to characterization of heterogeneous aggregation processes of other proteins.

### Keywords:

single-molecule fluorescence lifetime imaging, deep learning, amyloid- $\beta$ , Alzheimer's disease

## Characterization of single DNA loop extrusion steps by condensin

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### Abstract:

Condensin is a structural maintenance of chromosomes (SMC) protein complex that uses ATP to govern chromosome formation. To clarify how it functions to utilize ATP to extrude DNA, we applied high-resolution magnetic tweezers to study extrusion behavior of single condensins bound to single double-stranded DNA. When the DNA was stretched with very small forces, we found that condensin extrudes DNA in single steps of 20-45nm, which is comparable to the holocomplex size of condensin. Furthermore, ATP hydrolysis mutants showed that this behavior is powered by binding of ATP to the condensin complex, unlike typical ATP motors. Our results suggest that condensin behavior can be explained with a scrunching model, where loop extrusion occurs by engagement of the globular domain and the hinge of the SMC complex.

### Keywords:

SMC proteins, Force spectroscopy, DNA dynamics

## Active diffusion of self-propelled particles in flexible polymer networks

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### Abstract:

Biopolymer networks having a meshwork topology, e.g., extracellular matrices and mucus gels, are ubiquitous. It is an open question to understand how self-propelled particles diffuse through such a biopolymer network. Here, we computationally explore this issue in-depth by explicitly modeling three-dimensional biopolymer networks and performing Langevin dynamics simulations of active diffusion of the self-propelled tracers therein. We show that the active tracer performs distinct diffusion dynamics depending on the mesh-to-particle size and Péclet number (Pe). When the particle is smaller than the mesh size, it moves as if in free space with a decreased mobility depending on the polymer occupation density and Pe. However, when the particle size is increased to be comparable to the mesh size, the active particles explore the polymer network using the trapped-and-hopping mechanism. We study the trapped time distribution, flight length distribution, the mean-squared displacement, and the long-time diffusivity at varying Pe. If the particle is larger than the mesh, it captures the collective viscoelastic dynamics from the polymer network at short times and the simple diffusion of the total system at large times. Finally, we discuss the scaling behavior of the long-time diffusivity with Pe, where we find a range of Pe that yields a nontrivial power law.

### Keywords:

active particle, polymer network, diffusion

## Affleck-Dine Leptogenesis from Higgs Inflation

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### Abstract:

We investigate the possibility of simultaneously explaining inflation, the neutrino masses and the baryon asymmetry through extending the Standard Model by a triplet Higgs. The neutrino masses are generated by the vacuum expectation value of the triplet Higgs, while a combination of the triplet and doublet Higgs' plays the role of the inflaton. Additionally, the dynamics of the triplet, and its inherent lepton number violating interactions, lead to the generation of a lepton asymmetry during inflation. The resultant baryon asymmetry, inflationary predictions and neutrino masses are consistent with current observational and experimental results.

### Keywords:

Baryogenesis, Leptogenesis, Neutrinos, Higgs

## Lepto-axiogenesis in minimal SUSY KSVZ model

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### Abstract:

We study the lepto-axiogenesis scenario in the minimal supersymmetric KSVZ axion model. Only one Peccei-Quinn (PQ) field and vector-like fields are introduced besides the MSSM with the type-I see-saw mechanism. The PQ field is stabilized by the radiative correction induced by the Yukawa couplings with the vector-like fields introduced in the KSVZ model. We develop a way to follow the dynamics of the PQ field, in particular we found a semi-analytical solution which describes the rotational motion under the logarithmic potential with including the thermalization effect via the gluon scattering which preserves the PQ symmetry. Based on the solution, we studied the baryon asymmetry, the effective number of neutrino, and the dark matter density composed of the axion and the neutralino. We found that the baryon asymmetry is successfully explained when the mass of PQ field is about 1 PeV (100 TeV) with the power of the PQ breaking term being 10 (8).

### Keywords:

baryogenesis, axion, supersymmetry, cosmology

## Axion dark world

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### **Abstract:**

We discuss various astrophysical and cosmological aspects of axion dark world.

### **Keywords:**

암흑 물질, 중입자 생성

## Dark World beyond WIMP

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### **Abstract:**

We discuss the recent researches on the dark world beyond WIMP and highlight representative experimental efforts to probe the new dark matter theories.

### **Keywords:**

Dark Matter, Dark Sector

## The Status of experimental systems of RAON

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### **Abstract:**

The RAON heavy ion accelerator facility is at the stage of preparing for the first beam commissioning of low energy superconducting linear accelerator (SCL3) and ISOL system on 2022. Therefore, the preparation for RAON ISOL system, which is the major rare isotope(RI) production system connected to a mass measurement system(MMS) and collinear laser spectroscopic system(CLS), is discussed. Also SCL3 is also expected to provide low energy accelerated stable ion beams to a low energy experimental system KoBRA(KOrea Broad acceptance Recoil spectrometer & Apparatus) for a beam commissioning on next year. The status of experimental systems of RAON is reported.

### **Keywords:**

RAON, ISOL, MMS, CLS, KoBRA

## Recent progress and plans at RIBF

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### Abstract:

"Exotic nuclei" far from the stability line are unique objects of many-body quantum system, where ratios of neutron number to proton number are much larger or much smaller than those of nuclei found in nature. The large isospin asymmetry causes their exotic properties and phenomena, and even affects scenarios of nucleosynthesis in the universe.

To access nuclei far from the stability line, especially neutron-rich nuclei, the "Radioactive Isotope Beam Factory (RIBF) " facility at RIKEN, Japan was constructed to deliver intense radioactive isotope (RI) beams and the operation started in 2007. The RIBF facility is highly optimized for in-flight production of fission fragments via a U beam. Super-conducting Ring Cyclotron (SRC) in the accelerator complex delivers a 345 MeV/u U beam. The U nuclide is converted at a target to fission fragments. The in-flight separator BigRIPS was designed to collect about 50% of the fragments and to separate fragments of interest. The RI beams produced at BigRIPS are then delivered to several experimental devices.

In this talk, special emphasis would be given to selected recent highlights obtained in terms of "shell evolution", "the r-process path", "neutron-correlation" and "equation-of-state in asymmetric nuclear matter". Future projects with new setups would be introduced. In addition, a facility upgrade plan of RIBF would be shown.

### Keywords:

Radioactive Isotope Beam, Nuclear Structure and Reactions

## Exploring the limits of nuclear existence

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### Abstract:

Exploring the limits of nuclear existence plays an important role in understanding the particle stability of neutron-rich and proton-rich nuclei. It provides many opportunities to study exotic nuclear structures, nuclear reactions and nuclear astrophysics, and it can be a benchmark for theoretical mass models at the extremely exotic region.

The Rare Isotope Accelerator complex for ON-line experiments (RAON) has a unique feature of utilizing both Isotope Separation On-Line (ISOL) and In-Flight (IF) fragmentation systems for the production of rare isotope beams, and a new ISOL+IF combined method can produce rare isotope beams different from the one produced by either ISOL or IF technique. RAON has a beam commissioning plan to provide stable beams at the first operational stage and RI beams at the second stage in 2023.

In this talk, we will introduce the recent research topics and issues, and discuss about current status and future plans for the rare isotope beam production and possible experiments.

### Keywords:

RI beam production, Nuclear Reactions, Nuclear Structures, Nuclear Astrophysics, RAON

## Key Nuclear Physics Studies using CENS Instruments at RAON

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### Abstract:

The study of exotic nuclear properties is one of the most important topics in the Nuclear Physics Community to understand nuclear structure evolution, the origin of elements in the Universe, and the forces that shaped the evolution of the Universe. For example, astrophysical observations, such as the luminosity of X-ray bursts and the abundance pattern of stars, can be explained by nuclear reactions occurring in the stars. While the nuclear reaction rates of isotopes involved in nucleosynthesis have a direct impact on stellar evolution, our understanding of astronomical observables is still very limited due to large uncertainties in calculated reaction rates and a lack of measurements with radioactive ion beams for the reaction rates. Nevertheless, there are now many opportunities to address the challenges with advances in rare-isotope productions around the world, including FRIB in the U.S. and RIBF in Japan.

The Rare isotope Accelerator complex for ON-line experiments (RAON) is a facility to produce stable and rare heavy isotope beams in 2023, enabling scientists to find new nuclear properties of rare isotopes. In order to take advantage of the RAON, the Center for Exotic Nuclear Studies (CENS) is preparing many experimental devices such as Korea Broad acceptance Recoil spectrometer and Apparatus (KoBRA) Wien Filter, CryoSTAR, ASGARD, STARK, ATOM-X and so on. With a combination of stable and rare isotope beams at the KoBRA experimental facility and the CENS new instruments, we would like to propose key nuclear physics experiments to study the properties of exotic nuclei. Details of the proposed experiments will be presented. We will also discuss plans to develop the detector systems optimized for experiments of nuclear reactions using radioactive ion beams.

### Keywords:

RAON, Nuclear Physics, CENS Instruments, Nuclear Astrophysics, RI beams

## Black Hole Physics: Introduction

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### **Abstract:**

Black holes are now one of the most interesting topics in astrophysics. Particularly, with the detection of the gravitational wave, the interests on black holes are not only theoretical, but also observational and experimental. In this focus session, we present black holes in various prospects with recent progress.

### **Keywords:**

Black Hole, Gravity Theory, Gravitational Wave

## Diving into a black hole

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### **Abstract:**

While the exterior physics of black holes has been extensively investigated in the literature, the interior structure of black holes behind the event horizon has not been well understood. In this talk, I will introduce our recent progress towards understanding the interior of black holes, including the no Cauchy-horizon theorem, the interior dynamics of a hairy black hole, and the constraint on the number of horizons with energy conditions.

### **Keywords:**

Black holes, Interior of black holes, No Cauchy-horizon theorem

# Black holes in effective field theory extensions of general relativity

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## Abstract:

Effective field theory methods suggest that some rather-general extensions of General Relativity include higher-order curvature corrections, with small coupling constants. In this talk, we discuss black hole solutions in such a framework.

After reviewing effective field theory methods, we construct spherically symmetric black hole solutions and study gravitational perturbation around them. Despite the higher-order operators of the theory, we show that linearized field equations obey second-order differential equations. We also introduce recent development which includes scalar fields.

## Keywords:

Alternative gravity theories, Black holes, Effective field theory, Gravitational waves

## Chaotic orbits in Kerr-Newman black hole

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### **Abstract:**

We investigate the chaotic motion of a charged particle around a Kerr-Newman black hole. The Lyapunov exponent is measured larger than expected when the angular momenta of the black hole and particle are considered. Here, the location of the maximum is also related to the extremal and non-extremal states of the black hole. Furthermore, we introduce our recent progress.

### **Keywords:**

Kerr-Newman black hole, Chaos, Lyapunov exponent, Orbit

## Enhancing spin-orbit torque efficiency via orbital currents

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### Abstract:

Current-induced spin-orbit torque (SOT) is regarded as a promising mechanism for driving magnetic memories. In principle, to achieve high SOT efficiency in magnetic heterostructures, materials systems with strong spin-orbit coupling (SOC)-induced spin Hall effect (SHE) or spin Rashba-Edelstein effect (SREE) are employed, from which pure spin currents can be generated to produce spin-transfer torques. Very recently, several SOC-free mechanisms, such as the orbital Hall effect (OHE) and orbital Rashba-Edelstein effect (OREE), are proposed to produce sizable orbital currents and SOTs [1-7]. These SOC-free or SOC-light mechanisms allow us to incorporate light 3d transition metals such as V, Cr, and Cu into the conventional heavy metals to enhance the spin-orbital Hall conductivity therein. In this talk, I will present some of our recent results [8] on enhancing the overall SOT efficiency by employing both the SHE and the OHE of the materials systems.

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### Keywords:

spin-orbit torque, spin Hall conductivity, orbital Hall conductivity, orbital current

## Efficient conversion of orbital Hall current to spin current for spin-orbit torque switching

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### Abstract:

Spin Hall effect, an electric generation of spin current, allows for efficient control of magnetization. Recent theory revealed that orbital Hall effect creates orbital current, which can be much larger than the spin Hall-induced spin current. However, orbital current cannot directly exert a torque on a ferromagnet, requiring a conversion process from orbital current to spin current. In this talk, we report two effective methods of the conversion in normal metal (NM)/ferromagnet (FM) structures through spin-orbit coupling engineering of either an FM or an NM/FM interface, which allows us to unambiguously demonstrate orbital-current-induced spin torque, or orbital Hall torque (OHT). First, we employ a rare-earth FM of Gd with strong spin-orbit coupling, which increases the OHT in Cr/Gd heterostructures by ten times compared to that in Cr/Co heterostructures, indicating that the orbital current generated in Cr is efficiently converted to spin current in the FM Gd layer. Second, we modify the Cr/CoFeB interface by inserting a 1 nm Pt layer to facilitate the orbital-to-spin current conversion. This leads to an enhancement in OHT, allowing us to demonstrate OHT-induced magnetization switching of perpendicular magnetization in Cr/Pt/CoFeB heterostructures. Our results demonstrating the significant OHT generated through the conversion techniques broaden the scope of material engineering to improve spin-torque switching efficiency for the development of low-power spintronic devices.

### References

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### Keywords:

orbital current, orbital Hall torque, spin-orbit torque

## Observation of the orbital Hall effect in a light metal Ti

CHOI Young-Gwan <sup>1</sup>, JO Daegeun <sup>2</sup>, KO Kyung-Hun <sup>1</sup>, GO Dongwook <sup>3,4</sup>, KIM Kyung-Han <sup>2</sup>, PARK Hee Gyum <sup>5</sup>,  
KIM Changyoung <sup>6,7</sup>, MIN Byoung-Chul <sup>5</sup>, CHOI Gyungmin <sup>\*1,8</sup>, LEE Hyun-Woo <sup>2,9</sup>

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### Abstract:

Fast electrical control of magnetism can be achieved by injecting a spin current into nanomagnets. The spin Hall effect (SHE) generates a spin current perpendicular to an external electric field by inducing spin-dependent transverse motion of electrons. Theoretical studies indicate that the SHE arises in  $4d$  and  $5d$  transition metals due to the orbital Hall effect (OHE), which induces orbital-angular-momentum-dependent transverse flows [1]. The OHE-origin of the SHE explains the systematic variation of the spin Hall conductivity sign in  $5d$  transition metals.

In light metals with negligible spin-orbit coupling, the SHE becomes negligible but the OHE can remain strong provided the orbital character of wave functions varies fast with crystal momentum (orbital texture) [2]. We measure the orbital moment accumulation for the light metal Ti using the magneto-optical Kerr effect (Fig. 1a). The measured Kerr rotation comes from the large orbital Hall conductivity  $\sigma_{\text{OH}} \sigma_{\text{OH}} [3800 \hbar/e\Omega \cdot \text{cm}^{-1} (\hbar/e)(\Omega \cdot \text{cm})^{-1}]$  of Ti and high sensitivity of light for orbital magnetization [3]. As an independent test, we also measure the orbital torque that arises when an OHE-induced orbital current is injected into an adjacent ferromagnet (Fig. 1b).

### Keywords:

orbital Hall effect, orbital texture, orbital accumulation, orbital torque

## Chirality-induced Orbital Polarization in DNA-like Chiral Materials

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### Abstract:

In chemistry and biochemistry, chirality is the geometric asymmetry of a large group of molecules with a non-superposable mirror image, either left- or right-handed. In physics, chirality usually refers to the spin-momentum locking, for example, in Weyl fermions and neutrinos. We discover that the structural chirality generally leads to an electronic chirality, the orbital – momentum locking in the wave function. Such a chiral topology can lead to orbital polarization when electrons transmit through DNA-type chiral molecules, and eventually induce spin selectivity in the presence of spin-orbit coupling from heavy-metal contacts. Beyond chiral molecules, we anticipate that the orbital polarization could induce unidirectional magnetoresistance in emerging materials such as the twisted bilayer graphene. We also suggests a way to detect the orbital current from the orbital Hall effect.

### References

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- [2] Y Liu, T Holder, B Yan, The Innovation 2 (1), 100085 (2021).
- [3] J Xiao, Y Liu, B Yan, Memorial Volume for Shoucheng Zhang, 353-364 (2022).
- [4] J Xiao, B Yan, arXiv:2201.03623 (2022).

### Keywords:

Chirality, orbital, spin, topology

## Twofold van Hove singularity and origin of CDW in a kagome superconductor $\text{CsV}_3\text{Sb}_5$

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### **Abstract:**

The layered vanadium antimonides  $AV_3Sb_5$  ( $A = \text{K, Rb, Cs}$ ) are a recently discovered family of topological kagome metals with a rich phenomenology of strongly correlated electronic phases including charge density wave and superconductivity. Understanding how the singularities inherent to the kagome electronic structure are linked to the observed many-body phases is a topic of intense study. Here, by combining angle-resolved photoemission spectroscopy and density functional theory, we identified multiple kagome-derived van Hove singularities ( $\nu\text{Hs}$ ) coexisting near the Fermi level of  $\text{CsV}_3\text{Sb}_5$  and analyzed their role in driving electronic instabilities.

### **Keywords:**

kagome superconductor

## Single crystal growth and physical properties of several Kagome metals

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### Abstract:

Kagome metals (or magnets) refer to a new class of magnetic quantum materials hosting Kagome lattice and topological band structure. Various forms of Kagome lattices have been recently documented; they include 3-1 (e.g. paramagnet  $\text{Ni}_3\text{In}$ , antiferromagnet  $\text{Mn}_3\text{Sn}$ ), 1-1 (e.g. paramagnet  $\text{CoSn}$ ), 1-6-6 (e.g. ferrimagnet  $\text{TbMn}_6\text{Sn}_6$ ), 3-2-2 (e.g. hard ferromagnet  $\text{Co}_3\text{Sn}_2\text{S}_2$ ), and 3-2 materials (e.g. soft ferromagnet  $\text{Fe}_3\text{Sn}_2$ ), thus demonstrating a variety of crystal and magnetic structures. They generally feature a 3d transition metal-based magnetic Kagome lattice with an in-plane lattice constant  $\sim 5.5\text{\AA}$ . Their 3d electrons dominate the low-energy electronic structure in these quantum materials, thus exhibiting electronic correlation. Most importantly, the Kagome lattice electrons generally feature Dirac band crossings and flat band, which are the source for nontrivial band topology. Moreover, they all contain the heavy element Sn, which can provide strong spin-orbit coupling to the system. Therefore, the system can be an ideal platform to explore the rich interplay between geometry, correlation, and topology.

In this presentation, we summarize our group's efforts to grow all of the above-mentioned structures that have formed Kagome metallic magnets. In particular, we focus on how the Ti and Te doping into  $\text{Cs}_3\text{V}_2\text{Sb}_2$  compounds to form  $\text{Cs}_3(\text{V,Ti})_2(\text{Sb,Te})_2$  have changed their electrical and magnetic properties, partially combined with recent electronic spectroscopy results. Moreover, we provide temperature-dependent transport/magnetism in Ni shandites ( $\text{Ni}_3(\text{Tl,In})_2\text{S}_2$ ) materials. Finally, by looking at details of temperature-dependent Raman scattering, we trace out the phonon spectra and quasi-elastic electronic Raman spectra in  $\text{Ni}_3\text{In}$  to discuss the implications of the electron carries in this compound.

Finally, we end up with our plans to investigate systematically the Hall effects of these materials to uncover the signs of possible Dirac/Weyl fermions, Berry curvature, and spin-orbit coupling. Our research efforts are likely to provide promising hints for the development of technologies in quantum computing, spin superconductors, and low power electronics based on the Kagome metals.

### Keywords:

Kagome metals, shandites, flat band, dirac fermions, Weyl fermions

## Intertwining orbital current order and superconductivity in Kagome metal

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### Abstract:

The nature of superconductivity in newly discovered Kagome materials,  $AV_3Sb_5$  ( $A=K, Rb, Cs$ ), has been a subject of intense debate. Recent experiments suggest the presence of orbital current order on top of the charge density wave (CDW) and superconductivity. Since the orbital current order breaks time-reversal symmetry, it may fundamentally affect possible superconducting states. In this work, we investigate the mutual influence between the orbital current order and superconductivity in Kagome metal with characteristic van Hove singularity (vHS). By explicitly deriving the Landau-Ginzburg theory, we classify possible orbital current order and superconductivity.

It turns out that distinct unconventional superconductivities are expected, depending on the orbital current ordering types. Thus, this information can be used to infer the superconducting order parameter when the orbital current order is identified and vice versa. We also discuss possible experiments that may distinguish such superconducting states coexisting with the orbital current order.

### Keywords:

kagome, orbital current, superconductivity, van Hove singularity, topology

## Moiré quasicrystals

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### Abstract:

When 2D materials having different periodicities are overlaid with each other, an interference pattern of the lattice mismatch often gives rise to unusual electronic properties. In a twisted bilayer graphene (TBG) with a small twist angle, in particular, a moiré pattern gives rise to the flat band formation and emergent superconductivity. The electronic structure of a small angle TBG can be well described by the effective continuum approach which exclusively extracts the long-period moiré pattern. In larger twist angles, however, the atomic scale and the moiré period are no longer separable, and the system becomes truly quasiperiodic, i.e., the conventional Bloch theory breaks down.

In this talk, we present our recent theoretical works on the electronic properties of quasiperiodic twisted bilayer systems, including the 30-degree TBG [1] and also double moiré system of hBN/graphene/hBN [2].

In particular, we show that the electronic spectrum plotted against the twist angle generally contains a number of fractal minigaps, where each gap can be characterized by a set of integers associated with a quasi Brillouin zone. These quantum numbers can be expressed as second Chern numbers by considering a formal relationship between an adiabatic charge pumping under the interlayer slide and a topological nonlinear electromagnetic response in 4D band insulators.[3]

[1] P. Moon, M. Koshino, Y.-W. Son, Phys. Rev. B 99, 165430 (2019).

[2] H. Oka and M. Koshino, Phys. Rev. B 104, 035306 (2021).

[3] M. Koshino, H. Oka, Phys. Rev. Research 4, 013028 (2022).

### Keywords:

Twisted bilayer graphene , moiré superlattice , quasicrystal

## Electronic structures and interactions in twisted graphene layers

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### Abstract:

Twisted graphene layers show large-scale moiré superlattices in their atomic structures and have almost flat bands in their electronic structures. Detailed band structures of the almost flat bands are sensitive to the twist angle, the number of layers, the stacking configuration, doping, and applied electric fields [1-4]. Here, we discuss band dispersions of the almost flat bands as a function of doping, electric fields, the twist angle, and the number of layers. We also discuss strength of the electron-phonon interaction and the superconductivity in different twisted graphene layers [3]. We further discuss spin-valley polarized phases as a function of doping, based on the density functional theory calculations [4]. This work was supported by NRF of Korea (Grant No. 2020R1A2C3013673) and KISTI supercomputing center (Project No. KSC-2021-CRE-0384).

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### Keywords:

twisted graphene layers, moiré superlattice, electronic structure, electron-phonon interaction, spin-valley polarization

## Berry curvature dipole senses topological transition in a moiré superlattice

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### Abstract:

Topological aspects of electron wavefunction play a crucial role in determining the physical properties of materials. Berry curvature and Chern number are used to define the topological structure of electronic bands. While Berry curvature and its effects in materials have been studied detecting changes in the topological invariant, Chern number, is challenging; particularly changes of valley Chern type. In this regard, twisted double bilayer graphene (TDBG) has emerged as a promising platform to gain electrical control over the Berry curvature hotspots and the valley Chern numbers of its flat bands. In addition, strain induced breaking of the three-fold rotation ( $C_3$ ) symmetry in TDBG, leads to a non-zero first moment of Berry curvature called the Berry curvature dipole (BCD), which can be sensed using nonlinear Hall (NLH) effect. We reveal, using TDBG, that the BCD detects topological transitions in the bands and changes its sign. In TDBG, the perpendicular electric field tunes the valley Chern number and the BCD simultaneously providing us a tunable system to probe the physics of topological transitions.

### Keywords:

Berry curvature dipole, topological transition, Chern number

## Piezoelectric response and nonlinear optical properties of twisted graphene systems

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### Abstract:

Twisted graphene systems have drawn great attention recently due to the discoveries of various intriguing states such as correlated insulators, superconductivity, and quantum anomalous Hall states. Most of these phenomena are attributed to the presence of topologically nontrivially flat bands, which typically have nonzero valley Chern numbers. In this talk, we try to tackle with two problems: (a) how to directly and quantitatively probe the valley Chern numbers of the topological flat bands in moire graphene systems; and (b) how to experimentally identify the nature of the numerous “featureless” correlated insulator states discovered at both integer and fractional fillings in magic-angle twisted bilayer graphene (TBG). Our solution to the first problem is that the topological flat bands with nonzero valley Chern numbers in moire graphene systems would contribute to a nearly quantized piezoelectric response that is exactly proportional to the valley Chern numbers [1]. Thus, we propose that piezoelectric response can serve as a direct experimental probe to measure the valley Chern numbers of the system. As for the second problem, we find that although most of the correlated insulators are featureless in the linear response regime, they can exhibit distinct nonlinear optical responses [2]. To illustrate our idea, we have comprehensively studied the correlated insulator and density wave states at various integer and fractional fillings of the flat bands in magic-angle TBG, and find that most of these states exhibit nonzero valley polarization that can induce giant nonlinear optical response in the terahertz-infrared frequency regime. We further analyze the nonlinear optical properties of all 16 types of ordered states in the orbital space, and find that only three of them exhibit non-vanishing nonlinear optical response [2].

### References:

- [1] Ran Peng and Jianpeng Liu, arXiv:2109.09529
- [2] Shihao Zhang, Xin Lu, and Jianpeng Liu, arXiv:2109.12823

### Keywords:

Valley Chern numbers , twisted graphene , density wave state

## Competing orders in monolayer AV<sub>3</sub>Sb<sub>5</sub> (A=Na, Rb, Cs)

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### Abstract:

Recent years have noticed a surge of research interest in layered kagome metals AV<sub>3</sub>Sb<sub>5</sub> (A = K, Rb, and Cs), which have been emerged as a fertile platform for exploring correlations and topology. Using a combination of first-principles and mean-field calculations, we explore possible competing orders in monolayer AV<sub>3</sub>Sb<sub>5</sub> (A = Na, Rb, Cs). We argue that two-dimensional monolayer preserves intrinsically different symmetries from the three-dimensional layered bulk, enforced by stoichiometry. Due to this, enrichment of the van Hove singularities, a logarithmic divergence of electronic density of states, consequently appears in their numbers and types, leading to a dramatic consequence on the correlated states. We show that the monolayer hosts a variety exotic phases, including doublets of charge density waves and s- and d-wave superconductivity. Our results suggest the monolayer kagome metal AV<sub>3</sub>Sb<sub>5</sub> as a novel two-dimensional platform for correlated topological phenomena.

### Keywords:

kagome metal, first-principles calculations, correlated electrons, topology, mean-field theory

# The charge density wave collective excitations in Weyl semimetal (TaSe<sub>4</sub>)<sub>2</sub>I

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## Abstract:

The correlation effects in topological material is one of important themes in recent fields of condensed matter physics. One of them is CDW-Weyl motif, in which a pair of Weyl fermions is coupled by a charge density wave (CDW) wavevectors, thereby opening a gap at Weyl crossing points. The model predicts the phason, the phase part of the CDW collective mode, follow the axion electrodynamics described by  $\theta\mathbf{E}\cdot\mathbf{B}$  [1,2]. A variety of topological magneto-electric phenomena are proposed from this correlated topological band structure, such as negative magnetoresistance and dynamical piezomagnetic effects [2,3]. Among real materials, (TaSe<sub>4</sub>)<sub>2</sub>I is a promising candidate to explore CDW-Weyl phenomena. It hosts Weyl fermions near the Fermi level on its structurally chiral lattice, and undergoes the CDW phase transition near  $T_C \sim 260$  K [2,4,5]. In this work, we will investigate the low-energy excitations in (TaSe<sub>4</sub>)<sub>2</sub>I using ultrafast terahertz emission spectroscopy. Possible assignment of optic phason and its implication on the CDW-Weyl phenomena will be discussed.

[1] D. M. Nenzo *et al.*, Nat. Rev. Phys. **2**, 682 (2020).

[2] J. Gooth *et al.*, Nature **575**, 315 (2019).

[3] Yu *et al.*, Phys. Rev. B **104**, 174406 (2021).

[4] W. Shi *et al.*, Nat. Phys. **17**, 381 (2021).

[5] S. Kim *et al.*, arXiv:2108.10874

## Keywords:

(TaSe<sub>4</sub>)<sub>2</sub>I, charge density wave, ultrafast optical spectroscopy

## Spin-Split Band Hybridization in Graphene Proximitized with $\alpha$ - $\text{RuCl}_3$ Nanosheets

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### Abstract:

Proximity effects induced in the two-dimensional Dirac material graphene potentially open access to novel and intriguing physical phenomena. Thus far, the coupling between graphene and ferromagnetic insulators has been experimentally established. However, only very little is known about graphene's interaction with antiferromagnetic insulators. Here, we report a low-temperature study of the electronic properties of high quality van der Waals heterostructures composed of a single graphene layer proximitized with  $\alpha$ - $\text{RuCl}_3$ . The latter is known to become antiferromagnetically ordered below 10 K. Shubnikov-de Haas oscillations in the longitudinal resistance together with Hall resistance measurements provide clear evidence for a band realignment that is accompanied by a transfer of electrons originally occupying the graphene's spin degenerate Dirac cones into  $\alpha$ - $\text{RuCl}_3$  band states with in-plane spin polarization. Left behind are holes in two separate Fermi pockets, only the dispersion of one of which is distorted near the Fermi energy due to spin selective hybridization with these spin polarized  $\alpha$ - $\text{RuCl}_3$  band states. This interpretation is supported by our density functional theory calculations. An unexpected damping of the quantum oscillations as well as a zero-field resistance upturn close to the Néel temperature of  $\alpha$ - $\text{RuCl}_3$  suggest the onset of additional spin scattering due to spin fluctuations in the  $\alpha$ - $\text{RuCl}_3$ .

### Keywords:

Graphene,  $\alpha$ - $\text{RuCl}_3$ , Heterostructure

## Hyperbolic plasmon polaritons propagating in metallic delafossite PdCoO<sub>2</sub>

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### Abstract:

The ability to strongly couple to light makes plasmons most the promising quasiparticles for modern photonics and quantum information technology. However, the short lifetime of plasmon polaritons has limited the palette of plasmonic materials to highly conductive metals such as silver and gold. In this talk, we will show that metallic delafossites are good plasmonic materials where low-loss hyperbolic plasmon polaritons propagate. The presence of hyperbolic plasmon polaritons is demonstrated by carrying out monochromated scanning transmission electron microscopy and electron energy loss spectroscopy (monochromated STEM-EELS) experiments on the slits of metallic delafossites fabricated using focused ion beam (FIB) techniques. This work provides a basis to open a new area of plasmonics of complex delafossite oxides which may be coupled to other degree of freedom at the single crystal level. To note, metallic delafossites exhibit interesting transport phenomena at low temperature, e.g., hydrodynamic electron flow<sup>1</sup>, unconventional anomalous Hall effects<sup>2</sup>, and giant Rashba-like spin splitting<sup>3</sup>. We should also note the recent successes in growing these materials as thin films<sup>4-6</sup>, which opens tantalizing prospect for future development of functional delafossite plasmonics.

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<sup>3</sup> Sunko, V. et al. Nature, 549, 492-496 (2017).

<sup>4</sup> Harada, T. et al. APL Materials 6, 046107 (2018).

<sup>5</sup> Sun, J. et al. APL Materials 7, 121112 (2019).

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### Keywords:

Delafossite oxides, Hyperbolic plasmons, Polaritons, Monochromated STEM-EELS

## Fluctuating Antiferromagnetic Domains in $\text{Ni}_2\text{MnTeO}_6$

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### Abstract:

Magnetic domains play a fundamental role in the physics of magnetism. Despite the growing importance of antiferromagnetic materials in future electronic devices, the dynamics of antiferromagnetic domains are poorly understood. The dynamics of antiferromagnets also feature prominently in the studies of topological quantum matter. Real-space imaging of fluctuating antiferromagnetic domains is therefore highly desired. In this talk, I present the Real Space and Time Coherent Resonant X-ray Imaging (ReST-CRXI) technique. Using this technique, we obtained videos of fluctuating micrometer-scale antiferromagnetic domains in  $\text{Ni}_2\text{MnTeO}_6$  on timescales from  $10^{-1}$  to  $10^3$  s. We found that, in the collinear phase, thermally activated domain wall motion is observed in the vicinity of the Néel temperature. The fluctuations persist through the full range of the higher-temperature helical phase.

### Keywords:

ReST-CRXI, X-ray Imaging

## **Study of a transient normal state of the superconducting YBCO: Bridging the knowledge gap between equilibrium state and non- equilibrium state in high- $T_c$ cuprates**

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### **Abstract:**

One of the central issues in high- $T_c$  cuprates is an understanding of nature on the mysterious pseudogap, which occurs at the normal state where it is a much higher temperature than the superconducting critical temperature ( $T_c$ ). It naturally becomes a common belief that a proper understanding of the normal state (i.e., ground-state problems) would shed light on a direction to approach the room temperature superconductivity. Experimentally, to investigate the normal state of the cuprates at low temperature, the superconductivity (i.e., Cooper pairs) must be quenched by either a much high magnetic field or an optical pump. However, there is a challenging issue. This is because the pump-probe approach deals with the non-equilibrium state while the magnetic field approach represents the equilibrium state, being premature to reach a common ground between the two approaches. In this presentation, I would like to discuss how to overcome such a challenge. For this purpose, I will highlight a comprehensive x-ray scattering study on ortho-VIII  $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$  (YBCO) performed at both Free-electron-laser (FEL) and Synchrotron facilities, such as time-resolved resonant soft x-ray scattering (tr-RSXS), elastic resonant x-ray scattering, and high-magnetic field scattering. We found the existence of competition between superconductivity and charge density wave (CDW) even in the non-equilibrium state. We further observed that the broken pairing states in the superconducting  $\text{CuO}_2$  plane led to nucleation of three-dimensional CDW precursor correlation. Ultimately, we proved that a transient normal state triggered by the laser-driven quench of the YBCO superconducting state is possible to represent phenomena of the equilibrium state. This result provides clues on addressing the challenge, although we were not touching on all examples. At the final stage of this presentation, I will also extend the discussion about our scientific consideration even under the equilibrium state into the fact that the non-equilibrium approach could generate a transient superconducting state nearly up to room temperature.

### **Keywords:**

superconducting YBCO, high- $T_c$  cuprates

## Dimensionality-control and giant enhancement of the electron-phonon coupling in SrRuO<sub>3</sub> films

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### Abstract:

In condensed matters, an electron-phonon coupling is one of the most important couplings among fundamental degrees of freedom, and plays crucial roles in a variety of novel phenomena, such as superconductivity, ferroelectricity, insulator-metal transition, and so on. Whereas researchers usually have tried to reveal working principles of such phenomena based on the given coupling strength, it will be meaningful for both fundamental and application researches if the coupling strength can be controlled with experimentally accessible knobs. In this work, we discuss coupling effects among electron, phonon, and spin in SrRuO<sub>3</sub> films and SrRuO<sub>3</sub>/SrTiO<sub>3</sub> superlattices by examining relaxation processes of photo-excited electron states by using a conventional pump-probe technique. As the film thickness decreases down to the atomic thickness limit, we observe that the electron-phonon coupling can be enhanced by three orders of magnitude. Such a dimensionality-control and giant enhancement of the electron-phonon coupling in SrRuO<sub>3</sub> is attributed to the distinct film-thickness-dependent evolutions of  $d_{xy}$  and  $d_{yz}/d_{zx}$  orbital states. We expect this demonstration can provide an important clue in understanding various novel phenomena observed in ruthenates, such as superconductivity in Sr<sub>2</sub>RuO<sub>4</sub>, bad metallicity in SrRuO<sub>3</sub>, and so on.

### Keywords:

electron-phonon coupling, nonequilibrium state, ultrafast pump-probe technique, SrRuO<sub>3</sub>, thin film

## Femtosecond X-ray scattering and imaging to study light-induced ultrafast phase transition using X-ray Free Electron Laser

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### Abstract:

The recent advance of X-ray free electron laser (XFEL) opens the area of ultrafast structural dynamics with a few tens of time resolution due to its unique characteristics of X-rays. XFEL makes it possible to obtain critical information on the intermediate states or pathways during the phase transformation, which only measured the initial and final states with many existing techniques. In my talk, I present the recent results of expectation of band inversion related topological phase transition in  $\text{Bi}_2\text{Se}_3$  followed by carrier-induced contraction and vibration modes, the crystalline-amorphous phase transformation of a phase change material and light-induced phase transition in  $\text{VO}_2$  as examples.

This research was supported by the National Research Foundation of Korea (NRF-2021R1A3B1077076).

### Keywords:

phase transformation, ultrafast, X-ray free electron laser, time-resolved x-ray scattering, dynamics

## Manipulation of ultrafast hot carrier dynamics for 2D optoelectronic applications

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### **Abstract:**

One of the key aims for enhancing the performance of advanced optoelectronic devices is to convert photoexcited hot carriers to electricity in semiconductors. To realize efficient hot carrier devices, efforts focus on elongating the relaxation time of hot carriers and on understanding the dynamics of hot carriers at the interface between 2D material and metal electrodes. Here, we explore the mechanism of hot carrier extraction, relaxation, and diffusion processes at the MoS<sub>2</sub>/metal interface via ultrafast transient reflection spectroscopy. Furthermore, by integrating graphene with MoS<sub>2</sub>, we demonstrate an efficient interfacial hot-carrier transfer from MoS<sub>2</sub> to graphene with a prolonged hot carrier relaxation time.

### **Keywords:**

hot carrier, 2D optoelectronics, ultrafast spectroscopy

## Probing Deep-UV Optoelectronic Processes in vdW Wide Bandgap Semiconductors

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### Abstract:

Hexagonal boron nitride (hBN) is a van der Waals (vdW) semiconductor with a wide bandgap of ~ 5.96 eV. Despite the indirect bandgap characteristics of hBN, charge carriers excited by high energy electrons or photons efficiently emit luminescence at deep-ultraviolet (DUV) frequencies via strong electron-phonon interaction. In this work, we probe optoelectronic processes at a band edge in hBN by means of optical imaging and spectroscopy at deep ultraviolet frequencies. Our laser excitation spectroscopy shows that strong radiative recombination and carrier excitation processes originate from the pristine structure and the stacking faults in hBN. We further demonstrate prominent electroluminescence and photocurrent generation from hBN by fabricating vdW heterostructures with graphene electrodes. Our work provides a pathway toward efficient DUV light emitting and detection devices based on hBN.

### Keywords:

hexagonal boron nitride, excitons, Deep-ultraviolet optoelectronic properties

## Manipulating exciton dynamics in 2D-TMDC with high quality factor dielectric metasurfaces

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### Abstract:

Two-dimensional transition metal dichalcogenides (2D-TMDC) exhibit strong light-matter interactions due to their tightly bound excitons arising from the large in-plane quantum confinement and reduced dielectric screening. However, their photonics applications are limited by relatively low quantum yield and strong exciton-exciton annihilation that further reduces their quantum efficiency at high fluences. In this work, we attempt to address such challenges by integrating monolayer WSe<sub>2</sub> with high quality factor dielectric metasurfaces via Purcell effect. When the exciton resonance spectrally overlaps with the high quality factor resonance of the metasurface, we observe a robust photoluminescence enhancement of ~1 order of magnitude and radiative rate enhancement of 3.5. This also leads to 1.6-fold reduction of exciton-exciton annihilation rate, which is observed as longer exciton lifetime at high densities. Our results suggest that metasurfaces can support strong dynamic light-matter interactions in 2D-TMDCs for photonics applications in ultrafast sensors, modulators, and emitters.

### Keywords:

transition metal dichalcogenides, metasurfaces, Purcell effect, exciton-exciton annihilation, high-Q resonances

## Dominant role of ferroelectric dipoles for mechanical energy harvesting and acoustic energy transfer

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### Abstract:

With the rapid depletion of fossil fuels and consequent environmental problems, energy harvesting system from the environment has become one of the most critical issues for the sustainable development of civilization. Among renewable energy resources, mechanical energy is abundant, ubiquitous, and less dependent on environmental parameters, like time and geological locations, in contrast to solar and thermal energies. The mechanical vibrations of low frequency under ambient condition have been effectively converted to electricity by recently developed triboelectric nanogenerators to power small electronic devices without traditional batteries.

In this presentation, we show that ferroelectric dipoles play a domain role for the mechanical energy harvesting and energy transfer efficiencies through the modulation of surface potential of polymer. Such enhanced efficiency provides triboelectric nanogenerator with new functionalities of contactless power generation [1] and acoustic energy transfer through liquid and solid media [2].

[1] H. S. Kim, D. Y. Kim, J. E. Kim, J. H. Kim, D. S. Kong, Gonzalo Murillo, G. H. Lee, J. Y. Park and J. H. Jung, *Adv. Funct. Mater.* **29**, 1905816 (2019).

[2] H. S. Kim, S. Hur, D-G. Lee, J. Shin, H. Qiao, S. Mun, H. Lee, W. Moon, Y. Kim, J. M. Baik, C-Y. Kang, J. H. Jung, and H-C. Song, *Energy Environ. Sci.* (2022) (in press).

### Keywords:

Ferroelectric dipoles, Mechanical energy harvesting, Acoustic energy transfer

## **Magneto-Mechano-Electric energy harvesting by magnetoelectric composite for IoT sensor systems**

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### **Abstract:**

The deployment of wireless sensor networks (WSNs) for the internet of things (IoT) and remote monitoring devices has made tremendous progress in the last few years. At the same time, energy harvesters are also being developed to satisfy the power requirement of WSNs and other low power consumption electronics. Among various resources for energy harvesting, the magnetic noise produced by power transmission infrastructures and associated mechanical vibrations are ubiquitous energy sources that could be converted into electricity by energy conversion materials or devices. This naturally brings up the question: "How can we efficiently convert this waited and harmful energy source for IoT devices?"

In this presentation, the status and prospects of an emerging magnetic energy harvesting technology, the so-called magneto-mechano-electric (MME) generators, are reviewed. A magneto-mechano-electric (MME) generator is an effective way to get an improved electric power density using with magnetoelectric (ME) composite composed of piezoelectric single crystal and magnetostrictive shim. Since the piezoelectric phase in the MME generator also responds to mechanical vibration directly, an ME-based energy harvester can harness energy from both mechanical vibrations and magnetic fields simultaneously. The MME generator can be a ubiquitous power source for WSNs and low power electronic devices by harvesting energy from the tiny magnetic fields present as parasitic magnetic noise in an ambient environment.

### **Keywords:**

energy harvesting, magnetoelectric, piezoelectric, magnetic field

# Triboelectrification for New Energy Solution and Tribotronics

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## Abstract:

Energy harvesting systems based on triboelectric nanomaterials are in great demand, as they can provide routes for the development of self-powered devices which are highly flexible, stretchable, mechanically durable, and can be used in a wide range of applications. Our recent research interest mainly focuses on the fabrication of high-performance triboelectric nanogenerators (TENGs) based on various kinds of nanomaterials. Flexible TENGs exhibit good performances and are easy to integrate which make it the perfect candidate for many applications, and therefore crucial to develop. In this presentation, I firstly introduce the fundamentals and possible device applications of TENGs, including their basic operation modes. Then the different improvement parameters will be discussed. As main topics, I will present a couple of recent achievements regarding highly robust and efficient TENGs with multifunctional materials, etc. In addition, the presenter will report transcutaneous ultrasound energy harvesting using capacitive triboelectric technology. A major challenge for implantable medical systems is the inclusion or reliable delivery of electrical power. Ultrasound was used to deliver mechanical energy through skin and liquids and demonstrated that a thin implantable vibrating triboelectric nanogenerator is able to effectively harvest it. Finally The presenter is going to introduce a 2D materials-based tribotronics for possible future application toward tactile sensors, robots, security, human-machine interfaces, etc. The triboelectric charging behaviors of various 2D layered materials including graphene, MoS<sub>2</sub>, MoSe<sub>2</sub>, etc were investigated in order to decide the triboelectric position of each 2D material using the concept of a triboelectric nanogenerator, which provides new insights to utilize 2D materials in triboelectric devices, allowing thin and flexible device fabrication.

## Keywords:

Triboelectrification, Energy Harvesting, Nanogenerator, Tribotronics, 2D Materials

## Emerging optoelectronics based on the quantum-dots and oxide semiconductors

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### **Abstract:**

This talk will focus to introduce a new type of optoelectronics based on nanomaterials, such as quantum-dots and nanoparticles of oxide semiconductors. These kinds of optoelectronics are considered as an emerging science and technology due to the potential applications including transparent and soft interactive devices. During the presentation, the interfacial physics of quantum-dots light emitting diodes(QLEDs) will be considered as well as the fabrication process of high-performance QLEDs. In addition, a method to fabricated highly transparent photosensors, which can be perfectly turned on and off by a visible and near-IR light, based on quantum-dots and oxide semiconductors will be discussed in detail. The measurements and analysis of interfacial electronic structure of optoelectronics based on X-ray and UV photoelectron spectroscopy will be introduced in detail as well.

### **Keywords:**

Quantum-dots, oxide semiconductor, transparent, interfacial electronic structure, photosensors

## On-chip Brillouin scattering and its applications

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### Abstract:

On-chip Brillouin scattering has been investigated in various photonic platforms. I will review the platforms and present our recent experimental results of active information manipulation via optically driven acoustic-wave interference.

Harnessing well-developed micro-/nano-fabrication technologies to optics makes impossible possible, opening new era of light-matter interaction. At micro/nanoscales, coupling between light and different particle/quasi-particle domains can be enhanced dramatically and controllable with unprecedented design space, and such nano-systems can be integrated with other components on chip. In this talk, I will introduce a novel study about photon-phonon interaction, opto-mechanics and Brillouin scattering. The phenomena of optically driven mechanical vibration have been observed with either extremely high optical power or micro-/nano-sized structures. I will present pioneering demonstrations in opto-mechanics and my recent achievements of hybrid photonic-phononic systems. The controllable photon-phonon interactions in such hybrid systems could provide new science and technologies. In addition, I will present our recent experimental results of active information manipulation via optically driven acoustic-wave interference [1]. This approach will open a new era of photon-phonon-microwave systems.

### Acknowledgements

This work was supported by the National Research Foundation of Korea (NRF) (NRF-2019M3E4A1079780), Korea Institute of Science and Technology's Open Research Program (2E30620-20-052), and Institute for Information & communications Technology Promotion (IITP) (2020-0-00947).

### References

[1] H. Kim and H. Shin, "Active information manipulation via optically driven acoustic-wave interference," *Nano Letters* 21, 7270-7276 (2021).

### Keywords:

Brillouin scattering, silicon photonics, photon-phonon interaction, optical forces, opto-mechanics

## Plug-and-play single-photon source with highly efficient fiber interface

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### Abstract:

Future quantum information processing would rely on quantum systems that connect multiple qubits, control units, and measurement systems, and therefore all quantum operations are efficiently possible in an all-connected and integrated platform. Solid-state quantum emitters have attracted much attention as sources of both photonic and spin qubits. Integrating these artificial atoms onto practical optical channels such as optical fiber offers a new possibility for achieving long-distance quantum interaction and distributing quantum information across conventional fiber networks. In this talk, I present recent advances on fiber-integrated quantum devices and possible quantum applications using them [1]

Ref[1]. Jeon, Woong Bae, et al. "Plug-and-play quantum devices with efficient fiber-quantum dot interface". arXiv preprint [arXiv:2202.13127](https://arxiv.org/abs/2202.13127) (2022).

### Keywords:

Quantum photonics, Single-photon source, Quantum dot, Fiber integrations

## Time-dependent entropy production estimator

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### Abstract:

In this talk, we present multi-dimensional entropy production bound, an estimator for time-dependent entropy production. We verify our method on three examples, including the RNA unfolding process. The estimation results via multi-dimensional entropy production bound are comparable to a machine-learning-based method. In addition to that, this invented method is faster than the machine-learning-based method even with lower computational power.

### Keywords:

Entropy production, Nonequilibrium physics, Langevin dynamics

## Solving generalized Langevin equations violating the fluctuation-dissipation theorem: numerical simulation and exact theory

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### Abstract:

A viscoelastic system is governed by a generalized Langevin equation (GLE), in which viscoelastic interactions are described by a memory kernel  $K(t-t') \sim |t-t'|^{-\alpha}$  and the particle is driven by an effective noise  $\zeta(t)$  with the autocorrelation  $\langle \zeta(t)\zeta(t') \rangle \sim |t-t'|^{-\beta}$ . Using the GLE, we study the active particle moving through a viscoelastic environment where the active particle's motion violates the fluctuation-dissipation theorem (FDT). Performing the numerical simulation, we solve the GLE violating the FDT for several types of the memory kernel and effective noise. Both the exponents of the memory kernel and the autocorrelation in  $\zeta(t)$  determine the dynamics of the particle in the active viscoelastic system. We find that our exact theory excellently our simulation results. We demonstrate that the active particle's motion is non-stationary and non-ergodic process having the out-of-equilibrium steady state. Our results can give an insight into related problems such as the active diffusion of the particle in a polymeric network.

### Keywords:

Generalized Langevin equation, Anomalous diffusion, Fluctuation-Dissipation theorem, Ergodicity breaking, Polymeric network

## Analytical results for power and efficiency of active Brownian heat engine

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### Abstract:

Recent experiments have reported that, by utilizing active particles as working substance, colloidal heat engines can apparently achieve a super-Carnot efficiency. To obtain a full thermodynamic picture of how such engines operate, we have introduced a simple, thermodynamically consistent model of an active dimer driven by a chemical fuel, whose composite efficiency accounting for both dissipated heat and chemical work is bounded from above by the second law of thermodynamics. In this talk, we present a few analytical results regarding the properties of the composite efficiency. First, we show that the maximum composite efficiency is unattainable at finite power due to the entropic bounds of energetic currents, ruling out the realizability of the so-called "dream engine". Second, we examine how the efficiency at maximum power (EMP) depends on the thermodynamic forces driving the system out of equilibrium. Of particular interest is the effects of the parity of the self-propulsion force. Finally, based on these observations, we discuss design principles which optimize the engine's performance under prescribed spatiotemporal scale and self-propulsion mechanism.

### Keywords:

active matter, heat engine, efficiency, efficiency at maximum power, stochastic thermodynamics

## Correlation between concurrence and mutual information

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### Abstract:

We investigate a two-qubit system to understand the relationship between concurrence and mutual information, where the former determines the amount of quantum entanglement, whereas the latter is its classical residue after performing local projective measurement. For a given ensemble of random pure states, in which the values of concurrence are uniformly distributed, we calculate the joint probability of concurrence and mutual information. Although zero mutual information is the most probable in the uniform ensemble, we find positive correlation between the classical information and concurrence. It suggests that the destructive measurement of classical information can be used to assess the amount of quantum information.

### Keywords:

entanglement, concurrence, mutual information, quantum information

## Continuous phase transition in Brownian Potts Model: Suppression of phase coexistence by particle diffusion

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### Abstract:

We investigate the phase transitions of the  $q$ -state Brownian Potts model in two dimensions (2d) comprising Potts spins that interact ferromagnetically with other spins within a fixed distance and diffuse like Brownian particles.

With extensive Monte Carlo simulations, we find that the Brownian Potts model undergoes a continuous phase transition even for  $q > 4$ .

This is contrasted with a discontinuous phase transition in the equilibrium Potts model with  $q > 4$  in 2d lattices.

In order to understand the absence of phase coexistence, we compare the time scales associated with density fluctuations and spin fluctuations.

Based on the time scale comparison, we present a theoretical argument for the absence of phase coexistence.

### Keywords:

phase transition, Potts model, Brownian motion

# Upgrading performance of Quantum Network by using Hypergraph

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## Abstract:

Research on communication that exchanges information with each other using quantum entanglement is being actively implemented.

In order to constantly perform quantum communication, it is very important to maintain quantum entanglement stably. However, quantum entanglement is very sensitive to the external environment and is easily broken even by very small shocks, so it cannot implement or maintain a perfect quantum entanglement state in real system. So we need to investigate how quantum communication will be performed in a situation where quantum entanglement is somewhat broken.

The degree to which information can be transmitted through quantum communication depends on the degree to which quantum entanglement is broken. Therefore, the important topic here is to propose a efficient structure that enables quantum communication in globally even though quantum entanglement is broken locally. Therefore, many researchers have conducted research on structures like as network or graph in which quantum communication is possible globally in network even though there are regions where quantum communication is not possible locally due to breaking of quantum entanglement state. By using the properties of percolation transition, many studies show that even if quantum entanglement is broken locally a lot, quantum communication is possible through out a whole network.

A recent paper published by Nature Physics in 2014 revealed that quantum communication is possible globally even if quantum entanglement is more broken when we conduct quantum communication on multiplex networks. In this presentation, I would like to show that hypergraphs structures are much more efficient than multiplex networks in quantum communication.

## Keywords:

LOCC, Entanglement State, Quantum Network, Hypergraph

## 최덕인 교수님을 기리며

최은하\*1

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### Abstract:

최덕인 교수님께서 2000년, KAIST 에서 퇴임한 이후, 광운대학교의 플라즈마 연구개발 및 교육에 거의 20년 동안 힘쓰신 자취와 더불어 후학의 양성에 힘쓰신 업적을 살펴보고자 한다. 2004년 12. -2009. 12. 기간에는 PDP 공동연구 기반센터의 설립 및 운영에 자문위원으로서 기업체간의 산학협력연구의 중요성을 강조하여, PDP 연구의 핵심기관으로 성장하게 하였다. 2010. 8- 2017. 12. 및 2016.8.- 2022. 1 기간에는 광운대학교의 SRC 우수연구센터인 "플라즈마바이오효리연구센터 (PBRC)" 및 독일 라이프니츠 저온플라즈마연구소 (INP)의 해외우수연구소 유치사업인 "응용플라즈마의과학센터 (APMC)" 의 운영위원 및 기술자문위원으로서 플라즈마 바이오효리 및 의학의 플라즈마 연구에 많은 관심 및 조언을 아끼지 않으셨다. 또한 2021. 6- 2030. 12 기간의 대학중점연구소 "플라즈마 바이오효리 및 환경연구" 에 많은 격려와 좋은 말씀으로 이끌어 주셨으며, 올해 2022년 3월28일에 별세하셨다.

최덕인 교수님은 광운대학교를 포함한 광운학원의 재단이사로서 2011. 3-2015. 2. 기간에 대학 및 관련부속학교의 교육 및 발전에 지대한 공헌을 하셨으며, 이때 광운대학교의 과학기술 및 교육의 방향에 큰 기틀이 잡혔다. 1992년에 설립된 광운대학교의 대전입자빔 및 플라즈마 연구실은, 신희명 교수님 (서울대학교 1996년 은퇴, 2012년 8월 별세)의 1997. 8-2012.12 의 15년 동안 전자빔의 고출력 마이크로파 발생기술, 이자현 교수님 (2020. 2. 별세) 의 플라즈마 포커스의 EUV 기술 및 자문, 그리고 최덕인 교수님 (2022. 3 별세)의 플라즈마 연구의 큰 가르침에 발전하게 되었으며, 이제 우리 플라즈마 과학계는 큰 스승을 잃었다. 특히 최덕인 교수님은 2004. 12. 부터 설립된 광운대학교 플라즈마 실험실 PDP 연구센터, 플라즈마바이오효리연구센터 (PBRC), 응용플라즈마의과학센터 (APMC)" 및 플라즈마바이오효리연구소(PBRC)의 발전 및 어려움을 모두 지켜보셨으며, . 이에 힘입어 제자 및 제자의 제자에 이르는 후학들이 현재 열심히 일하고 있다. 이와 같은 위대한 스승들은 우리 제자들에게 무언의 애뜻한 사랑을 많이 베풀셨으며, 이에 우리 후학 및 제자들은 어떻게 이 고마움을 제대로 표현할지 모르겠고, 또한 깊은 아쉬움 및 슬픔을 이겨낼지 모르겠다.

## 우리나라 핵융합 연구에서 고 최덕인 교수님의 업적 - 플라즈마 불안정성 및 난류 연구와 KSTAR 프로그램을 중심으로

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### Abstract:

본 발표에서는 고 최덕인 교수님께서 우리나라 핵융합 연구에 기여한 바를 살펴보고자 한다. 핵융합 장치의 성능을 결정짓는 플라즈마의 미세 불안정성과 난류 연구에서 고 최덕인 교수님을 중심으로 한 연구자들이 여러 중요한 기여를 하였다. 토카막에서 발생하는 ITG(Ion Temperature Gradient) 모드, RBM(Resistive Ballooning Mode) 등 핵심 불안정성 현상의 물리적 성질 규명에서부터 현대 핵융합 플라즈마 난류 시뮬레이션의 근간을 이루는 자기선회동역학 모델 개발에 이르기까지 고 최덕인 교수님이 핵융합 연구에 기여한 바를 살펴보고자 한다. 더불어 관련 연구가 현재 핵융합 연구의 최전선에서 활용되는 모습 또한 살펴본다. 고 최덕인 교수님께서서는 핵융합 이론 연구와 더불어 KSTAR와 같은 우리나라의 핵심 핵융합 연구 프로그램에도 기여하신 바가 크다. 관련한 업적을 미래 전망과 더불어 살펴보고자 한다.

## 핵융합로 재질의 수소동위원소 permeation 및 retention 연구와 노승정교수

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### Abstract:

1979년 당시 서울대학교 대학원 원자핵공학과 석사과정생 노승정은 (고) 정기형 교수님의 지도하에 박사과정생 (고) 인상렬과 함께 SNUT-79 개발에 참여한 것을 계기로 핵융합 연구와 인연을 맺게 되었다. 1994년 단국대학교 응용물리학과 교수로 부임한 이후 연구와 후학양성에 매진하여 반도체, 플라즈마, 핵융합 분야에 우수한 연구성과를 창출하였다. 교내에서는 교육행정가로서 자연과학대학장을 교외에서는 과학행정가로서 한국연구재단 핵융합단장, 거대과학단장, 국책연구본부장을 겸임하였고 한국물리학회 이사, 한국가속기및플라즈마연구협회 회장, 한국핵융합대학협의회 회장, 한국양성자가속기이용자협의회 회장 등을 역임하며 온화한 품격과 리더십으로 관련분야의 발전에 기여하였다. 또 대중적인 과학저술가로서 나노 테크놀러지 관련서적이 문화관광부 추천 기술과학 교양도서로 지정된 바 있으며 다양한 분야의 발명가로서 반도체, 가속기, 핵융합 관련분야의 특허를 다수 출원등록하였다. 특히 핵융합로 재질의 수소동위원소 permeation 및 retention 연구에 대하여 독보적인 연구성과를 이룩하였다. 노승정교수의 정년퇴임을 맞이하여 그간의 학문적 업적을 기리며 교육과 연구외길의 인생을 감사의 마음을 담아 조명한다.

### Keywords:

노승정 교수, 핵융합, 수소동위원소, permeation

## Direct writing of structural-color graphics with colloidal photonic inks

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### Abstract:

Nature has created regular nanostructures to develop structural colors for communication, camouflage, or mating competition. Ordered colloidal arrays have been used to artificially produce structurally-colored materials. The structural colors are iridescent, tunable, nonfading, and nontoxic, unlike chemical pigments, which makes them useful for various applications. However, it is challenging to produce high-quality structural-color patterns practically. Here, we report a pragmatic approach to producing single- and multi-colored structural-color graphics through direct writing with photocurable colloidal inks. The inks are formulated by dispersing silica particles in carefully-selected photocurable resins at optimum volume fractions to satisfy rheological properties for the direct writing and spontaneously produce ordered arrays of colloidal particles for structural coloration. The optimized inks are dispensed from a nozzle by applying pneumatic pressure while the nozzle moves along the predefined trajectory to deposit the ink on a target surface. The inks show shear-thinning and fast thixotropic relaxation, which secures ease of dispensing and high resolution of line drawing. The controlled fusion of the line segments produces faces. The fusion causes the shear flow in the deposited inks along the direction perpendicular to the drawing, which induces the reorganization of the particle arrangement to have a uniform direction of the crystalline lattice, improving the reflectivity up to 90%. Moreover, the inks do not allow the mixing at the boundary of two different inks due to their high viscosity, which enables the production of multi-color graphics by single-step photocuring. Direct writing can be done on various target surfaces, including plastic, glass, metals, and even papers and fabrics. The high mechanical stability of the printed graphics allows the surface transfer and origami-folding. We believe this direct writing method potentially serves as a pragmatic means to create customized structural-color graphics with an unprecedented level of controllability.

### Keywords:

colloids, crystals, glasses, photonic bandgap, diffraction

## Structural color as a tool to investigate structure and formation pathways of colloidal clusters

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### Abstract:

The spontaneous organization of individual building blocks into ordered structures is extensively used in nature and found at all length scales, from crystallization processes, via composite materials, to living cells constituting complex tissue. Understanding the relationship between building blocks, environmental conditions, and resulting structure is of fundamental importance for controlling materials properties. Confining elements imposed upon the self-organizing particles can significantly alter the assembly process and may lead to entirely different crystals. Emulsion droplets are interesting confinements in that respect, as the spherical nature prevents the formation of periodic structures by introducing boundaries and curvature.

Here, we explore the surprising diversity of crystal structures and symmetries that can form in this confining element. We create a phase diagram of observed crystal phases in dependence of the number of colloidal particles within the confinement and support our model by event-driven molecular dynamics simulations of hard-spheres in a spherical confinement.

A key challenge to characterize such confined self-assembly processes and understand the formation pathways in detail is to gain insights into the internal structure and order. Electron tomography can provide highly accurate reconstructions, but is time-consuming and requires sophisticated instrumentation and expertise. To overcome this limitation, we take advantage of the structural coloration that can be observed in such colloidal clusters. Since the optical pathways in a light microscope only collect light that is reflected (near) parallel to the optical axes, colloidal clusters with defined symmetries show characteristic, anisotropic color patterns. These color patterns allow a facile identification of the internal structure of such clusters and, importantly, can be used to observe the formation pathway of the clusters in situ.

## Creating Photonic Architectures by Nanoimprinting Unconventional Materials

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### Abstract:

Photonic and plasmonic architectures can concentrate the electric field through resonances, increase the light optical path by strong diffraction and exhibit many other interesting optical phenomena that cannot be achieved with traditional lenses and mirrors. The use of these structures within actual devices will be most beneficial for enhanced light absorption solar cells, photodetectors and improved new sensors and light emitters. However, emerging optoelectronic devices rely on large area and low cost fabrication routes to cut manufacturing expenses and increase the production throughput. If the exciting properties exhibited photonic structures are to be implemented in these devices then, they too have to be processed in a similar fashion as the devices they intend to improve.

In this presentation, I will illustrate how the technique of soft nanoimprinting lithography provides an exciting opportunity for the fabrication of nanostructures in a scalable, fast and inexpensive way. In our group, we use pre-patterned soft elastomeric stamps to induce a nanostructure onto a variety materials such as conductive polymers<sup>1</sup> and cellulose<sup>2</sup>. We also use our patterned stamps to induce the long range ordering of metal colloids<sup>3,4</sup> and perovskite nanocrystals<sup>5</sup> in what is known as template induced self assembly. In all cases, the resulting photonic architectures can exhibit a resolution below 100 nm while covering an area of 1 cm<sup>2</sup>. This fabrication route allows us to combine the photonic properties of the pattern with those of the original material resulting in a new generation of inexpensive photonic components such as biodegradable photonic films, highly efficient SERS platforms for sensing, chiral metamaterials, improved efficiency solar cells and more.

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## Manipulating light and color with soft and structured matter

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### **Abstract:**

Investigations of nature's most fascinating light manipulation strategies can inspire design concepts for synthetic, hierarchically structured, functional optical materials and devices. While soft and fluid matter frequently enables tunable and stimuli-responsive optical characteristics in biological photonic systems, soft and fluid components still represent an underutilized class of materials in the optical engineers' toolbox. My group tries to understand how organisms grow and form light-manipulating material architectures to translate useful biological design concepts into bioinspired dynamic optical materials. In this presentation, I will briefly discuss our efforts on visualizing butterfly scale structure formation and will then focus on the manufacture of bio-inspired dynamic photonic materials with nano-scale feature control and macroscale area throughput.

## Contextual advantages and certification for maximum confidence discrimination

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### Abstract:

One of the most fundamental results in quantum information theory is that no measurement can perfectly discriminate between non-orthogonal quantum states. In this work, we investigate quantum advantages for discrimination tasks over noncontextual theories by considering a maximum confidence measurement that unifies different strategies of quantum state discrimination, including minimum-error and unambiguous discrimination. We first show that maximum confidence discrimination, as well as unambiguous discrimination, contains contextual advantages. We then consider a semi-device independent scenario of certifying maximum confidence measurement. The scenario naturally contains undetected events, making it a natural setting to explore maximum confidence measurements. We show that the certified maximum confidence in quantum theory also contains contextual advantages. Our results establish how the advantages of quantum theory over a classical model may appear in a realistic scenario of a discrimination task

### Keywords:

Quantum information, Quantum foundation, Quantum state discrimination

## Detecting Entanglement Generating Circuits in Cloud-Based Quantum Computing

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### Abstract:

Entanglement, a direct consequence of elementary quantum gates such as controlled-NOT or Toffoli gates, is a key resource that leads to quantum advantages. In this work, we establish the framework of certifying entanglement generation in cloud-based quantum computing services. Namely, we present the construction of quantum circuits that certify entanglement generation in a circuit-based quantum computing model. The framework relaxes the assumption of the so-called qubit allocation, which is the step in a cloud service to relate physical qubits in hardware to a circuit proposed by a user. Consequently, the certification is valid no matter how unsuccessful qubit allocations may be in cloud computing or how untrustful the service may be in qubit allocations. We then demonstrate the certification of entanglement generation on two and three qubits in the IBMQ and IonQ services. Remarkably, entanglement generation is successfully certified in the IonQ service that does not provide a command of qubit allocations. The capabilities of entanglement generation in the circuits of IBMQ and IonQ are also quantified. We envisage that the proposed framework is applied when cloud-based quantum computing services are exploited for practical computation and information tasks, for which our results would find if it is possible to achieve quantum advantages.

### Keywords:

cloud-based quantum computing, entanglement certification, qubit allocation

## Coherent Control of Motion in a Trapped Ion System

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### Abstract:

The coherent control of phonon modes is a prerequisite to utilize trapped ions for various practical quantum information applications. It enables quantum sensing [1], quantum logic spectroscopy [2], analog simulation of quantum systems [3], and universal quantum computation [4]. While the spin degree of freedom of a trapped ion qubit can be relatively easily controlled, manipulation of its motion is more challenging, as it usually requires coherent laser fields, good understanding of micromotion, and low heating rate.

In this presentation, we discuss the current status of our efforts towards the coherent control of the motion of an ion chain. By using a frequency comb generated by a ultraviolet pulse laser, we successfully sideband-cooled a single ion down to its motional ground state. Also, we realized spin-dependent force and observed the periodic entanglement and disentanglement of an ion's spin and motional states. Lastly, a preliminary result of the implementation of Mølmer-Sørensen interaction in a two-ion chain will be presented.

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### Keywords:

Quantum Information, Quantum Computing, Trapped Ion, Atomic Physics

## Interpretable Shadow Neural Network for Entangled Many-Body States

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### Abstract:

Classical shadows provide a succinct classical description of quantum many-body states, reducing the cost for quantum simulations and computations on near-term quantum devices. Here we show classical shadows, when used as datasets for various machine learning architectures, can be used to classify quantum states and identify their classifying features. Several numerical experiments are conducted, including symmetry-breaking transitions, topological order, spin liquids, and measurement-induced entanglement phase transitions, identifying features such as order parameters and quantum information measures.

### Keywords:

Machine Learning, Quantum Simulation, Phase Transitions, Topological Order, Toric Code

# Maximum-Independent-Set Experiments with Random Arrays of Rydberg Atoms

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## Abstract:

Artificial quantum many-body systems are being expected to revolutionize the humankind's computational capability from digital computing to probabilistic Turing computing. There are experimental efforts to challenge NP-hard combinatorial problems with currently available noisy-intermediate-scale quantum systems, among which the Maximum-Independent-Set (MIS) problem is proposed and experimentally tested for Rydberg-atom arrays [1,2]. Here we present our 9-by-23 grid-graph quantum simulation experiments for MIS problems. Up to 136 atoms are randomly captured and their many-body ground states, which intrinsically correspond to the MIS solution, are probed by a quantum annealing method. We obtain experimental results of total 1285245 events of up to 123 qubits on various grid graphs. Statistical analysis reveals that the necessary measurement cycle to obtain the MIS size of a specific graph within finite confidence is given linear to the size of the graph. This means that hypothetically a perfect Rydberg system can compute 100-qubit-scale graphs within one hour and a 10,000-qubit-scale graphs within a few days.

## Keywords:

Rydberg atom, Quantum computing, Quantum annealing

## A fast quantum algorithm for computing matrix permanent

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### Abstract:

In my talk, I will present the first polynomial-time quantum algorithm for computing permanents of arbitrary  $N$ -dimensional square matrices. We transformed the well-known classical algorithm, Ryser's formula, computing a matrix permanent with an exponential cost to sums of quantum amplitudes to develop the quantum algorithm. It requires  $O(N)$  or  $O(N^3)$  independent quantum circuits, respectively for real or complex matrices, composed of  $2N+1$  qubits and a quadratic number of CNOT gates and depth to approximate permanents with additive errors. Depending on the size of a matrix norm of interest, we can obtain an exponentially small additive error estimation and a better estimation against the Gurvits' classical bounded-error probabilistic polynomial time (BPP) algorithm. Moreover, our quantum algorithm directly connected the boson sampling and the instantaneous quantum polynomial (IQP) problems by invoking the quantum Ising Hamiltonian propagators.

### Keywords:

quantum algorithm, matrix permanent

## Trapping Yb ions in a segmented-blade linear trap

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### Abstract:

본 발표에서는 분할된 날(segmented-blade) 형태의 ion trap 장치 개발과 이를 이용한 이터븀 이온 포획 과정에 대하여 보고한다. 포획 장치를 구성하는 전극의 제작은 알루미늄 세라믹을 수 마이크로미터의 분해능으로 레이저 미세 가공 후 금 증착 및 전해 도금 공정을 거쳐 완성하였다. 이후 4개의 날을 초고진공 챔버 내부에 정렬하였으며, 기존의 분할된 날 구조의 이온 트랩에 전극을 추가적으로 설치하여 다른 장치들과 이온의 미세운동 보상 방식에서 차별성을 두었다 [1]. 이러한 실험 장치에서  $^{174}\text{Yb}^+$  포획에 성공하였고, 이를 이용한 앞으로의 계획에 대해 논의한다.

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\*These authors contributed equally to this work

### Keywords:

Ion Trap, Quantum Computing

## Quantum simulation of 2D arranged Platonic graph Ising spins

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### Abstract:

There is a growing interest in using quantum simulation to find the ground states of complex quantum systems. Here we present Rydberg-atom experiments performed for Ising ground states of Platonic graphs. A direct physical implementation of the three-dimensional Ising-spin structures is experimentally daunting. Instead, we use quantum wires [1-3] to conduct topology-preserving transformations of the structures from 3D to 2D. The quantum wires maintain the qubit connectivities of the flattened structures. In experiments, we construct three Platonic graphs, tetrahedron, cube, and octahedron, with up to twenty atoms. The probability distributions of the graphs are measured to obtain their ground state spin configurations, which are verified by numerical simulations. The result agrees well with the expected solutions of the graphs.

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### Keywords:

Quantum simulation, Platonic graph, Quantum annealing

## Rydberg wire gates for universal quantum computation

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### Abstract:

Rydberg atom arrays offer flexible geometries and topologies of strongly-interacting neutral atoms, useful for quantum applications including quantum simulation and quantum computation [1, 2]. One drawback of Rydberg atoms in quantum computing applications is the short-ranged interactions. Here we utilize quantum wires to overcome the given drawback by coupling remote atoms, which are not directly adjacent with each other. For example, the CNOT gate between two qubit atoms is constructed by a sequence of individual atom addressing area pulses of the qubit atoms and in-between wire atoms [3]. We construct standard one-, two-, and multi-qubit gates for universal quantum computation. Furthermore, we provide a detailed resource estimate for an experimental implementation of the gates of this scheme for Rydberg-atom arrays.

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### Keywords:

Rydberg atom, Quantum Computation, Quantum gates, CNOT, Toffoli

## Perovskite Semiconductors for Photonics and Polaritonics

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### Abstract:

Halide perovskite semiconductors exhibit exceptional optical gain properties, large oscillator strength and high external quantum efficiency, thus they have shown tremendous potentials in a wide range of photonic and optoelectronic applications, such as solar cells, light-emitting diodes, photodetectors, and nanophotonics. In 2D hybrid perovskites and some 3D all inorganic perovskite systems, robust exciton formation at room temperature has been recognized, suggesting a bright future for strong light-matter coupling towards room-temperature polaritonics. We will present an exciting journey in the discovery of exciton polariton in perovskite semiconductor microcavities, resulted from a strong light-matter coupling. Particularly we will discuss recently progress in polariton laser and condensate, nonlinear properties and quantum optics control based on artificial potential landscapes, demonstrating the significant promise in future photonics, polaritonics and integrated photonic devices based on those new quasiparticles.

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### Keywords:

Perovskite, Polariton, Photonics

## Direct polariton coupling in single hexagonal microcavity at room temperature

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### Abstract:

It has been known that parity–time reversal (PT) symmetry in non-Hermitian systems realizes spontaneous symmetry breaking. To introduce PT symmetry into a photonic system, a coupled system with antisymmetric gain/loss profiles is necessary. Owing to non-interactive nature of photons, two or more photonic components have been used for the indirect coupling via near-fields. Meanwhile, exciton-polaritons formed in a semiconductor microcavity can condense into a coherent ground state, which can be directly interactive via excitonic components due to the hybrid nature of excitons and photons. We have shown the room-temperature polariton condensate caused by strong coupling between excitons and whispering gallery mode photons in GaN-based single hexagonal microcavity system [1, 2]. In this talk, based on this GaN-based single microcavity system, we demonstrate the room-temperature polaritonic PT symmetry, showing the lowest threshold of polariton condensates despite increasing loss [3]. The hexagonal symmetry of the GaN microrod plays an important role to use degenerated modes between upwards and downwards triangular-whispering gallery polaritons. An integration of the coupled polariton pair into the loss-manipulated substrate satisfies antisymmetric gain/loss profiles. As a result, a room-temperature polaritonic PT-symmetric system with a phase transition from unbroken to broken was achieved within a single microcavity.

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### Keywords:

Polariton, PT symmetry, GaN

# Femtosecond Dynamics of a Polariton Bosonic Cascade at Room Temperature

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## Abstract:

Whispering gallery modes in a microwire are characterized by a nearly equidistant energy spectrum. In the strong exciton–photon coupling regime, this system represents a bosonic cascade: a ladder of discrete energy levels that sustains stimulated transitions between neighboring steps. In this work, by using a femtosecond angle-resolved spectroscopic imaging technique, the ultrafast dynamics of polaritons in a bosonic cascade based on a one-dimensional ZnO whispering gallery microcavity are explicitly visualized. Clear ladder-form build-up processes from higher to lower energy branches of the polariton condensates are observed, which are well reproduced by modeling using rate equations. Remarkably, a pronounced superbunching feature, which could serve as solid evidence for bosonic cascades, is demonstrated by the measured second-order time correlation factor. In addition, the nonlinear polariton parametric scattering dynamics on a time scale of hundreds of femtoseconds are revealed. Our understandings pave the way toward ultrafast coherent control of polaritons at room temperature.

## Reference:

Fei Chen, Hang Zhou et al, Nano Lett. 22, 2023-2029 (2022)

## Keywords:

Polariton, Ultrafast dynamics, Bosonic cascade

## Tip-enhanced cavity-spectroscopy

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### Abstract:

Plasmonic nano-cavity enables to induce light-matter interactions and tip-enhanced nano-spectroscopy enables to probe them at the nanoscale. However, these two approaches have developed independently with their own weaknesses so far. In this talk, I provide a novel concept of "tip-enhanced cavity-spectroscopy (TECS)" overcoming the limitations of previous approaches to induce, probe, and dynamically control ultrastrong light-matter interactions in the quantum tunneling regime. Furthermore, I provide several new directions of nano-spectroscopy and -imaging. First, we exploit extremely high tip-pressure (~GPa scale) to directly modify the lattice structure and electronic properties of materials. Second, we dynamically control the near-field polarization by adopting adaptive optics technique to near-field optics. Third, we develop conductive TECS to modify electrical properties of materials by directly flowing an electric current through the cavity junction.

### Keywords:

tip-enhanced cavity-spectroscopy, TECS, plasmonic nano-cavity, tip-enhanced nano-spectroscopy

## Resonant tunneling through twisted black phosphorus heterostructures

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### Abstract:

The advent of atomically thin 2D material's heterostructures open new opportunities for rethinking conventional semiconductors heterostructure devices. In this work, we explored electronic transport in heterostructures based on anisotropic material, black phosphorus, and demonstrate the unprecedented degree of control that the relative stacking twist angle between anisotropic layers has on the vertical transport behavior, i.e. from Ohmic to tunneling regime. Utilizing high quality heterostructures made of orthogonally stacked anisotropic black phosphorus multilayers, we demonstrate resonant tunneling through quantum well states without the need of any physical tunneling materials, hence achieving the largest tunneling conductance and peak-to-valley ratio in negative differential resistance characteristics reported for resonant tunnel diodes based on van der Waals heterostructures. Hence, our work advances a new approach to realize RTD devices with twisted anisotropic vdW materials, without the need of any high-bandgap barriers.

### Keywords:

Black phosphorus, Twisted stack, Resonant tunneling diode

# Strain-induced electronic structure and functionality changes in MoTe<sub>2</sub> - Understanding the nanomechanical underlying mechanisms governing strain engineering

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## Abstract:

Two-dimensional (2D) materials offer technologically relevant properties such as strong light–matter interactions and tunability of their electronic structure. For example, the band gap of MoTe<sub>2</sub> can be modulated by 0.2 eV through the application of linear strain [1], which can potentially enable applications based on technologically relevant light wavelengths. In the past, changes in electronic structure have also been demonstrated in other 2D materials, such as in the reversible generation of quantum dots in graphene through application of axisymmetric strain via a scanning tunneling microscope probe [2]. Strain engineering thus offers opportunities for designing new and exotic nanoelectronic systems. However, the determination and application of the appropriate strain field on specific discrete 2D structures is by no means a trivial matter. In the above studies strain has emerged naturally from the experimental geometry, offering little control and therefore little opportunity for precise engineering design. This talk discusses the two mechanisms for strain generation introduced above for graphene and MoTe<sub>2</sub>, as well as the prospects for more intricate strain designs enabled by, (i) understanding of the fundamental quantitative relationships between strain changes and electronic structure changes, as well as (ii) harnessing of specific nanoscale mechanical behaviors [3].

[1] Maiti, R. et al., Nature Photonics 14, 578 (2020).

[2] Klimov, N.K. et al., Science 336, 1557 (2012).

[3] Solares, S.D. and Blanco, M., Nanotechnology 15, 1405 (2004).

## Keywords:

2D materials, strain generation, electronic structure, graphene, MoTe

## Epitaxial growth, exfoliation, and heterostructuring of complex-oxide membranes

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### Abstract:

Remote epitaxy, a recent discovery allowing epitaxial growth of thin films on single-crystalline substrates through graphene, has clearly shown that the utility of graphene goes far beyond the established applications. This novel process allows creation of freestanding and flexible single-crystalline membranes of exotic materials not possible previously. In particular, complex-oxide materials exhibit many desirable physical properties that can advance conventional electronics, photonics, and quantum devices. Moreover, the combination of two or more of these materials could lead to a discovery of new physical coupling phenomena and functionalities. However, monolithic growth of dissimilar single-crystalline complex-oxide films have been impossible due to the widely different crystalline lattice structure as well as the thermal budget.

To solve these restrictions, we carried out and optimized remote epitaxial process of complex-oxide materials and succeeded in producing freestanding single-crystalline membranes with crystalline structures such as perovskite, spinel, and garnet. Moreover, we were able to artificially integrate two very dissimilar complex-oxide membranes together via a simple transfer process, creating new heterostructures consisting of 2D and 3D materials. We hope such demonstration of artificial 3D-3D and 2D-3D heterostructures will open up a new playground for material scientists, physicist, and device engineers to explore these materials with unrestricted manipulation and integration possibilities.

### Keywords:

Remote epitaxy, complex-oxide, epitaxial lift-off, heterogeneous integration

## Current Status and Challenges in Genome Editing

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### Abstract:

Genome editing tools such as ZFNs, TALENs, and CRISPR-Cas9/Cas12/Cas13 derived RNA-guided endonucleases have been broadly used for biomedical research, biotechnology, and plant transformation. CRISPR nucleases are widely exploited due to the ease of use and inexpensive cost; researchers can induce gene editing at different sites by simply altering guide RNAs. Ultimately, the Nobel Prize in Chemistry 2020 was awarded for discovering one of gene technology's sharpest tools. However, CRISPR-mediated DNA double-stranded breaks (DSBs) frequently cause unexpected large chromosomal deletions or genomic rearrangements, and also induce the p53-mediated DNA damage response. In parallel, new genome editing tools are constantly being developed. DNA base editing tools, including cytosine base editors (CBEs) and adenine base editors (ABEs), enable the direct conversion of DNA bases without producing DNA DSBs were developed. Furthermore, a prime editor (PE) that enables generating small insertion and deletion in addition to substitution of several nucleotides at target sites, was recently developed. While the gene editing mechanism is different for each tool, all tools have been developed based on the CRISPR effectors. Here I present current trends in genome editing tools along with on-going studies of my group such as development of web-based programs in CRISPR RGEN Tools ([www.rgenome.net](http://www.rgenome.net)), protein engineering for enhancing specificity of base editors, and versatile application of genome editing tools for plant transformation and gene editing therapy in vivo and ex vivo.

### Keywords:

CRISPR, Genome editing, Base editing, Prime editing, Gene therapy

## Self-sufficient minimalism in CRISPR technology: Target with TaRGET

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### Abstract:

In spite of the developments and advancements of CRISPR technology, the present CRISPR system shows several hurdles in the clinical applications, which include patent wars between patent holders, risks in safety aspect and limitations in viral delivery. Here we introduce a new genome-editing platform, Transposase B/augment RNA-based Genome Editng Technology, termed TaRGET. We uses TnpB instead of Cas9, which is an ancestral protein for type V Cas proteins together with an engineered guide RNA, named an augment RNA. TaRGET is a self-sufficient minimalist in genome-editing technology due to its deliverability, high efficiency, persistency, high safety, and expandability. The expandability is associated with hyper-compactness of the TaRGET system, which we leveraged to create an AAV-deliverable adenine base editing system. The TaRGET-ABE system allows specific, and flexible base editing via AAV delivery *in vitro* as well as *in vivo*. We expect that these hypercompact toolsets would harness the development of *in vivo* gene-editing therapy and thus offer hope in life for patients with various genetic defects.

### Keywords:

AAV, CRISPR, Gene therapy, Genome editing, TaRGET

## **Predicting the Efficiencies and Outcomes of Genome Editing and time-recording using Cas9**

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### **Abstract:**

We developed high-throughput methods for evaluating activities of AsCas12a, SpCas9 including the high-fidelity or protospacer-adjacent motif variants, base editors, and prime editor 2. Based on the large data sets of these genome editing tool activities, we developed computational models that predict the activities and, in some cases, editing outcomes of these genome editing tools based on target sequence composition in mammalian cells. In addition, we recently recorded elapsed time using the indel generation by Cas9 and guide RNAs. As applications of this time-recording system, we recorded the duration of chemical exposure and the lengths of elapsed time since the onset of biological events (e.g., heat exposure and inflammation) by combining event-responsive Cre expression systems.

### **Keywords:**

genome editing, CRISPR, base editors, prime editors, deep learning

## In vivo Genome Editing for Vision

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### Abstract:

From the FDA approval of anti-VEGF aptamer to wet-type age-related macular degeneration (AMD) of choroidal neovascularization, anti-VEGF aptamer and antibody have been widely used against all kinds of vaso-proliferative retinopathy. Actually, current therapies directed at controlling vascular abnormalities in vaso-proliferative retinopathy target VEGF and can slow the progression of these diseases. While the general role of VEGF in development has been well described, the specific function of locally synthesized VEGF in the eye is incompletely understood. Recently, RNA-guided genome surgery using CRISPR-Cas9 nucleases has shown promise for the treatment of diverse genetic diseases. Yet, the potential of such nucleases for therapeutic applications in non-genetic diseases including AMD, diabetic retinopathy (DR) as well as retinopathy of prematurity (ROP) is largely unexplored. Those vision-threatening retinopathies such as AMD, DR, and ROP are leading causes of blindness in adults and children, which is associated with retinal over-expression of, rather than mutations in, the VEGFA gene.

Herein I would like to provide some my recent experimental results of therapeutic applications such as small peptide, small molecule as well as nanoparticles beyond anti-VEGF antibody. In addition, some results of *in vivo* genome editing in vision-threatening retinopathy would be provided.

### Keywords:

Eye, Genome editing, In vivo, Retinopathy, Vision

## 주요국가의 핵융합 연구개발 동향

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### Abstract:

탄소중립을 위한 다양한 기술 중에 핵융합에너지는 중장기 기술로써 각광을 받고 있다. 특히 최근에는 북미 권역에서 스타트업을 중심으로 하는 핵융합 분야의 조기 상용화에 대한 관심이 높다. 또한 영국도 탄소중립 기술로써 2040년까지 핵융합 상용화를 최초로 달성하는 국가가 된다는 목표를 설정하고 공격적 투자를 진행하고 있다. 미국, 영국, 중국, 일본, EU 등 주요국가의 핵융합 연구개발 정책과 투자 동향을 알아보고 한국의 상황도 점검한다.

### Keywords:

핵융합, 주요국가, 동향

# Global Trends on Non-Electric Application using SMR for Carbon Neutrality

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## Abstract:

In the fossil fuel age, most of nuclear power has produced electricity by large Light Water Reactor (LWR). For carbon neutralization, nuclear energy should be utilized not only for electricity generation but also for hydrogen and industrial heat production. Currently, the advanced nuclear countries are developing various non-LWR Small Modular Reactors (SMRs), which have a higher operating temperature than existing LWRs. Especially, a Very High Temperature gas-cooled Reactor (VHTR) is a helium-cooled reactor whose outlet temperature is above 700 °C. Its high temperature heat can be applied to the various industrial areas including massive hydrogen production. VHTR had always attracted attention as an alternative to fossil fuels in the era of high oil prices such as the 1970s and 2000s. Each time, it was intensively studied as the alternative energy for fossil fuel combustion. Recently, the Paris agreement and carbon dioxide emission regulations are increasing interest in nuclear heat as alternative energy although low oil prices due to shale gas. Therefore, unlike in the past, the heat energy from SMRs should be used to stop using fossil fuels regardless of the low oil price. This presentation will introduce non-LWR SMRs for non-electric applications and their recent global trends.

## Keywords:

SMR (Small modular Reactor), non-electric applications, Very High Temperature gas-cooled Reactor (VHTR), Carbon Neutrality

## Catalyst Designs and Nanoarchitecture for Hydrogen and Fuel Cell Applications

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### **Abstract:**

A variety of novel composite materials have been used/tested for next-generation energy conversion devices. However, in many cases little is known about their properties and performance, although such fundamental understanding is essential for further advances in energy conversion technologies. Experiments may yield many clues to the behavior of those materials, but the interpretations are often controversial due largely to the difficulty of direct characterization. Under such circumstances, first principles-based computational approaches have emerged as one of the most powerful tools for design and development of new energy materials. This talk will focus on introducing our ongoing efforts in first principles modeling of energy conversion materials. In the first part of my talk, I will discuss the properties and performance of Pt-based nanomaterials and composites PEMFCs, particularly the dissolution mechanisms of Pt-based nanomaterials near the surface and interface, with comparisons to those in bulk Pt, as well as the surface and interface effects on the anode and cathode performance, such as oxidation/reduction reaction rate and stability. In the second part, I will present recent progress in our collaborative theoretical and experimental efforts to explore electrolysis catalysts with the stability, costs, and abundance for electro-powered hydrogen/oxygen production.

## 태양광 미래 기술

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### Abstract:

탄소중립을 위해서는 온실가스를 배출하지 않는 무탄소 전원의 보급이 확대되어야 한다. 그리고 잉여의 무탄소 전기를 사용하여 열과 수소 등을 만들어서 건물, 수송, 제철 등 다양한 분야에 활용을 해야 한다. 따라서 기본적으로 무탄소 전원의 확대가 매우 중요하다. 태양광발전은 빛을 전기로 직접 변환하는 기술로 온실가스를 배출하지 않으며 연료비가 들지 않는다. 최근에는 대량생산 체계 확립과 기술 고도화로 경제성까지 개선되고 있으며, 가장 값싼 발전원으로 자리매김한 국가들이 늘어나고 있다. 다만 상대적으로 넓은 설치 면적이 필요하고 일사조건에 따른 불안정성을 가지고 있다. 이러한 태양광 발전의 한계는 기술 개발로 해결해야 한다.

우선 설치부지의 부족을 해결하기 위한 초고효율 태양전지 기술이 활발히 진행 중이다. 결정질 실리콘 태양전지, 화합물 박막 태양전지 등 이미 시장에 진출한 태양전지의 고효율화와 함께 페로브스카이트 등의 유무기 하이브리드 태양전지의 고효율 기술이 매우 빠르게 개발되고 있다. 그리고 각기 태양전지가 가지는 이론효율을 극복하기 위한 다중접합 태양전지 기술의 실용화도 매우 활발하게 진행되고 있다.

태양광 시스템의 측면에서는 다양한 영역에서 응용이 가능한 기술이 개발되고 있다. 농사와 발전을 병행하는 영농형 태양광, 호수 바다 등 수상위에 태양광을 설치한 수상 태양광에 대한 개발이 활발하다. 또한 건물 자재로 활용되는 건물일체형 태양광 뿐만 아니라 자동차 일체형, 도로 일체형 등 다양한 형태의 모듈과 시스템이 개발 중이다. 이를 통해 태양광 보급의 확대를 꾀할 수 있을 뿐만 아니라 새로운 시장도 개척할 수 있다.

그리고 간헐적인 태양광 발전으로 인한 계통 불안정성 문제를 극복하기 위해 다양한 형태의 에너지 저장 기술이 개발되고 있으며, 스마트 인버터 기술의 적용을 통해 계통문제 해결을 시도하고 있다. 또한 잉여의 전기를 활용하여 열, 수소 등으로 변환하는 섹터커플링 기술도 개발되고 있다.

이러한 기술들을 통해 태양광의 경제성과 활용성은 더욱더 개선될 것으로 전망되어 탄소중립을 위한 핵심 전원으로 자리매김 할 것으로 보인다. 본 발표에서는 이러한 태양광 분야의 미래기술에 대해 살펴보고 탄소중립에 대한 기여도와 함께 신산업 창출가능성에 대해 토의하고자 한다.

### Keywords:

태양광 (pv), 태양전지 (solar cells), 탄소중립 (carbon neutrality), 다중접합(multi-junction), 건물일체형 태양광 (bipv)

## Reduction of systematic error sources with rf phase-space matching in the muon g-2 experiment at Fermilab

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### Abstract:

The muon g-2 experiment at Fermilab aims to measure the magnetic anomaly of the muon to the precision of 140 parts-per-billion. Its first result, which was announced in 2021, confirmed the previous experiment at BNL, increasing the tension between the Standard Model prediction and the combined experimental average to 4.2 standard deviations. Since the systematic errors still limit the experimental sensitivity, understanding and reducing them is crucial in precision physics experiments. We developed a novel phase-space matching technique with a resonant rf electric field to reduce the systematic effects related to the beam dynamics, namely Coherent Betatron Oscillations (CBO) and muon losses. Currently, the experiment is in its fifth stage of the scientific run (Run-5) and is fully operating our rf matching technique, with which the CBO amplitude and muon losses have been reduced by approximately an order of magnitude and by a factor of 5, respectively. We highlight a preliminary estimate of the impact on the corresponding systematic uncertainties.

### Keywords:

Muon anomaly, Muon g-2, phase-space matching

## Study of $B \rightarrow \rho \gamma$ at Belle and Belle II

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### Abstract:

FCNC of B meson decays are highly sensitive to new physics beyond the Standard Model. Comparing with  $b \rightarrow s$  transition,  $b \rightarrow d$  transition has currently large experimental uncertainty due to its lower statistics. Belle II experiment, however, will decrease statistical uncertainty dramatically, and will allow us to access the new  $b \rightarrow d$  field to be explored.  $B \rightarrow \rho \gamma$  is one of the golden channels of pure  $b \rightarrow d$  transition, and thus crucial step of Belle II progress, as  $K/\pi$  identification is highly important for this study.

In this study, we plan to use Belle and Belle II combined dataset to get the world best sensitivity to  $B \rightarrow \rho \gamma$  study. The target observables are: branching ratio of charged and neutral modes ( $\mathcal{B}(\rho^+ \gamma)$  and  $\mathcal{B}(\rho^0 \gamma)$ ), isospin asymmetry ( $A_{\text{I}}$ ) and CP asymmetry ( $A_{\text{CP}}$ ). Since the CKM angle  $\phi_2$  is close to 90 degree, the isospin asymmetry of  $B \rightarrow \rho \gamma$  should be close to that of  $B \rightarrow K^* \gamma$ , while the current world average of  $A_{\text{I}}$  of  $B \rightarrow \rho \gamma$  shows a slight tension from the expectation.

Belle II experiment is now ongoing and collected  $\sim 180/\text{fb}$  data so far. We would assume 360/fb for Belle II dataset which will be collected until the summer 2022 and estimate the possible sensitivity to those observables by the study based on MC.

Main source of background come from  $ee \rightarrow qq$  events, which can be suppressed by MVA technique. In addition, combinatorial background due to  $\pi^0 (\eta) \rightarrow \gamma \gamma$ , where one of the  $\gamma$  is misidentified as primary photon, can be removed by  $\pi^0/\eta$  veto technique. Those MVA trainings are performed independently Belle and Belle II dataset to get the highest sensitivity.

Number of signal is extracted by three dimensional simultaneous fitting using beam constrained mass ( $M_{bc}$ ), energy difference of beam and B energy ( $\Delta E$ ) and invariant mass of two pions with Kaon assumption ( $M_{K\pi}$ ), among the  $B^{+}$ ,  $B^{-}$  and mixed  $B^0$  distributions of Belle and Belle II; i.e. 18 distributions are simultaneously fitted to determine  $\mathcal{B}(B^{+} \rightarrow \rho^+ \gamma)$ ,  $\mathcal{B}(B^{-} \rightarrow \rho^- \gamma)$ ,  $A_{\text{I}}$  and  $A_{\text{CP}}$ .

I will report the current status of the  $B \rightarrow \rho \gamma$  study based on MC. The optimization of MVA, fitting procedure, and the results of Toy-MC study for the sensitivity estimation will be shown.

### Keywords:

Belle, Belle II, EWP, Radiative, FCNC

## AMGA를 활용한 Belle II 분산데이터처리 시스템 연구개발

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### Abstract:

일본 KEK Belle II 실험의 분산데이터처리 시스템의 연구개발에 관한 과거, 현재 및 계획에 관하여 소개한다. Belle II 실험은 기존 Belle 실험보다 50배나 많은 데이터를 생산하고 이를 분산 컴퓨팅 위에 처리해야 하기 때문에 새로운 데이터 처리시스템이 필요하였다. 이에 여러 저장장치에 분산되어 있는 데이터의 요약정보를 관리하는 AMGA(ARDA Metadata Grid Application)라는 미들웨어를 활용하였다. 본 연구진은 KISTI에서 개발한 AMGA를 손쉽게 실험데이터에 활용할 수 있도록 본 시스템 개발을 주도하였다. 지난 10여간 MC 시뮬레이션 데이터를 생산하고 처리한 본 시스템은 가속기충돌실험이 시작됨에 맞춰 새 운영체제로 성능이 향상되었다. 또한, 2021년부터 KISTI에 Belle II 원격제어실을 구축하여 온라인뿐만 아니라 오프라인 shift인 Data production shift를 수행하여 본 시스템을 체계적으로 모니터링하며 연구개발하고 있다.

### Keywords:

가속기충돌실험, 데이터처리, 분산컴퓨팅

## Recent results on tau leptons from Belle

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### Abstract:

The Belle experiment uses  $e^+ e^-$  collision at the KEKB collider at KEK and is a very good place to study tau leptons and search for new physics beyond the Standard Model. In this presentation, we discuss recent highlights from the Belle experiment on the properties of tau leptons. The subjects we discuss will include lepton-flavor-violating  $\tau \rightarrow \ell \gamma$  decays, electric dipole moment (EDM) of  $\tau$  lepton, and rare  $B$ -meson decays to  $\tau$  in the final state, e.g.  $B^0 \rightarrow \ell^+ \tau^-$ ,  $B \rightarrow K^* \tau^+ \tau^-$ .

### Keywords:

Belle, tau lepton,  $e^+ e^-$ , EDM

## Status of the SUB-Millicharge Experiment (SUBMET)

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### Abstract:

SUB-Millicharge Experiment (SUBMET) sensitive to low-mass millicharged particles produced at the 30 GeV proton fixed-target collisions at J-PARC has been proposed. The detector is composed of long scintillators that allow the particles with a small electric charge to produce photons by ionization energy loss. With the number of protons on target of  $5 \times 10^{21}$ , the experiment is sensitive to particles with electric charge  $6 \times 10^{-5} e$  for mass less than  $0.2 \text{ GeV}/c^2$  and  $1.0 \times 10^{-3} e$  for mass less than  $1.6 \text{ GeV}/c^2$ . The status of this experiment will be discussed in this talk.

### Keywords:

millicharged particles, J-PARC, scintillator, PMT

## Studies on the detector modules for SUBMET

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### Abstract:

The detector of the SUBMET is composed of long scintillators that allow the particles with a small electric charge ( $Q$ ) to produce photons by ionization energy loss. One detector module is composed of a scintillator bar with an optically coupled PMT. The main background is expected to be due to the PMT dark current, so understanding and controlling this rate is crucial for the experiment. In addition, for the particles with  $Q < 10^{-3}e$ , a single photon is produced in the scintillator. Therefore, the PMT should have gain large enough for the identification of single photoelectrons. In this talk, the studies on the detector modules will be discussed.

### Keywords:

SUBMET, PMT, dark current, dark count rate, scintillator

## Readout system for SUBMET

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### Abstract:

The Main Ring at J-PARC provides proton spills every  $\sim 1$  s and each spill is about 5  $\mu$ s long. The goal of the readout system of SUBMET is to read the whole spill using the beam trigger provided by the accelerator. For the particles with  $Q < 10^{-3}e$ , a single photon is produced in the scintillator of the detector, so a high sample rate is required. To meet these challenging requirements, we are developing a readout system based on the Domino Ring Sampler (DRS) chip. In this talk, the result of the extensive tests on the prototype readout board will be discussed.

### Keywords:

SUBMET, readout, DRS

## Update of DUNE experiment

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### **Abstract:**

Deep Underground Neutrino Experiment(DUNE) is a long-baseline oscillation experiment that aims to measure CP violation phase and neutrino mass ordering in a single experiment. Progress in the designs and the constructions of both far detectors(FD) and near detectors(ND) and data analysis of ProtoDUNE have been collected. This talk will update the overall status of DUNE and show the recent activities and accomplishments of Korean researchers on ND and FD.

### **Keywords:**

Deep Underground Neutrino Experiment(DUNE), leptonic CP violation, neutrino oscillation

## Neutron detection and application with a novel 3D projection scintillator tracker in the DUNE

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### Abstract:

Neutrino oscillation experiments require a precise measurement of the neutrino energy. However, the kinematic detection of the final state neutron in the neutrino interaction is missing in current neutrino oscillation experiments. The missing neutron kinematic detection results in a feed-down of the detected neutrino energy compared to the true neutrino energy. A novel 3D projection scintillator tracker, which consists of a large number of optical opaque scintillator cubes, is capable of detecting the neutron kinetic energy and direction on an event-by-event basis using the time-of-flight technique thanks to the fast timing, fine granularity, and high light yield. The muon anti-neutrino interaction channels in DUNE induce neutrons in the final state predominately. With the neutron detection, the muon anti-neutrino energy can be reconstructed precisely. Furthermore, the interaction channel, such as the low-energy transfer, can provide a neutrino flux measurement due to the flat neutrino interaction cross-section. This paper shows the neutron kinematic detection performance and a low-energy transfer interaction channel study with simulation data. A quantitative flux constraint is presented with the muon anti-neutrino low-energy transfer channel.

### Keywords:

neutrino

## Update of the GBAR experiment status

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### Abstract:

The GBAR experiment aims to measure the gravitational acceleration of antihydrogen at rest. As a fundamental question, the gravitational interaction between matter and anti-matter is an interesting topic although it never has been directly measured. Using ultra-cold antihydrogen, the GBAR experiment plans to do a freefall test as a classical way. Here, I present the status of the GBAR experiment and plan during beamtime.

### Keywords:

antihydrogen, gravity

## AMoRE-I Status and Performance

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### Abstract:

AMoRE (Advanced Mo-based Rare process Experiment) is an international project to search for the neutrinoless double beta decay of  $^{100}\text{Mo}$  in enriched Mo-based scintillating crystals using metallic magnetic calorimeters in a mK-scale cryogenic system. The project aims at operating the detector in a zero-background condition to detect this extremely rare decay event in the region of interest near 3.034 MeV. The simultaneous measurement of phonon and photon signals based on the metallic magnetic calorimeter (MMC) read-outs is performed at a few tens mK temperatures to achieve a high resolution and a good background rejection. AMoRE-I, the phase following the successfully completed AMoRE-pilot, has been running with thirteen  $^{48}\text{depletedCa}^{100}\text{MoO}_4$  and five  $\text{Li}_2^{100}\text{MoO}_4$  crystals in the Yangyang underground laboratory; since the beginning of the experiment in Sep. 2020, we have accumulated more than 300 days of physics data. We present the current status of the experiment, its analysis method and the most recent performance results.

### Keywords:

AMoRE, Underground Experiment, Neutrinoless Double Beta Decay

## AMoRE-II construction at Yemilab

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### Abstract:

The AMoRE project is an experiment to search for neutrinoless double beta decay of  $^{100}\text{Mo}$  using molybdate scintillation crystals and a cryogenic detection technique. To reach the goal of this experiment, we are trying to advance the current state-of-the-art methods in background rejection, radio-pure crystal growing, and cryogenic radiation detector techniques.

This project runs the first phase, AMoRE-I, an experiment using about 6kg of crystals, and now we are preparing the final phase, AMoRE-II. AMoRE-II will be operated at the Yemilab, which is a new underground laboratory of CUP at Jeongseon, using about 200kg crystals. In this talk, the construction status of AMoRE-II in Yemilab and its schedule will be presented.

### Keywords:

neutrinoless double-beta decay, AMoRE, AMoRE-II

## Measurement of the smallest neutrino mixing angle using reactor antineutrino events with neutron capture on hydrogen at RENO

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### Abstract:

RENO has been taking data since August, 2011 and successfully measured the smallest neutrino mixing angle,  $\theta_{13}$ . The measured value is obtained from the observed reactor anti-neutrino events with neutron captures on gadolinium (n-Gd) in the target detector region. The experiment has also measured the mixing angle using an independent sample of neutron captures on hydrogen (n-H). Because of a large accidental background in the n-H sample, an improved technique has been developed to make an effective removal of the background. For example, flashing PMTs make a contribution to an accidental background against a reactor neutrino signal. By effectively removing the flashing events, we can make better extraction of the n-H reactor antineutrino signal.

In particular, the (n-H) analysis utilizes events in both target and gamma-catcher and thus obtains a larger reactor antineutrino sample, twice more than that of (n-Gd). This independent measurement provides an important cross-check on the systematic uncertainties of the n-Gd  $\theta_{13}$  measurement. In this talk, we will present a new measurement of  $\theta_{13}$  using 2800 days of n-H data.

### Keywords:

RENO, reactor neutrino, neutrino mixing angle, neutrino

## Measurement of cosmogenic $^9\text{Li}$ and $^8\text{He}$ production rates at RENO

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### Abstract:

We report the measured production rates of unstable isotopes  $^9\text{Li}$  and  $^8\text{He}$  produced by cosmic muon spallation on  $^{12}\text{C}$  using two identical detectors of the RENO experiment. Their  $\beta$ -decays accompanied by a neutron make a serious contribution to backgrounds of the inverse beta decay events in precise determination of the smallest neutrino mixing angle. The mean muon energy of its near (far) detector with an overburden of 120 (450) m.w.e. is estimated as  $33.1 \pm 2.3$  ( $73.6 \pm 4.4$ ) GeV. Based on 3100 days of data, the cosmogenic production rate of  $^9\text{Li}$ ( $^8\text{He}$ ) isotope is measured to be  $44.2 \pm 3.1$  ( $10.6 \pm 7.4$ ) per day at near detector and  $10.0 \pm 1.1$  ( $2.1 \pm 1.5$ ) per day at far detector. This corresponds to yields of  $^9\text{Li}$  ( $^8\text{He}$ ),  $4.80 \pm 0.36$  ( $1.15 \pm 0.81$ ) and  $9.9 \pm 1.1$  ( $2.1 \pm 1.5$ ) at near and far detectors, respectively, in a unit of  $10^{-8}\mu\text{--}1\text{g--}1\text{cm}^2$ . Combining the measured  $^9\text{Li}$  yields with other available underground measurements, an excellent power-law relationship of the yield with respect to the mean muon energy is found to have an exponent of  $\alpha = 0.76 \pm 0.05$ .

### Keywords:

$^9\text{Li}$ ,  $^8\text{He}$ , RENO

## Status of NEOS-II

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### Abstract:

The energy spectrum of the inverse beta decay of reactor antineutrinos has been measured for one complete fuel cycle at a 24 m distance from the Hanbit-5 reactor. The observed IBD candidate rate is about 1900 per day, with a signal to background ratio of 23. In addition to searching for a short-baseline oscillation by the existence of a light sterile neutrino, utilization of the evolution of the fuel components during a fuel cycle allows us to extract the isotope-dependent antineutrino yields and spectra, especially for uranium-235 and plutonium-239.

### Keywords:

neutrino oscillation, sterile neutrino, reactor neutrino, inverse beta decay

## **Pulse shape discrimination in NEOS II with a convolutional neural network**

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### **Abstract:**

This study describes the pulse shape discrimination (PSD) with signals from Neutrino Experiment for Oscillation at Short baseline II (NEOS II). In NEOS II, PSD is crucial to identify the signal of electron-induced events from those of fast neutron-induced events so that it improves the signal-to-background ratio. Conventionally, The PSD has been done by comparing the ratio of the tail part to the total area of the waveform. As an alternative way, we apply a convolutional neural network (CNN) trained from Fast Fourier-Transformed waveform selected in NEOS II data to the PSD. The CNN model was evaluated on the Na gamma source and showed an improvement in terms of the signal-to-background ratio on the low energy range.

### **Keywords:**

pulse shape discrimination, convolutional neural network, machine learning

## Status of Neutrino Elastic-scattering Observation with NaI(Tl) experiment (NEON)

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### Abstract:

Neutrino Elastic scattering Observation with NaI (NEON) is an experiment to detect a coherent elastic neutrino-nucleus scattering (CEvNS) using reactor electron antineutrinos. NEON is based on an array of six NaI(Tl) crystals corresponding to a total mass of 15 kg, located at the tendon gallery of the Hanbit nuclear reactor that is 24 m far from the reactor core. The installation of the NEON detector was completed in December 2020 and the detector is currently taking data with full power of the reactor since May 2021. The current status of the NEON experiment will be presented in this talk.

### Keywords:

Neutrino, NaI crystal, NEON, CEvNS, reactor

## Integrating the Camera System to the IceCube Upgrade

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### Abstract:

The IceCube neutrino observatory, located at the geographic south pole, is currently the largest volume among underground detectors. IceCube detects and observes neutrinos using Cherenkov light emissions from charged particles produced in neutrino interactions. There is a necessity of studying Antarctic ice properties to reduce a major uncertainty of event reconstructions in IceCube. The Neutrino Astro Particle Physics Laboratory(NAPPL), located in Sungkyunkwan University(SKKU) and University of Utah, is currently running a mass production of camera systems which will be installed into the IceCube Upgrade for the use of calibration and interpretation of Antarctic ice properties. The test procedure of the camera system has been done for three batches of more than 1600 cameras. During this mass production, the NAPPL is also simulating the geometries and images of camera systems. We will present how we reconstruct the geometry and image with our new simulation.

### Keywords:

IceCube, Camera System

## Novel Camera System to Improve Analysis of Neutrino Events in the IceCube Upgrade

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### Abstract:

The IceCube Neutrino Observatory consists of over 5,000 digital optical modules (DOMs) evenly spaced in 1 km<sup>3</sup> of the purest ice on Earth, more than 1.5 km below the surface of the South Pole. Each DOM is equipped with one photomultiplier tube (PMT) that detects Cherenkov light emitted by high energy charged particles produced in the neutrino-nucleon interactions within the vicinity of the telescope. The IceCube Upgrade - deployment scheduled to begin in early 2023 - will add seven strings of novel photosensors at denser spacings, and is expected to enhance the detection and improve the reconstruction of neutrino events in the "low energy" 1-100 GeV range. Towards this goal, the Neutrino Astroparticle Physics Laboratory (NAPPL) at Sungkyunkwan University has designed and is manufacturing a camera system which will be installed into each DOM to improve said reconstructions by probing the local optical properties of both the surrounding pristine and refrozen ice from the drill holes. We will show our testing procedure, report on the status of the camera system mass production, and talk about what useful information we could learn through analyzing the images taken once the integrated cameras are deployed in the Antarctic ice.

### Keywords:

IceCube, IceCube Upgrade, Camera System, Detector Calibration, Cherenkov Detector, Astroparticle Physics, Neutrinos

## Detection of Cosmic Rays under latitude & altitude dependence in South Korea

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### Abstract:

In this study we conducted on experiments to confirm the locational dependence of cosmic rays in South Korea using the SiPM detector (Silicon Photomultiplier). The data include the measurements at latitude 33, 34, 35, 36, 37 degree and at altitude 826m, 74m. As there was a limitation of measuring time, we introduced comparison data of the entire week measurement at a fixed place. We find that there is no apparent dependence on latitude but altitude.

### Keywords:

cosmic ray, cosmic muon, sipm

## Exploring EOS in heavy-ion collisions with transport models

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### Abstract:

Heavy-ion collisions (HICs) provide a unique opportunity to study nuclear matter under various conditions, e.g., densities and isospin asymmetries. However, we must understand the nontrivial many-body dynamics in HICs by developing reliable transport models. We are making efforts in the worldwide collaboration of the transport model evaluation project (TMEP) and also in individual transport models such as the antisymmetrized molecular dynamics (AMD). In this talk, I will report some recent results from TMEP and our work with AMD, including the comparisons with the SpiRIT experimental data for the pion and cluster observables.

### Keywords:

heavy-ion collisions , equation of state , symmetry energy , transport models , antisymmetrized molecular dynamics, pion production, cluster production

## KIDS Energy Density Functional and Symmetry Energy

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### Abstract:

I present the recent work on constraining the density dependence of the nuclear symmetry energy with KIDS (Korea-IBS-Daegu-SKKU) nuclear density functional theory. Calibrating the parameters of the symmetry energy with standard nuclear data and recent astronomical observations, we obtain  $J=30.9\pm 0.6$  MeV,  $L=49.8\pm 5.2$  MeV, and  $K_{\text{sym}}=-82.4\pm 33.7$  MeV at the  $1\sigma$  level. Neutron skin thickness of  $^{48}\text{Ca}$ ,  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$  are considered in comparison with the recent PREX-II result.

### Keywords:

Density functional theory, Symmetry energy

## **Apha cluster formation in the surface of stable and unstable nuclei.**

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### **Abstract:**

Cluster formation at dilute densities is one of the interesting topics in nuclear physics. It is also closely related to the equation of state of nuclear matter as well as the decay lifetime of the heavy elements. Recently, an innovative method to measure cluster formation on the nuclear surface has been proposed, and based on this method, the study of cluster formation in nuclear matter is going to make a great progress.

In this contribution, I will discuss the recent results and future prospects of this topic.

### **Keywords:**

nuclear matter EOS , cluster formation , neutron-rich nuclei

## Probing the expansion history of the universe with gravitational waves

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### Abstract:

Standard candles such as Cepheids or type Ia supernovae are the most common objects to measure cosmological distances, but they have to be calibrated against other distance indicators. Gravitational waves originating from merging binaries composed of compact objects such as neutron stars are known as standard candles which can also be used to measure the distances to these sources. Contrary to the standard candles, the distance measurements using gravitational-waves do not suffer from the calibration uncertainty since the waveforms for given set of the binary parameters, such as masses and spins of the binary components, can be obtained from general relativity alone. Discrepancy of Hubble constant between that measured in the local universe and that implied by the Cosmic Microwave Background (CMB) radiation, poses serious challenge to our understanding of the universe. Gravitational waves can be used to determine the local Hubble constant independently from other methods based on the standard candles if we can identify the host galaxy of the gravitational-wave event, and therefore could provide clues to the current Hubble tension. More sensitive detectors in the future can observe the gravitational-waves coming from very distant objects and therefore would allow us to measure acceleration or deceleration of the universe in the past. We discuss the promises and challenges in utilizing gravitational waves to resolve Hubble tension and to probe the expansion history of the universe.

### Keywords:

gravitational-waves, cosmology, black holes

## Multi-messenger Astronomy with 7-Dimensional Telescope

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### Abstract:

With the expected start of the LIGO/Virgo O4 run in late 2022, the expectation is high for multi-messenger astronomy with gravitational-wave (GW) and electromagnetic wave (EM). To prepare for future GW observing runs, our group is constructing the 7-dimensional telescope (7DT) which is capable of carrying out spectral mapping of the sky in 40 wavelength elements over a wide field of view ( $1.4 \text{ deg}^2$ ). 7DT will be made of twenty, 0.5-m class wide field telescopes, and it is now being constructed at the El Sauce Observatory, Chile. With its spectral mapping capability, 7DT will gather spectra for all of 60 million pixels (60 million spectra in one shot) in its field of view, allowing rapid identification of peculiar features kilonova, the EM counterpart of binary neutron merger events. With 7DT identification, we will be able to use the GW events as standard sirens for constraining cosmological parameters, trace to the early evolution of EM signal to constrain the EM emission signals, and constrain the environment of binary star mergers. Additionally, 7DT will carry out large area, time-domain spectral mapping survey, the 7-dimensional sky survey (7DS), which will open a new window to understand the dynamic nature of the Universe in many subdisciplines of astronomy.

### Keywords:

multi-messenger astronomy, gravitational-wave astronomy, instrumentation, galaxy evolution, cosmology

## aLIGO Gravitational-Wave Detector Science: Room Temperature Ground-Based Detector

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### **Abstract:**

According to the Theory of General Relativity, gravitational waves are ripples in spacetime caused by the asymmetrical acceleration of mass. 100 years since Einstein first predicted the existence of gravitational waves, the Advanced LIGO detectors succeeded in first direct detection in 2015. The most important contribution that made the detections possible was the upgrade to the Advanced LIGO, including a quadruple pendulum system, and monolithic fused silica final stage suspensions. To further improve the sensitivity of the detectors, world-wide collaboration works on various experimental and modelling are under progress to investigate. As a general introduction of experimental gravitational wave research, instrumental science side of the aLIGO detectors will be discussed. aLIGO detectors are ground-based detectors operated under room temperature. Following this talk, Dr. Junkyu Park will cover cryogenic underground detectors such as KAGRA and ET.

### **Keywords:**

Gravitational Wave, aLIGO

## KAGRA and Einstein telescope : the underground cryogenic gravitational wave telescope

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### Abstract:

The first gravitational wave detection(GW150914) by advanced LIGO, confirmed that merging of the binary black holes can be detected with a interferometric gravitational wave detector. Since then, the binary neutron star merger, the intermediate mass black hole merger and gamma rays burst were detected by multiple gravitational wave detector which means gravitation wave detection has begun in earnest.

KAGRA is interferometric gravitational wave detector located in Kifu, Japan. Construction of KAGRA was completed in 2019 became the fourth completed large scale gravitational wave detector. The key characteristics of KAGRA are that it was built underground, operated at cryogenic temperature, and use of sapphire mirrors.

KAGRA is built to minimize seismic noise, gravity noise and other environmental noise. Other gravitational wave detectors are built on the ground and next-generation detectors such as Einstein telescope are planning to build underground. Operating at cryogenic temperature is effective in reducing thermal noise. Since KAGRA is operated at cryogenic temperature(20K), a sapphire mirror is used to optimize thermal characteristic instead of fused silica. KAGRA joined the observation at end of O3 and is currently adjusting the system to join the O4.

Einstein telescope (ET) is a next generation gravitational wave detector which is planning to build in Europe. ET will be built underground and operated at cryogenic temperature same as KAGRA. It has an arm length of 10 km and is designed as a triangular shape. This is expected to be able to detect improved sensitivity and signals in frequency bands that have not been previously detected. ET is in the design stage and is planning necessary research by forming teams for each area to be developed.

### Keywords:

Gravitational wave detector, Interferometer, Frequency dependent squeezing, KAGRA

## Orbital torque in magnetic bilayers

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### Abstract:

The orbital Hall effect [1] describes the generation of the orbital current flowing in a perpendicular direction to an external electric field, analogous to the spin Hall effect. As the orbital current carries the angular momentum as the spin current does, injection of the orbital current into a ferromagnet can result in torque on the magnetization [2], which provides a way to detect the orbital Hall effect. With this motivation, we examine the current-induced spin-orbit torques in various ferromagnet/heavy metal bilayers by theory and experiment [3]. Analysis of the magnetic torque reveals the presence of the contribution from the orbital Hall effect in the heavy metal, which competes with the contribution from the spin Hall effect. In particular, we find that the net torque in Ni/Ta bilayers is opposite in sign to the spin Hall theory prediction but instead consistent with the orbital Hall theory, which unambiguously confirms the orbital torque generated by the orbital Hall effect.

### References

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### Keywords:

Orbital Hall effect, Spin Hall effect, Orbital torque

## Long-range orbital transport in ferromagnets: Theory and experiment

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### Abstract:

While it is often assumed that the orbital transport is short-ranged due to strong crystal field potential and orbital quenching, we show that orbital propagation can be remarkably long-ranged in ferromagnets. In contrast to spin transport, which exhibits an oscillatory decaying behavior by spin dephasing, we find that the injected orbital angular momentum does not oscillate and decays slowly [1]. This unusual feature is attributed to nearly degenerate states in the momentum space, which form hot-spots for the intrinsic orbital response. We demonstrate this in a bilayer consisting of a nonmagnet and a ferromagnet, where the orbital Hall current is injected from a nonmagnet into a ferromagnet. Interaction of the orbital Hall current with the magnetization in the ferromagnet results in an intrinsic response of the orbital angular momentum which propagates far beyond the spin dephasing length. This gives rise to a distinct type of orbital torque on the magnetization, increasing with the thickness of the ferromagnet.

Following the theoretical prediction, we have experimentally confirmed that orbital currents propagate over longer distances than spin currents by more than an order of magnitude not only in ferromagnets but also in nonmagnets [2]. Furthermore, we find that the orbital current enables electric manipulation of magnetization with efficiencies significantly higher than the spin counterpart. Our findings open the possibility of using long-range orbital transport in orbitronic device applications. These findings open the door to orbitronics that exploits orbital transport and spin-orbital coupled dynamics in solid-state devices.

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### Keywords:

orbital current, spin current, spin-orbit torque

## Generating Orbital Currents and Densities

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### Abstract:

Orbitronics, based on the generation and manipulation of orbital angular momentum, offers interesting perspectives for the conception of alternative microelectronic components. Nonetheless, before any workable device can be realized, efficient means to generate, propagate and detect orbital information must be identified. In this presentation, I will discuss two methods to generate orbital angular momentum out of equilibrium: the orbital Rashba effect and the orbital Hall effect. The former generates nonequilibrium orbital densities whereas the latter unlocks flows of charge-neutral orbital momentum. I will examine these two mechanisms in different classes of materials, using toy model and realistic calculations. We consider a large range of materials including narrow-gap semiconductors, large-gap semiconductors as well as in transition metals. I will pay particular attention to discussing the local and non-local origin of the nonequilibrium orbital moment.

## Orbitronics: new torques and magnetoresistance effects

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### Abstract:

Experimentally, orbital currents for efficient manipulation of magnetization have only recently started to be explored. We studied spin orbit torques generated in TmIG/Pt/(Cu(O)x) heterostructures. Varying the CuOx and Pt layer thicknesses, we realized a 16x increase of the spin orbit torques exerted on the TmIG compared to conventional TmIG/Pt [1]. Such an enhancement is extremely surprising if one considers only conventional spin-charge interconversion based on spin orbit coupling effects and given the low spin-orbitcoupling of Cu and Cu(O)x one does not expect large torques. However, the results can be naturally explained as Cu(O)x can generate large orbital currents that are then converted to spin currents in the Pt layer, which then manipulate the TmIG extremely efficiently. In addition, we found in Py/Cu(O)x a Orbital Rashba-Edelstein Magnetoresistance effect related to the conventional spin Hall magnetoresistance [2]. In particular in this work, the length scale of the orbital to spincurrent conversion in Py could be identified as a key step to harnessing orbital currents efficiently even without a heavy metal-based orbital to spin conversion layer [3].

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- [3] D. Go, MK et al., Perspectives Review in EPL 135, 37001 (2021)

### Keywords:

Orbitronics, orbital torques, orbital magnetoresistance effects, spin-orbit torques

# The critical role of Sb-*p* state in the Van Hove singularity formation and the electronic correlation for superconducting Kagome metal CsV<sub>3</sub>Sb<sub>5</sub>

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## Abstract:

Recently discovered V-based Kagome metal family,  $AV_3Sb_5$  ( $A = K, Rb, Cs$ ), gained a lot of interest due to its superconductivity, charge density wave (CDW), and the interplay between them. The van Hove singularities (VHSs) near Fermi level and electron-electron interaction strength are pointed out as keys to understanding the superconductivity and time-reversal symmetry breaking with CDW. In this work, we found that the *p* orbitals of Sb atoms play a crucial role in forming VHSs and correlation strength in CsV<sub>3</sub>Sb<sub>5</sub> in a first-principles manner. First, we found that one of three VHSs near the Fermi level has dominant Sb-*p* character while the other two mainly consist of V-*d* orbitals. By the tight-binding model generation with maximally localized Wannier function method, only one of three VHSs is reproducible when only V-*d* orbitals are considered. To obtain all three VHSs, the Sb-*p* and V-*t*<sub>2g</sub> orbitals must be considered. Moreover, we performed constrained random phase approximation to extract interaction parameters for V-*d*. We found that Sb-*p*, especially out-of-plane Sb-*p*, screens a large part of on-site and inter-site interaction, making the CsV<sub>3</sub>Sb<sub>5</sub> less correlated. Finally, we examined the strain and pressure effect on electronic features and VHS character in CsV<sub>3</sub>Sb<sub>5</sub>. Interestingly, Sb-*p* dominant VHS energy level depends on the out-of-plane lattice constant, while energy levels of V-*d* dominant VHSs depend on the in-plane lattice constant. Our results that Sb atoms are important for understanding VHS physics in the superconducting Kagome family.

## Keywords:

Kagome metal, density functional theory, van Hove singularity, cRPA

## Flat band, Dirac fermions, and CDW formation in Kagome Lattices

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### Abstract:

The two-dimensional Kagome lattice composed of uniformly tiled triangles and hexagons possesses a unique electronic structure characterized by symmetry-enforced flat bands, Dirac points, and Saddle points, thereby providing a novel platform to investigate various topological and correlated phenomena, such as quantum anomalous Hall effect, charge fractionalization, and spin liquid. Based on the first-principles calculations, we introduce three experimentally studied Kagome lattices. First, the layered  $\text{Fe}_3\text{Sn}_2$  crystal consisting of two Fe Kagome lattices separated by a Sn spacing layer features a striking flatband near the Fermi level originating from the local destructive interferences of Bloch wave functions within the Kagome lattices [1]. The high-temperature ferromagnetic ordering in  $\text{Fe}_3\text{Sn}_2$  can be interpreted in terms of the consequence of the synergetic effects of electron correlation and peculiar lattice geometry. Secondly, we reveal that massless Dirac fermions are present in a layered FeSn crystal containing antiferromagnetically coupled ferromagnetic Fe Kagome layers, where each of the  $P$  and  $T$  symmetries is individually broken but the combined  $PT$  symmetry is preserved [2]. The presence of Dirac fermions is protected by the combined  $PT$  symmetry with additional nonsymmorphic  $S_{2z}$  symmetry. Finally, we identify the origin of the observed charge density wave (CDW) formation in a layered Kagome metal  $\text{CsV}_3\text{Sb}_5$  [3]. It is revealed that the structural distortion of Kagome lattice forming the trimeric and hexameric V atoms is accompanied by the stabilization of quasimolecular states, which gives rise to the opening of CDW gaps for the V-derived multibands lying around the Fermi level. Thus, we propose the Jahn-Teller-like instability having the local lattice distortion and its derived quasimolecular states as a driving force of the CDW order, rather than the widely accepted Peierls-like electronic instability due to Fermi surface nesting.

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### Keywords:

First-principles calculations, Kagome Lattices

# A first-principles study of kagome superconductors $AV_3Sb_5$ (A = K, Rb, Cs): exchange-correlation functional and van Hove singularity

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## Abstract:

The  $AV_3Sb_5$  (A=K, Rb, Cs) family is recently discovered and found to have intriguing properties, including the unconventional charge order and the superconductivity. The first-principles study found that multiple van Hove singularities (VHSs) exist near the Fermi level, which could be important to understand physical properties. In this work, we performed density functional theory (DFT) calculations for these superconducting kagome metals via different exchange-correlation functional. The DFT-optimized lattice parameters are compared to experimental ones. The electronic structures from various functionals were also examined with both experimental and DFT-optimized structures. Especially, we focused on the VHS energy levels and orbital characters in  $AV_3Sb_5$ . Our results would provide a useful guide to study  $AV_3Sb_5$  with DFT and information for understanding experimental properties related to VHSs.

## Keywords:

van Hove singularities, Density functional theory, Superconducting kagome metals

## **Studies of emerging materials using time-resolved resonant X-ray scattering at PAL-XFEL**

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### **Abstract:**

The interplay among fundamental physical degrees of freedom such as lattice, charge, spin and orbital leads to a rich array of intriguing quantum states in condensed matter. These four physical degrees of freedom are entangled one another and often complicate identification of the microscopic origins for the emergent states. Recent development of X-ray free electron lasers (XFEL) opens a gateway to ultrafast dynamics of the phenomena via the femtosecond X-ray pulses. I will discuss time-resolved resonant X-ray scattering as a powerful probe to study each individual degree of freedom with examples obtained using soft and tender X-rays at PAL-XFEL.

### **Keywords:**

XFEL, ultrafast dynamics, resonant X-ray scattering

## Two-temperature and *ab initio* molecular dynamics study of ultrafast nonequilibrium structural transformation of nanoparticles

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### Abstract:

Femto-second laser irradiation induces states far-from-equilibrium through mode-selective electronic excitation. In metals, lattice heating by the photo-excited electrons occurs via thermal activation of the atoms resulting from electron-phonon coupling, whereas, in semimetals and semiconductors, photo-excitation of the bonding electrons can modify the interatomic potential energy surface, leading to sub-picosecond lattice melting. In this talk, I will show that two-temperature and *ab initio* molecular dynamics calculations can be used to study the thermal and nonthermal kinetics-driven lattice melting to which the two above-mentioned mechanisms respectively belong. I will discuss the results of our recent experimental and computational studies on the ultrafast structural transformation of the gold, bismuth, and germanium nanoparticle systems.

### Keywords:

Ultrafast phenomena, Nonequilibrium, Two-temperature molecular dynamics, Ab initio molecular dynamics, Femtosecond laser

## Ultrafast lattice control and electron phonon correlation spectroscopy

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### **Abstract:**

The concept of ultrafast control of material properties is of fundamental interests as well as of technological relevance. High-intensity fs laser sources and phase stable pulse technologies allow for an active, selective, and ultrafast control over electronic, optical, magnetic properties, or properties that are not accessible in static materials. Ultrashort electromagnetic radiations can be employed to modulate atomic positions, in particular, in sync with one another, and in turn, the electronic band structure. In order to secure the selectivity, it is essential to have mode-resolved information of accessible phonon modes and each of their couplings with electronic degrees of freedom. Multidimensional spectroscopies, where a coupling between resonances manifests itself as an off-diagonal peak, could provide such mode-resolved details. In this talk, I'll introduce our recent development of two-dimensional spectroscopy, which reveals the correlation between electronic transitions and phonon modes in an element-resolved fashion, and present the potential of this technique towards fundamental understanding of intriguing condensed matter systems.

### **Keywords:**

Ultrafast, electron phonon

# First-Principles Studies on Ultrafast Excited-State Dynamics in Materials

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## Abstract:

Density functional theory (DFT) is one of the most successful approaches to simulating the properties of molecules and condensed matters. However, DFT is a theory for electronic ground state, and it cannot be applied to investigate the dynamical processes in materials. Here, we discuss recent developments in the first-principles program based on time-dependent density functional theory, which can overcome the limit of DFT. Without any input parameters, which are necessary for model calculations, the program can be readily applied to real system involving nanostructures and condensed matters. As examples, we provide two interesting results: a charge transfer dynamics in two-dimensional materials, which shows a coherent oscillation of the charge carriers, and an excitation-induced structural change of phase change materials, which shows non-thermal phase transition.

This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) (Grants No. NRF-2018R1D1A1B07044564 and No. NRF-2020R1A4A1019566) and the National Research Council of Science & Technology (Grant No. CAP-18-05-KAERI).

## Keywords:

Ultrafast phenomena, Excited-State Dynamics, Time-Dependency Density Functional Theory

## Magnetic effects in graphene

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### Abstract:

Interactions between two different materials can produce strong electronic correlations that do not exist when each material stands alone. We search for such correlations from graphene, a non-magnetic semi-metal, in the vicinity of other materials such as a diamagnetic insulator and a topological Kondo insulator, using angle-resolved photoemission spectroscopy and additional complimentary tools. Sulfur-decorated graphene exhibits magnetic hysteresis and energy gap opening at low temperature concomitant with enhanced electron-phonon coupling that are clearly distinguished from the behavior observed from clean graphene. Graphene placed on top of  $\text{SmB}_6$  exhibits Kondo effect at low temperature that is found to be controlled by the charge carrier density of graphene. We discuss the magnetic effects in graphene, which will provide intriguing insights on the search for novel quantum phases in graphene-based compounds.

### Keywords:

Graphene, ARPES, Magnetic effects, Interface

## Correlated nodal surface semimetal in Mn-based kagome compound $\text{Sc}_3\text{Mn}_3\text{Al}_7\text{Si}_5$

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### Abstract:

Topological semimetals hosting zero-dimensional (Weyl, Dirac semimetals) and one-dimensional (nodal line, nodal link semimetals) Fermi surfaces have been actively investigated for their topological protections and interesting bulk-boundary correspondences. Recently a new kind of topological semimetal, the so-called nodal surface semimetal, has been reported where the two-fold degeneracy is enforced on a two-dimensional surface in the three-dimensional momentum space. Here we employ ab-initio electronic structure calculations to report that  $\text{Sc}_3\text{Mn}_3\text{Al}_7\text{Si}_5$ , a metallic compound with layered Mn-based kagome planes and with no reported magnetic order down to  $T = 1.8\text{K}$ , is a nodal surface semimetal protected by non-symmorphic symmetries. Even more interestingly, dynamical mean-field theory calculations reveal that electronic correlations flatten the band dispersion and induce magnetic fluctuations within the nodal surface bands. This compound can be a rare example hosting weakly-dispersive bands with the so-called Hund's metal character, manifesting a van Hove singularity close to the Fermi level and may give rise to interesting instabilities.

### Keywords:

nodal surface semimetal, Hund's metal, kagome lattice, dynamical mean-field theory, ab-initio electronic structure calculation

## 양자 스핀 액상 이종구조

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### Abstract:

키타에프 스핀 액상은 최근 많은 관심을 받고 있는 강상관 위상물질이다. 이 물질에서는 마요나라 페르미온과 비아벨 애니온 입자와 같은 쪼개진 입자가 나타날 수 있고, 이러한 입자는 위상 양자 컴퓨팅을 가능하게 한다는 점에서 양자 정보 소자 분야에 활용될 가능성이 있다. 하지만 이러한 키타에프 스핀 액상을 구현하고, 양자 정보 소자로서 활용하기 위해서는 후보 물질을 박막의 형태로 합성하는 것이 중요한 과제로 남아있다. 본 발표에서는 키타에프 스핀 액상 물질의 박막 합성과 물리적 특성을 소개하고, 더 나아가 쪼개진 입자를 관측하는 실험에 대해 논의할 것이다.

### Keywords:

강상관 이종구조, 양자 스핀 액상

## Search for Majorana Fermions in Quantum Magnets

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### **Abstract:**

Majorana fermions may appear in quantum magnets, revealing enormous entanglement of localized quantum spins. Search and control of the emergent quasi-particles are suggested as one significant step to advance quantum science and technology. Here, we discuss how to identify Majorana fermions in quantum magnets theoretically and experimentally.

### **Keywords:**

Majorana fermions, Quantum magnetism

# Topological band engineering for ultracold atoms in shaken optical lattices

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## Abstract:

Ultracold atoms in optical lattices provide a versatile platform to realize topological states and study their phase transitions in a clean and well-controlled manner. In this talk, I present our recent experiments with ultracold fermionic  $^{173}\text{Yb}$  atoms to realize a topological Creutz ladder in 1D optical lattices. The Creutz ladder is a cross-linked two-leg ladder system discussed as a minimal model for 1D topological insulators. In our experiment, the two-leg ladder consists of the two lowest orbital states of the optical lattice, and the cross interleg links are generated via two-photon resonant coupling between the orbitals by periodic lattice shaking. I will describe the interleg link tunability of the shaken lattice system and discuss the topological charge pumping effect and the possibility of flat band engineering in the Floquet system.

## Keywords:

Floquet engineering, Optical lattices, Ultracold atoms

# Topological phases and flat bands of quantized light

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## Abstract:

Topological phases and flat bands are important topics in condensed matter physics and photonics. In this talk I am going to introduce the topological phases and flat bands due to the particle nature of light, i.e., solely related to the quantized Fock states and the inhomogeneous coupling between them. In particular, we study a three-mode Jaynes-Cummings model, where three cavity modes are coupled to a two-level atom. The combinational Fock and atomic states form a two-dimensional honeycomb lattice, where the strain due to the inhomogeneity of the coupling strengths induces a Lifshitz topological phase transition between a semimetal and three band insulators within the lattice. In the semimetallic phase, the strain is equivalent to a pseudomagnetic field, which results in flat bands, i.e., pseudo Landau levels. We further construct a Haldane model where the topological phases can be characterized by the topological markers. This study demonstrates a fundamental distinction between the topological phases of bosons and fermions and provides a novel platform for studying topological physics in dimensions higher than three.

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## Keywords:

Topological phases, quantized light, Jaynes-Cummings model, Landau levels

## Flatband photonic lattices: from localized states to topological phenomena

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### Abstract:

Flat-band systems have attracted considerable interest in many different branches of physics in the past decade, providing a flexible platform for studying a variety of fundamental phenomena. Engineered flat-band structures have now been realized in different material systems, and in particular, in the realm of photonics. In this talk, I will present our recent work on flat-band localization and associated topological phenomena in photonic lattices, including momentum-to-real-space mapping of topological singularities, unconventional localized flatband states arising from real-space topology, and higher-order topological states in laser-written Lieb, Kagome, super honeycomb, and fractal-like photonic structures. Our results from flat-band photonic lattices may provide inspiration for exploring fundamentals and applications of flat-band physics in other materials or complex systems beyond photonics.

### Keywords:

flat-band localization, topological singularity, noncontractible loop states, higher-order topological insulators

# Exciton-polaritons in flatland: Controlling flatband properties in coupled optical resonator lattices

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## Abstract:

In recent years, novel two-dimensional materials such as graphene, bismuthene and transition-metal dichalcogenides have attracted enormous interest due to their unique physical properties. A range of physical effects can be transferred to the realms of photonics by creating artificial photonic lattices, emulating these two-dimensional materials. Here, exciton-polaritons in semiconductor microcavities offer an exciting opportunity to study a part-light, part-matter quantum fluids of light in complex lattice potentials.

In this presentation, we discuss exciton-polaritons in two-dimensional lattices of coupled microresonators. In particular, we will discuss the formation of virtually dispersionless flatbands in Honeycomb, Lieb and Kagome lattices [1-5]. The ground state S- and orbital  $P_{xy}$ - photonic orbitals give rise to the formation of flatbands which are of greatest interest for the distortion-free storage of compact localized states [3,4], topological effects [6,7] and flatband lasers [8].

By using a well controlled etch-and-overgrowth technique, we manage to control the trapping as well as the site couplings with great precision. This allows us to control the flatness of the flatbands across the full Brillouin zone. Furthermore, we demonstrate experimentally that these flatbands can be directly populated by condensation under non-resonant laser excitation. Finally, we demonstrate resonant and deterministic excitation of flatband modes in transmission geometry [3], increasing the control and opening new experimental possibilities. Our findings establish the exciton-polariton systems as a highly controllable, optical many-body system to study flatband effects with great perspectives for topological effects and flatband lasing.

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## Keywords:

Exciton-polaritons, polariton lattices, flatbands, band topology, lasers

## Quantum geometry and superfluidity in fermionic and bosonic systems: new twists

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### Abstract:

Quantum geometry, namely quantities such as quantum metric, Berry curvature, and Chern number, have become increasingly important in understanding interacting many-body systems in solid state and ultracold gas quantum matter. We have shown that supercurrents and superfluidity in a flat band are governed by quantum geometry, which opens new prospects for achieving high temperature superconductivity. These findings have become relevant for superconductivity in twisted bilayer graphene and other moiré systems. We present our newest results on the topic, showing for instance that to achieve the critical temperature enhancement, the flat band does not need to be isolated from other bands, which is promising from the experimental perspective [1]. Further, we show that quantum geometry governs the behaviour of bosonic condensates in flat bands as well, making quantum fluctuation effects remarkably strong [2]. The speed of sound of the condensate is found to be proportional to the quantum metric, and the excited state fraction governed by the quantum distance.

### Reference

1. K.-E. Huhtinen, and PT, in preparation (2022).
2. A. Julku, G.M. Bruun, and PT, Phys. Rev. Lett. 127, 170404 (2021).

### Keywords:

Quantum geometry, quantum metric, superfluidity, superconductivity, Bose-Einstein condensation

# Strained Graphene Optoelectronic Devices for Integrated Quantum Photonics

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## Abstract:

Graphene – often dubbed as a wonder material – has the crucial drawback of having no energy gaps, which prevents it from becoming a game-changing material in the real world. Subjecting graphene to very large magnetic fields using laboratory-size superconducting magnets has been one of the most promising ways to create energy gaps in graphene by utilizing Landau quantization. However, the necessity of using such giant-scale magnets for making energy gaps in graphene renders the approach impractical. Approximately a decade ago, there was a theoretical proposal predicting that the creation of spatially non-uniform strain in monolayer graphene can induce pseudo-magnetic fields. Following this striking idea, many research groups presented experimental demonstrations of generating very strong pseudo-magnetic fields of up to a few hundred teslas (T). Unfortunately, however, the spatial area of the induced pseudo-magnetic fields in those reports is limited to the nanometer scale, preventing the feasibility of harnessing such promising new properties for developing a new class of graphene optoelectronic devices. Due to the same reason, it has not either been feasible to study the effect of such pseudo-magnetic fields on the optoelectronic properties of graphene.

In this talk, we present our recent progress on the realization of large-area, strong pseudo-magnetic fields in strained graphene and study the effect of pseudo-magnetic fields on the ultrafast hot carrier dynamics. First, we demonstrate two distinct strain engineering platforms: periodically strained graphene nanopillars and triaxially strained suspended graphene. By using 2D Raman mapping and tight-binding simulations, we reveal the achievement of strong pseudo-magnetic fields. The strength of pseudo-magnetic fields in the graphene nanopillars can be higher than 100 T, which is far beyond a level that is possible with state-of-the-art superconducting magnets. By using time-resolved infrared pump-probe spectroscopy, we provide unambiguous evidence for a significant slow-down of the ultrafast hot carrier dynamics. Lastly, we also discuss the potential of strain-engineered graphene towards developing integrated graphene lasers harnessing pseudo-Landau energy levels. Our findings offer new opportunities for developing a new class of graphene optoelectronic devices.

## Keywords:

Graphene, Pseudo-magnetic field, strain, quantum photonics

# Strain-Engineered Quantum Interferometry and Qubits in Graphene

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## Abstract:

Graphene gives us a promising playground for strain-engineered quantum devices, thanks to the synergy from a combination of graphene's outstanding mechanical and transport properties. Especially, the emergent pseudo-magnetic field due to elastic strain in graphene has attracted research interests in the field of condensed matter and applied physics, with the possibility of controlling Dirac fermion transport via strain engineering. In this presentation, I will introduce the recent research results about effects of a nanobubble formed on graphene sheet, and address the possible quantum device applications based on strain effects. Being motivated from the analogy between real and pseudo-magnetic fields, quantum Hall conductance also exhibits the characteristic oscillatory behavior as a function of strain. Such a strain-induced conductance oscillation leads to a possible quantum sensing device to detect a nano-scale mechanical deformation like a nanobubble. Also, it is revealed that a circular-shape nanobubble on graphene can host strong localized states with the emergent non-uniform pseudo-magnetic fields, as if graphene quantum dots are created inside the nanobubbles. The presence of the strain-induced graphene quantum dots is measurable via apparent Fano resonances in the quantum Hall conductances across the p-n junction. Interestingly, two-level systems are created as a consequence of double-dot couplings, showing a typical avoided crossing nature via gate control. Thus, a nanobubble in graphene is expected to be a novel type of qubits for tunable quantum technology devices, by means of strain engineering. Owing to graphene's extraordinary coherent properties, the nanobubble-induced graphene qubit can be a high-speed quantum operation, not requiring ultra-low temperatures.

## Keywords:

Graphene, Elastic Strain, Conductance Resonance, Quantum Dots, Qubits

## Electro-mechanical properties of 2D crystals

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### Abstract:

The energy and length scales of electronic responses of typical bulk materials are order of magnitude different from those of their mechanical responses. On the other hand, for 2D crystals, such as graphene, hexagonal boron nitride and various transition metal dichalcogenides, the length scales along the direction perpendicular to the 2D plane have the same order of magnitude for both electronic and mechanical parts. Due to this, the correlation between mechanical and electronic behaviors such as piezoelectricity in 2D materials are much stronger compared to those in typical bulk materials. In this talk, I will introduce several of our works related to the electro-mechanical properties of 2D materials. Bilayer graphene shows exotic negative Poisson's ratio which is deeply related to its electronic wave function[1]. Maximal strain that graphene can endure is closely related to its electron-phonon interaction[2]. Uniaxial tensile stress and interlayer sliding of bilayer crystals are delicately correlated, which is attributed to their 2D piezoelectricity[3]. Such piezo effects have further correlation with pseudo magnetic field. I will also briefly mention straintronics, a newly emerging field.

[1] Phys. Rev. B 93, 075420

[2] Phys. Rev. B 87, 075419

[3] Nat. Comm. 8, 1370

### Keywords:

electro-mechanical, 2D material, piezoelectricity

## Thermal Hall response: violation of gravitational analogues and Einstein relations

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### Abstract:

The effect of strains in graphene is effectively described by Dirac particles coupled to gravity. One may relate this concept with the thermal transport from a gravitational analogue: a space-dependent temperature in solid can be modeled by a space dependent metric. Here we investigate the validity of this analogue in describing the bulk response of quantum Hall states and other gapped chiral topological states. To this end, we consider the prototypical Haldane model in two different cases of (i) a space-dependent electrostatic potential and gravitational potential and (ii) a space-dependent temperature and chemical potential imprinted by a weak coupling to non-interacting electron baths or phonons. We find that the thermal analogue is invalid; while a space dependent gravitational potential induces transverse energy currents proportional to the third derivative of the gravitational potential, the response to an analogous temperature profile vanishes in limit of weak coupling to the thermal bath. Similarly, the Einstein relation, the analogy between the electrostatic potential and the internal chemical potential, is not valid in such a setup.

### Keywords:

Thermal Hall response, Luttinger relation (gravitational analogue)

## Ultrahigh Strain and Piezoelectric Behavior in Gen III PMN-PZT Single Crystals ( $d_{33} > 5,000$ pC/N) Developed by SSCG Technique

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### Abstract:

Crystallographically engineered Relaxor-PT single crystals, specifically PMN-PT (Generation I) and PIN-PMN-PT/PMN-PZT (Generation II), offer much higher piezoelectric and electromechanical coupling coefficients ( $d_{33} > 1,500$  pC/N,  $k_{33} > 0.9$ ), when compared to polycrystalline PZT ceramics. Recently Ceracomp Co., Ltd. ([www.ceracomp.com](http://www.ceracomp.com)) has developed the solid-state single crystal growth (SSCG) technique and successfully fabricated Gen III PMN-PZT single crystals modified with acceptors or donors.

The piezoelectric constants ( $d_{33}$ ) of (001) Gen III PMN-PZT single crystals were measured to be higher than 5,000 pC/N and thus about two times higher than those of PMN-PT/PZN-PT (Gen I) and PIN-PMN-PT/PMN-PZT (Gen II) single crystals. The Gen III PMN-PZT single crystals have been firstly applied to single crystal-epoxy composites, ultrasonic transducers, piezoelectric sensors, and piezoelectric actuators. In this presentation, we will introduce the development of high performance piezoelectric sensors and actuators by using the Gen III PMN-PZT single crystals.

### Keywords:

Piezoelectric, Ultrasonic, Single Crystal, Transducer, Sensor

## Structural characteristics and applications of BNT-based relaxor ferroelectric ceramics

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### Abstract:

Relaxor ferroelectrics use excellent electromechanical coupling to be applied in various fields such as piezoelectric sensors, ultrasonic transducers for high-resolution medical images, high-precision actuators, and energy storage devices. Relaxor ferroelectrics are distinguished from typical ferroelectrics by their frequency dependence and diffuse phase transitions, and it is known that their excellent electromechanical coupling properties compared to typical ferroelectrics are due to the nanoscale order in the material. Recent studies suggest that the electrical properties of relaxor ferroelectrics are improved because polar nano-regions (PNRs) and/or polar nano-domains (PNDs) facilitate easy polarization rotation in the ferroelectric domains. However, it is very difficult to study the real-space atomic structure due to complex nanoscale chemical and structural heterogeneity. In this regard, we investigated the structural characteristics of  $(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3$  (BNT)-based relaxor ferroelectrics and studied their applications.

### Keywords:

Relaxor ferroelectrics, Polar nanoregions

## Emergence of isotropy at morphotropic phase boundary of relaxor ferroelectrics

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### Abstract:

The relaxor ferroelectric materials have received attention because of their gigantic piezoelectric coefficients and are utilized for high-performance electromechanical devices. The physics underlying its functionality, however, is not yet fully understood because of its complex nature such as microscopic heterogeneity and path dependence characteristics. We explored the subdomain structure of the PIN-PMN-PT single crystal sample by the angle-resolved resonance-tracking lateral PFM technique. Inhomogeneous polarization field distribution is observed inside the poled domain forming polar slush structures. Our simulation model suggests that the stoichiometric inhomogeneity at the atomic scale may generate the polar slush structure. Moreover, the simulation study predicts a window near the morphotropic phase boundary between tetragonal and rhombohedral phases that the system's Landau free energy becomes an isotropic Mexican hat shape with respect to the ferroelectric polarization. It implies the system can be poled along an arbitrary orientation on the macroscopic scale. This study may shed a light on understanding why the relaxor ferroelectric materials are found at morphotropic phase boundaries.

### Keywords:

Relaxors, Ferroelectrics, AFM, PFM, Phase field simulation

## Steady Floquet-Andreev states in graphene Josephson junctions

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### Abstract:

Engineering quantum states through light-matter interaction has created a new paradigm in condensed matter physics. A representative example is the Floquet-Bloch state, which is generated by time-periodically driving the Bloch wavefunctions in crystals. Previous attempts to realise such states in condensed matter systems have been limited by the transient nature of the Floquet states produced by optical pulses, which masks the universal properties of non-equilibrium physics. Here, we report the generation of steady Floquet-Andreev (F-A) states in graphene Josephson junctions by continuous microwave application and direct measurement of their spectra by superconducting tunnelling spectroscopy. We present quantitative analysis of the spectral characteristics of the F-A states while varying the phase difference of superconductors, temperature, microwave frequency and power. The oscillations of the F-A state spectrum with phase difference agreed with our theoretical calculations. Moreover, we confirmed the steady nature of the F-A states by establishing a sum rule of tunnelling conductance, and analysed the spectral density of Floquet states depending on Floquet interaction strength. This study provides a basis for understanding and engineering non-equilibrium quantum states in nano-devices.

### Keywords:

Floquet state, graphene Josephson junction, Andreev state

## Charge Induced Aharonov-Bohm Phase Modulation in Multiple Quantum Hall Edges Graphene Fabry-Pérot Interferometer

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### Abstract:

We have developed locally gated van der Waals (vdW) graphene heterostructure that allows observation of Fabry-Pérot interference of electrons propagating in quantum Hall edge channels [1]. Similar to recent experiments in semiconductors [2,3], the vdW heterostructure efficiently suppresses charging effects to reveal Aharonov-Bohm interference [1,4]. Moreover, the electron density in graphene channel can be tuned electrostatically using the local gates, which enables accessing a wider range of carrier densities, while also stabilizing fractional quantum Hall states. Here we report on the modulation of Aharonov-Bohm interference phase appeared in multi-quantum Hall edge configuration. We observe periodic phase jumps in the Aharonov-Bohm oscillations of the outer edge channel due to the controlled addition of electrons to the annular compressible region formed by the inner quantum Hall edge state. The proposed mechanism for this observation, arising from inter-edge interaction between the spin-split Landau levels, may shed light on pairing between edge channels [5]. In addition to their ability to operate in this unique regime, will discuss progress towards interference of fractional quantum Hall modes in these new devices.

[1] Ronen, Y., Werkmeister, T., Haie Najafabadi, D. *et al.* Aharonov-Bohm effect in graphene-based Fabry-Pérot quantum Hall interferometers. *Nature Nano.* **16**, 563-569 (2021).

[2] Nakamura, J., Fallahi, S., Sahasrabudhe, H. *et al.* Aharonov-Bohm interference of fractional quantum Hall edge modes. *Nature Phys.* **15**, 563-569 (2019).

[3] Nakamura, J., Liang, S., Gardner, G.C. *et al.* Direct observation of anyonic braiding statistics. *Nature Phys.* **16**, 931-936 (2020).

[4] Déprez, C., Veyrat, L., Vignaud, H. *et al.* A tunable Fabry-Pérot quantum Hall interferometer in graphene. *Nature Nano.* **16**, 555-562 (2021).

[5] Choi, H., Sivan, I., Rosenblatt, A. *et al.* Robust electron pairing in the integer quantum hall effect regime. *Nature Comm.* **6**, 7435 (2015).

### Keywords:

Condensed matter physics, quantum Hall effect, interference of edge states

## Floquet theory of multiterminal Josephson junctions

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### Abstract:

In this talk, I will consider two models of four-terminal Josephson junctions, in connection with a recent experiment [1]: single quantum dot coupled to four superconducting leads [2], and double quantum dot coupled to four superconducting leads and to normal leads [3]. Both models yield voltage-tunable inversion, i.e. the possibility of larger quartet critical current at half-flux quantum than in zero-field. At small bias voltage, the single quantum dot Hamiltonian [2] features repulsion among Floquet states and hybridization between the two time-evolving Andreev states. At larger bias voltage, the populations of the Floquet states are such as to produce  $\pi$ -shift in the quartet current-quartet phase relation. This produces dips in the voltage dependence of the quartet current. On the other hand, the double quantum dot model [3] shows sharp peaks in the voltage-dependence of the quartet critical current, due to the interplay between relaxation and degeneracies. Together with perturbation theory in the tunnel amplitudes [4] yielding  $h/4e$ -periodic quartet critical current due to interference between the quartets and the spin quartets, this work provides theoretical interpretation to the recent Harvard group experiment [1].

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[2] R. Mélin and B. Douçot, Inversion in a four terminal superconducting device on the quartet line: II. Quantum dot and Floquet theory, Phys. Rev. B 102, 245435 (2020).

[3] R. Mélin, Multiterminal ballistic Josephson junctions coupled to normal leads, arXiv:2110.09870 (2021).

[4] R. Mélin, Inversion in a four-terminal superconducting device on the quartet line: I. Two-dimensional metal and the quartet beam splitter, Phys. Rev. B 102, 245435 (2020).

### Keywords:

Multiterminal Josephson effect, Floquet theory, Quartets

## 가속기 포럼: 가속기 분야의 일관성 있는 장기전략 및 로드맵의 필요성

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### Abstract:

국내 가속기 분야 연구 인력들은 포항의 3세대/4세대 방사광가속기, 경주의 양성자가속기, 대전의 중이온 가속기 등의 구축에 핵심적인 역할을 해왔고, 추가로 오창에 4세대 원형방사광가속기의 구축이 추진되는 등, 관련 분야의 연구 활동, 인력과 예산, 중요도는 꾸준히 증가하고 있다. 앞으로는 변화하는 국내외 상황에 체계적인 대응을 할 수 있는 가속기 분야의 일관성 있는 장기전략 및 로드맵이 필요하다. 이를 위해서는 가속기 전문가들의 의견 수렴 및 국내 R&D 연구 현황 파악이 꾸준히 이루어져야 하며, 이를 위한 플라즈마 분과내 소모임으로 "가속기 포럼"이 시작되었다. 이 발표에서는 가속기 포럼의 소개 및 향후 활동 방향 등을 간단히 소개하고, 가속기 전문가 및 사용자 들의 다양한 의견을 듣고자 한다.

### Keywords:

가속기

## 양성자가속기 기반 핵파쇄 중성자원 기술현황

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### Abstract:

물성연구에 있어 중성자는 X선과 상보적인 역할을 하며 그 이용분야를 넓혀가고 있다. 물성연구를 위한 중성자원으로 기존에는 대부분 연구용 원자로를 사용하였으나, 대용량 양성자가속기 기술이 발전함에 따라, 첨두 열중성자 속을 기준으로 연구용원자로보다 높은 중성자속을 갖는 핵파쇄 중성자원이 개발되어 운영되고 있다. 본 발표에서는 대용량 양성자가속기를 이용한 핵파쇄 중성자원의 특징과 기술현황에 대해서 논한다.

### Keywords:

Accelerator, Proton, Spallation neutron source

## **Review and prospects of the laser-plasma accelerator research and applications for light source**

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### **Abstract:**

An intense laser pulse can produce a strong plasma wake wave when the laser pulse is focused in plasma, which can provide an ultrastrong electric field on the order of 100 GV/m. This ultrastrong electric field can be used for electron acceleration to high energy in table-top scale, leading to development of compact advanced accelerators. In recent years, diverse research activities have been performed around the world, including electron acceleration to multi-GeV level and applications of the high-energy electrons for light source. In this talk, we will review the recent progress of the world-wide laser-plasma accelerator research and their applications for light source development.

### **Keywords:**

laser-plasma acceleration, electron acceleration, light source, high power laser, plasma wave

## Critical issues in the 4th generation storage ring projects

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### Abstract:

There had been remarkable progress in developing third-generation electron storage rings as the main sources of very bright photon beams. Fourth-generation storage rings based on the multi-bend achromat lattice concept may be able to surpass the brightness and coherence that are attained using present third-generation storage rings. In this presentation, some critical issues in the fourth-generation storage ring projects will be discussed.

### Keywords:

electron storage ring, bright photon beam, multi-bend achromat lattice, 4GSR

## Structural Colors of Mie-Resonant Hollow Nanospheres

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### Abstract:

Hollow carbon-silica nanospheres that exhibit angle-independent structural color with high saturation and minimal absorption are made. Through scattering calculations, it is shown that the structural color arises from Mie resonances that are tuned precisely by varying the thickness of the shells. Since the color does not depend on the spatial arrangement of the particles, the coloration is angle-independent and vibrant in powders and liquid suspensions. These properties make hollow carbon-silica nanospheres ideal for applications, and their potential in making flexible, angle-independent coloured films and 3D printed films is explored.

### References

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3. Y. Lim et al., *Particle & Particle Systems Characterization* 37(4), 1900405 (2020).
4. N. X. V. Lan et al. *Chemistry of Materials* 33(5), 1714-1722 (2021).

### Keywords:

hollow carbon silica nanospheres, Mie scattering, photonic glass, self-assembly

## **Transformative applications enabled by the spherically symmetric chiral Bragg diffraction of cholesteric spherical reflectors**

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### **Abstract:**

The seemingly simple step of moulding a cholesteric liquid crystal into spherical shape has profound optical consequences, opening a range of potentially revolutionary application opportunities. In these Cholesteric Spherical Reflectors (CSRs), the chiral Bragg diffraction arising from the cholesteric's self-assembled helical structure becomes spherically symmetric, turning CSRs into selective retroreflectors that can be made invisible to human vision while at the same time being exceptionally easy to distinguish, regardless of background, by simple and low-cost machine vision. By arranging CSRs into QR-code-like labels in coatings on surfaces in our environment they can assist robots and Augmented Reality (AR) devices to make sense of their surroundings. At the scale of individual CSRs, unpredictable features within each coating turn CSR labels into Physical Unclonable Functions (PUFs), of great value for secure authentication. CSR labels can thus act as trustworthy yet unobtrusive links between the physical world (buildings, vehicles, packaging, ...) and its digital twin computer representation, with potential to address pressing challenges in logistics and supply chain management, recycling and the circular economy, reliable construction of the built environment, safe coexistence of humans and robots, and many other fields.

## Inorganic DNA origami particles

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### **Abstract:**

DNA origami is one of the most powerful self-assembly techniques to create well-defined nanoscale objects with atomic precision, high yields, and controlled stoichiometry. These properties make DNA origami uniquely capable of being used for single-molecule biophysics experiments, targeted delivery of therapeutics to tissues, investigating fundamental biological phenomena as well as studying fundamental nanophysics. However, the limited compatibility of DNA origami in biological media, as well as organic solvents, often restricts the applications of these nucleic acid nano-assemblies and devices. Here, we present a couple of approaches for creating DNA origami templated inorganic nanoparticles while preserving their shape, high yield as well as stoichiometric control over ligands and geometry. Further, we also demonstrate the use of this new technique to enable mono-functional magnetic particles as well as for ultra-precise molecular quantification.

## Observation of universal coarsening dynamics in a ferromagnetic spinor Bose-Einstein condensate

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### Abstract:

In this talk, we report the coarsening dynamics of a spin-1 superfluid system. After preparing a polar condensate ( $m_F = 0$  state) of Lithium-7 atoms in a two-dimensional harmonic trap, the spinor condensate is quenched to the easy-axis ferromagnetic phase by changing the quadratic Zeeman shift abruptly via microwave dressing. Short time after the quench, small size of spin domains, consist of  $m_F = 1$  and  $m_F = -1$  state, are generated because of dynamical instability for the initial state. In the long-time dynamics, these domains start to merge and the number of domains decreases, signaling the coarsening dynamics of the multi-component superfluid systems [1,2]. Investigating the spin correlation function, we observe dynamical scaling behavior, where the dynamical exponent is close to  $1/z=0.52(3)$  under various quadratic Zeeman energy.

[1] J. Hofmann, S. S. Natu, and S. Das Sarma, Phys. Rev. Lett. **113**, 095702 (2014).

[2] L. A. Williamson and P. B. Blakie., Phys. Rev. Lett. **116**, 025301 (2016)

### Keywords:

coarsening dynamics, universality, spinor Bose-Einstein condensate

## Towards degenerate NaK molecular gases with long-range dipolar interactions

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### Abstract:

Ultracold atomic gas experiments enable the quantum simulation of complex many-body phenomena with extreme precision and control. However, since the interactions between ultracold atoms are governed by the simple contact interaction, they have constraints on simulating more realistic Hamiltonians that feature anisotropic and/or long-range interactions. A quantum gas of strongly dipolar molecules holds exceptional promise in this regard, which may give access to exotic dipolar quantum phases of matter and also enable quantum information processing based on the molecules' strong dipole-dipole interactions.

In this presentation, we introduce our experimental apparatus to create a degenerate gas of strongly dipolar fermionic/bosonic  $^{23}\text{Na}^{40,41}\text{K}$  molecules. Na and K atoms are loaded into a magneto-optical trap from a Zeeman slower and a 2D MOT, respectively. By employing gray molasses cooling of  $^{23}\text{Na}$ , we aim to dramatically increase the phase space density of the atomic mixture. Once the atomic mixture is prepared in an optical dipole trap, we will perform stimulated Raman adiabatic passage (STIRAP) to coherently transfer the loosely bound NaK Feshbach molecules to the rovibrational ground state. By employing advanced cooling techniques such as molecular evaporative cooling, we aim to create deeply quantum degenerate gases of bosonic  $^{23}\text{Na}^{41}\text{K}$  and of fermionic  $^{23}\text{Na}^{40}\text{K}$  molecules.

### Keywords:

Ultracold quantum gases, Ultracold molecules, Dipole-dipole interaction

## Experimental Study of the Inhomogeneous Kibble-Zurek Mechanism

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### Abstract:

Inhomogeneous Kibble-Zurek Mechanism (IKZM) provides the framework for understanding the non-equilibrium, continuous phase transition of a system with an inhomogeneous density distribution as it is cooled beyond its critical temperature. Although the theory correctly predicts the power-law dependence of the defect number density on the thermal quench rate of the system, recent studies in <sup>87</sup>Rb Bose gas show significant deviation from the predicted scaling exponent as well as the observation of defect density saturation at rapid quench rates [1]. The study presented here extends our investigations into the IKZM in <sup>87</sup>Rb Bose gas and examines the effect of optical trapping potential geometry on certain key parameters such as the KZ scaling exponent, and the saturated defect number density. Our preliminary observations indicate a strong correlation between the trap geometry and the KZ scaling exponent with a trend contrary to what might be expected from the IKZM. We will discuss possible mechanisms to account for the experimental results.

[1] J. Goo *et. al.*, Phys. Rev. Lett. **127**, 115701 (2021)

### Keywords:

Inhomogeneous Kibble-Zurek mechanism, Bose-Einstein condensate, Quantum critical phenomena, Quantum vortex

## 변조전달분광신호를 이용한 불안정도 10-14 수준의 주파수 고안정화

LEE Sanglok<sup>1,2</sup>, PARK Sang Eon<sup>1</sup>, HONG Hyun-Gue<sup>1</sup>, HEO Myoung Sun<sup>1</sup>, LEE Jae Hoon<sup>1</sup>, SEO Sangwon<sup>1</sup>, KWON Taeg Yong<sup>1</sup>, MOON Geol<sup>2</sup>, LEE Sang Bum<sup>\*1</sup>

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### Abstract:

세슘이나 루비듐 같은 알칼리 금속 원자의 D<sub>2</sub> 전이선에 레이저 주파수 고안정화는 원자 간섭계, 원자시계 등의 실험에서 원자냉각 및 신호대잡음비를 개선하기 위해 필수적으로 요구된다. 우리 연구팀에서는 변조전달분광법에 사용되는 D<sub>2</sub> 전이선의 자연선폭이 수 MHz 임에도 불구하고 레이저 빔의 크기와 세기 등의 매개 변수를 최적화하여 수십 Hz 수준으로 안정화된 광 주파수를 구현하였다. 알란 편차에서 단기 안정도는  $6.5 \times 10^{-14} / \sqrt{\tau}$  수준에 도달하고, 장기 안정도는 특별한 온도 안정화 없이  $1 \times 10^5$  초 동안  $2 \times 10^{-12}$  를 넘지 않는다. 또한 광 검출기, RF 회로 등에서 오는 전기적 잡음과 레이저의 세기 안정도, 빔의 직경, 온도 요동, 주파수 고정 시스템의 offset 요동 등이 주파수 안정화에 미치는 궁극적 한계에 대해서 논의한다.

### Keywords:

MTS, Frequency stabilization

## Dynamic polarization response of polarization-maintaining optical fiber by a periodic temperature modulation

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### Abstract:

We investigated polarization-maintaining optical fiber of the dynamic responses by temperature modulation. The temperature modulation causes the continuous periodic change of polarization direction of the output laser without approaching to the steady-state of the resulting dynamic polarization response, and the response depends on the temperature modulation frequency and amplitude. Remarkably the dynamic responses provides us a new and convenient polarization alignment method and it would be utilized to measure properties of polarization-maintaining optical fiber.

### Keywords:

polarization-maintaining optical fiber, temperature modulation

## Observation of interplay between propagations of phase front and phase information during defect formation on a quenched inhomogeneous Bose gas

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### Abstract:

The Kibble-Zurek mechanism describes the formation of topological defects in the system quenched across a second-order phase transition. In an inhomogeneous system, the situation becomes different since the critical point is reached locally then the front of the transition spreads through the system with a finite velocity. It has been expected that the competition between the propagation of the symmetry breaking and the propagation of phase information from neighboring regions that had already made a phase domain determines the defect density, unlike the paradigmatic Kibble-Zurek mechanism. We experimentally investigate the defect formation in an oblate atomic Bose gas quenched through a Bose-Einstein condensate transition. We analyze the position of vortices on the condensate with the help of a machine learning algorithm, and find that the position distribution of vortices expands outward as the quench rate increases. This result is the first experimental evidence of the existence of the interplay between the phase front propagation and the phase information propagation in the inhomogeneous dynamics.

### Keywords:

Bose-Einstein condensate, Quantum vortex, Spontaneous defect formation, Inhomogeneous Kibble-Zurek mechanism

## Chiral induced spin selectivity enabling a spin light-emitting diode

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### Abstract:

In traditional opto-electronic approaches, control over spin, charge, and light requires the use of both electrical and magnetic fields. In a spin-polarized light-emitting diode (spin-LED), charges are injected and circularly polarized light is emitted from spin-polarized carrier pairs. Typically, injection of carriers occurs with the application of an electric field, while spin-polarization can be achieved using an applied magnetic field or polarized ferromagnetic contacts. Here we employ chiral induced spin selectivity (CISS) to produce spin-polarized carriers and demonstrate a spin-LED that operates at room temperature without magnetic fields or ferromagnetic contacts. The CISS layer consists of oriented self-assembled small chiral molecules within a layered organic/inorganic metal-halide hybrid semiconductor framework. The spin-LED achieves  $\pm 2.6\%$  circularly-polarized electroluminescence at room temperature. Thus, here we control of spin, charge, and light with only an applied electric field.

### Keywords:

Perovskite, spin, chiral, spin-polarization, light-emitting diodes

## 유기 반도체 첨가제 기반 결정 성장 제어 기술 기반 고효율 페로브스카이트 발광 소자

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### Abstract:

Organic-Inorganic halide perovskites as emerging next-generation light emitters are getting attention in academia and industries due to their advantages of low material cost, simple synthesis process, wide color gamut. Polycrystalline perovskites have fundamental limitations of long exciton diffusion length and small exciton binding energy. Moreover, passivating the defects at the grain boundary is also critical when the grain size becomes smaller. Making small nanograins in polycrystalline perovskite thin-films while passivating the grain boundary is critical to improving the luminescent efficiency in perovskite light-emitting diodes (PeLEDs). Small molecular additives can passivate the defects at grain boundaries by shielding the nanograins. However, uneven additive distribution causes imbalanced charge distribution and inefficient defect healing. In this work, we finally developed polycrystalline organic-shielded nanograins (OSN) with uniformly-distributed organic additives mimicking core-shell nanoparticles and thus high device efficiency of 21.8% and four-times increased device lifetime was achieved through the effective exciton confinement, improved radiative recombination, and efficient optical out-coupling by the low refractive index of the OSN emitting layer. Therefore, our novel strategy will provide a simple and efficient way to fabricate highly effective polycrystalline perovskite films and their optoelectronic applications.

### Keywords:

halide perovskites , nanograins , semiconducting additive , light-emitting diodes

## Perovskite and quantum dot light-emitting diodes for future realistic displays

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### Abstract:

In this talk, I will present my research to overcome limitations of high color-purity light-emitting diodes (LEDs) including metal halide perovskite LEDs (PeLEDs) and quantum dot LEDs (QLEDs) for next-generation realistic display applications.

Before 2014, room-temperature electroluminescence from metal halide perovskites was considered almost impossible. We have solved this problem by identifying fundamental efficiency-limiting factors and developing two novel strategies: (1) *In-situ* fabrication of perovskite nanocrystals based on crystallization control<sup>[1]</sup> and (2) introducing quasi-2D structures with ligand-like A-site cations (Ruddlesden-Popper phase).<sup>[2,3]</sup> Those strategies led to a world-first breakthrough in the brightness and efficiency of perovskite LED at room temperature. These works greatly stimulated PeLED research and totally changed the paradigm of the display industry that focused only on organic or QD emitters.

On the other hand, precision patterning of QDs is a critical step to fabricate displays incorporating QD color filters and QLED subpixels in form of RGB matrix. However, high-resolution patterning of solution-processed QD layers is fundamentally challenging because conventional patterning methods cannot simultaneously meet the requirements of high resolution, pattern uniformity, high throughput, and high photoluminescence quantum yield. To overcome this challenge, we developed a direct, scalable, and nondestructive route for high-resolution patterning of QDs and QLEDs.<sup>[4]</sup> A specially designed nanocrystal ink, "photopatternable emissive nanocrystals (PEN)", consists of gradient core/shell QDs and photoacid generators which enable photochemically activated reactions leading to in-situ ligand exchange in the QD films. Uniform electroluminescence patterns of RGB QLEDs with features size down to 1.5  $\mu\text{m}$  were demonstrated while preserving the structural, electronic, and emissive properties of patterned QDs.

### Keywords:

Metal halide perovskites, colloidal quantum dots, electroluminescence, direct optical patterning

## Preparation of Chemically Stable Ultrathin SiO<sub>2</sub>-Coated Core–Shell Perovskite QDs via Modulation of Ligand Binding Energy and PeLED Applications

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### Abstract:

Perovskite quantum dots (QDs) have attracted significant interest due to their outstanding opto-electrical properties, but their chemical and environmental instabilities impediments the development of the high-performance perovskite QD-based light-emitting diodes (PeLEDs). In this study, chemically stable SiO<sub>2</sub>-coated core–shell perovskite QDs are prepared to fabricate all-solution-processed PeLEDs. Controlling the SiO<sub>2</sub> thickness is essential to obtain core–shell perovskite QDs optimal for PeLEDs in an aspect of chemical and opto-electrical properties. Optimization of the APTES/OAm ratio affords less defective core-shell CsPbBr<sub>3</sub> QDs with an ultrathin SiO<sub>2</sub> shell, resulting in high PLQY. The all-solution-processed PeLED exhibited maximum current efficiencies of ~5.3 cd/A, compared with that of PeLED using pristine CsPbBr<sub>3</sub> QDs (~0.08 cd/A).

### Keywords:

Perovskite quantum dots, PeLED

## Self-Selective Ferroelectric Memory Realized with Semimetallic Graphene Channel

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### Abstract:

In this talk, the experimental works demonstrating a new concept of read-out method for ferroelectric random-access memory (FeRAM) using a graphene layer as the channel material of bottom-gated field effect transistor structure will be presented. The transconductance of graphene channel is found to change its sign as the spontaneous polarization (SP) direction in the underlying ferroelectric layer switches due to the ambipolar characteristics of graphene in its charge carrier transport. This indicates that the memory state of FeRAM, specified by the SP direction of ferroelectric layer, can be sensed unambiguously with transconductance measurements [1]. With the proposed read-out method, it is possible to construct an array of ferroelectric memory cells in the form of cross-point structure where the transconductance of a crossing cell can be measured selectively without any additional selector. This type of FeRAM can be a plausible solution for fabricating high speed, ultra-low power, long lifetime, and high density 3D stackable non-volatile memory.

Supported by Samsung (SRFC-TA1903-02) and NRF (2020M3F3A2A02082437)

### Keywords:

Ferroelectric Memory, Graphene, Ambipolar Carrier Type, Field Effect Transistor, Transconductance

## Making room temperature ferromagnetism of lead-free ferroelectric materials

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### Abstract:

Multiferroic materials have been promised to apply for the next smart electronic devices. However, multiferroic materials are rare because favorable interactions of ferroelectric and ferromagnetic properties usually are excluded in nature. Among lead-free ferroelectric materials,  $\text{Bi}_{1/2}\text{Na}_{1/2}\text{TiO}_3$ -based materials are environment friendly and less harmful to the human body than  $\text{Pb}(\text{Zr,Ti})\text{O}_3$ -based materials. Recently,  $\text{Bi}_{1/2}\text{Na}_{1/2}\text{TiO}_3$  materials promised to extend functional materials due to observation of room-temperature ferromagnetism. The observation of room-temperature ferromagnetism in lead-free  $\text{Bi}_{1/2}\text{Na}_{1/2}\text{TiO}_3$  ferroelectric materials is significant to transfer the materials to next generations of electronic devices, such as magnetic field sensors, mechanical ME antennas, or nonvolatile memories, etc. However, the current issue of using lead-free ferroelectric  $\text{Bi}_{1/2}\text{Na}_{1/2}\text{TiO}_3$  materials by converting magneto-electric behaviors is that the magnetization of about 1-2 memu/g at room temperature is too small and has a strong influence on diamagnetic components [1-3]. Thus, improving the magnetization of lead-free ferroelectric  $\text{Bi}_{1/2}\text{Na}_{1/2}\text{TiO}_3$ -based materials is an essential requirement for the development of their magnetic performance. Herein, we reported the new observation in room temperature ferromagnetism for lead-free ferroelectric  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  materials via using the solid solution with  $\text{ABO}_3$ -type materials such as  $\text{SrMnO}_{3-d}$ ,  $\text{CaFeO}_{3-d}$  or  $\text{BaFeO}_{3-d}$  [1-3]. The results are important to point out that the co-modification of *A*-site via alkaline-earth and *B*-site via transition metal has strongly improved the magnetic moments rather than that of single transition metal dopants. We expect our method to provide a flexible and straightforward approach to integrating the ferromagnetic properties in current advanced functional lead-free materials.

### Keywords:

multiferroic, lead-free ferroelectric, ferromagnetic, sol-gel method

## Modified Orbital Occupancy induced MIT of VO<sub>2</sub> films by Octahedral Symmetry

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### Abstract:

Vanadium dioxide (VO<sub>2</sub>) has received much attention due to its near room temperature (RT) metal-insulator transition (MIT). Even though the physical origin of the phase transition mechanism is still controversial in scientific, the presence of near RT phase transition offers many potential applications in sensors, smart windows, etc., in practice. Therefore, obtaining the controllability of phase transition characteristics such as temperature range and slope, and resistivity variation are crucial.

In this presentation, we showed the existence of transition characteristics variation of VO<sub>2</sub> film via film thickness variation. By carefully examining the structural and chemical variations, we found the correlation between the asymmetry octahedral structure, orbital occupancy, and the MIT temperature of monoclinic VO<sub>2</sub> films with different in-plane compressive strains. As a result, the octahedral structure with low asymmetry, caused by the in-plane compressive strain, increased the splitting between  $d_{||}$  and  $d_{||}^*$  orbitals and the bandwidth of  $\pi^*$ . The modified orbitals suppressed the hybridization of V 3d - O 2p and subsequently increased interdimer hopping energy, lowering the energy barrier for MIT. As a result, the VO<sub>2</sub> with the low asymmetric octahedral structure has a lower MIT temperature than the VO<sub>2</sub> with a high asymmetric one. These results provide the role of octahedral symmetry in tuning the MIT temperature of VO<sub>2</sub>.

This work is supported by NRF-2018R1D1A1B07045663 & NRF- 2021M3H4A6A02045432

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### Keywords:

MIT, VO<sub>2</sub>, Octahedral Symmetry

## Insight into the adsorption of hydrogen on Sc<sub>2</sub>C monolayers from the perspectives of first-principles

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### Abstract:

MXenes are two-dimensional, multilayered structures in that a monolayer consists of an atomic layer of carbon or nitrogen sandwiched by transition metals [1]. Due to their structural diversities and intriguing electronic properties, they become potential platforms for a wide range of applications as co-catalysts for hydrogen evolution, electrodes in Li-ion batteries, sensing material for gas detection, as well as medium for hydrogen storage [2, 3]. MXenes Sc<sub>2</sub>C monolayers have been reported to be an efficient medium for hydrogen capturing [4]. In this work, we have examined the adsorption properties of hydrogen on pristine Sc<sub>2</sub>C monolayers by DFT calculations [5]. Based on these calculations, we proposed a simple thermodynamic model to estimate the hydrogen storage capability within the typical ranges for the operating temperature and pressure. In addition, we also thoroughly evaluated the changes in the electronic structure of the Sc<sub>2</sub>C monolayer upon adsorbing hydrogen. Since the bandgap of Sc<sub>2</sub>C changes significantly upon adsorbing H<sub>2</sub>, Sc<sub>2</sub>C may have more potential as a hydrogen detector along with a hydrogen storage material.

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## Latest Advances and Prospective of Cryo-Electron Microscopy

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### Abstract:

Transmission electron microscope (TEM) is an optical instrument that utilizes electron wave as a beam source. Based on Rayleigh criterion, sub-nanometer wavelength of electron radiation allows for imaging at atomic resolution. Since its invention in the early 1930s by Ernst Ruska, TEMs have made enormous contributions in physics, chemistry, material science and life science.

In biological sciences, TEM offers high resolution and versatility that can visualize samples that range from atomic details of molecular structures of proteins to cellular ultrastructures. In particular, technology that can produce the reconstruction of 3D electron coulomb potential maps from the 2D projection images of TEM, so-called 3D electron microscopy (3DEM), has led significant advancements in our understanding of biological processes in recent years. Most pivotal breakthrough in high-resolution 3DEM is the development of cryo-electron microscopy (cryo-EM). Cryo-EM is a technique that involves combination of cryogenic sample preparation, low electron dose imaging and computational image processing. Developments in instrumentations and software algorithms in the past decade have dramatically improved achievable resolution by cryo-EM, which can now resolve individual atoms in frozen-hydrate proteins.

In this presentation, basic principles in cryo-EM and recent technical breakthroughs will be introduced, and current efforts in technical development of electron tomography for in situ biological imaging will be discussed.

### Keywords:

Cryo-electron microscopy, electron tomography, single particle analysis, transmission electron microscope

## Swimming bacteria in 2D confinement: Observing Stochastic and Deterministic Processes

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### Abstract:

Motile bacteria have been of keen interest not only from biomedical perspectives but also in statistical and biological physics, as a model system. Here I report our ongoing observations of bacterial motion in the 2D environment. First, utilizing extensive data from the automated tracking of their 2D motions, we propose a revision of common stochastic motility models, e.g., run-and-tumble motion, pinpointing the inherent heterogeneity in bacterial motility. Second, we find the interfacial tension-driven interactions between the bacteria and liquid-liquid interface can govern the motile behavior in a deterministic way, in contrast to the stochastic nature of 2D swimming. These observations reassure the usefulness and necessity of physics to understand the microbial world.

### Keywords:

Bacteria, Heterogeneity

## Structural basis for a dynamic metallocofactor in Mo-nitrogenase.

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### Abstract:

Nitrogenase converts inert nitrogen gas into an ammonia, a usable form by biological organisms using adenosine triphosphate and several iron-sulfur clusters. The enzyme pumps electrons into iron-molybdenum cofactor (FeMoCo) to reduce the substrates, but the mechanistic details of this reaction remain elusive. Recently, we reported a crystal structure of a N<sub>2</sub>-bound Mo-nitrogenase (Av1\*) captured under physiological N<sub>2</sub> turnover conditions. The structure reveals asymmetric displacements of the cofactor belt sulfurs with distinct N<sub>2</sub> species. The sulfur-displaced sites are distinct in the ability of protein ligands to donate protons to the bound N<sub>2</sub> species, as well as the R-homocitrate. It was further supported by the release of <sup>15</sup>N<sub>2</sub> from the acid-quenched nitrogenase that was isolated from the <sup>5</sup>N<sub>2</sub>-grown culture. Interestingly, we showed that Av1\* is clearly distinct from its resting-state counterpart in displaying previously unobserved, turnover-related S=1/2 electron paramagnetic resonance (EPR) features concomitant with a ~50% reduction of the magnitude of its 3/2 signal. Taken together, our observation that all three belt-sulfur sites are involved in catalysis is consistent with the dynamic nature of the FeMoCo, and provides evidence for participation of all belt-sulfur sites in this process.

### Keywords:

nitrogen cycle, nitrogen fixation, nitrogenase, FeMo cofactor, P-cluster

## Photoacoustic endomicroscopy as a new tool for the in vivo visualization of microvasculature

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### **Abstract:**

Blood vessel is an indispensable component that constitutes the circulatory system of our body to supply oxygen and nutrients to tissues and organs and also to take waste and carbon dioxide away from them. Not only the basic function, it also has been importantly recognized as the key element that it is closely related to the onset and progression of the well-known diseases, such as cancers, hypertension, Alzheimer's disease, and many other metabolic diseases including diabetes. In this talk, I will introduce our photoacoustic endomicroscopy technique developed for the in vivo visualization of microvasculature targeting all possible biomedical applications in a broad scope. Due to the importance of blood vessel in biological systems, developing a related visualization technique (i.e., angiography) has been an important subject always in biomedical engineering and physics. However, existing angiographic techniques suffer from either slow imaging speed (MRI) or shallow imaging depth (confocal microscopy) and also require a dedicated contrast agent in most cases. In this respect, we expect that our technique could make a viable contribution to biomedicine because it can provide capillary- or organ-level visualization of vasculature at a much higher speed and also without the aid of a contrast agent. In this talk, several biomedical application examples that we have been conducting will be presented.

### **Keywords:**

Biomedical imaging, photoacoustic imaging, endomicroscopy, microvasculature, angiography

## The equation of state of dense matter and nuclear physics constraints

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### Abstract:

The exceptional progress of multi-messenger astronomy on different astrophysical sources of dense matter has very recently led to quantitative measurements of various properties of neutron stars, such as the tidal polarizability from gravitational wave LIGO/Virgo data, and the correlation between mass and radius from X-ray timing with NICER. These observations, together with the plethora of upcoming data, are expected to unveil in the next future exciting open questions such as the structure and degrees of freedom of baryonic matter in extreme conditions, and in particular the presence of phase transitions and the existence of deconfined matter in the core of neutron stars.

This direct connection between astrophysical measurements and the microphysics of dense matter is due to the well-known fact that, under the realm of general relativity, there is a one-to-one correspondence between any static observable and the dense matter equation of state.

However, the task is complicated by the uncertainty on the effective energy functional, and similar equations of state can be obtained under different hypotheses on the underlying microphysics.

To identify the observables pointing towards more exotic constituents, it is important to quantitatively evaluate the space of parameters and observables compatible with the nucleonic hypothesis. We will review the different theoretical and experimental nuclear constraints that can be used to restrict the space of parameters, and show that both nuclear observables in the sub-saturation and super-saturation regime are needed to achieve a quantitative description of static astrophysical observables that will be challenged by the upcoming measurements.

### Keywords:

equation of state , symmetry energy , multi-messenger astronomy

## Experimental study of asymmetric nuclear matter equation of state by using heavy RI collisions at RIKEN-RIBF

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### Abstract:

Neutron star is believed to be created as a remnant of super nova explosion. In order to determine a thermodynamical character (EoS) of outer core of neutron star through terrestrial experiments, we have performed a series of measurements using RIKEN Radio Isotope Beam Factory (RIBF). Various central collisions between neutron-rich unstable tin nucleus and stable tin nucleus were measured. The density achieved by the collisions nearly corresponds to the one for the outer core of neutron star:  $\rho \sim 2 \times \rho_0$ .

As one of the probes for nuclear EoS, both positive and negative pions emitted from the high density nuclear matter were measured by using a newly developed large time projection chamber which can provide 3-dimensional image of their tracks.

Based on the comparison of spectral charged pion ratio with one of the transport models, we deduce the slope of the symmetry energy to be  $42 < L < 117$  MeV, which is consistent with the result given by the recent measurement of the neutron skin thickness of Pb-208.

### Keywords:

Heavy ion collision , nuclear EoS , pion , symmetry energy

## Status of LAMPS

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### **Abstract:**

Rare Isotope Accelerator complex for ON-line experiments (RAON) is expected to provide the RI beam optimized to study the equation of nuclear state, particularly exploring key parameters to understand the symmetry energy of the nucleus more precisely. The Large Acceptance Multi-Purpose Spectrometer (LAMPS) is designed for this research and is under construction in a high-energy facility room. In this presentation, we would like to report the current status and plan of LAMPS.

### **Keywords:**

RAON, LAMPS, Symmetry Energy

## Progresses in Metamaterials for Electromagnetic Radiation Applications: energy transfer and absorption

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### Abstract:

We report recent achievements related to our research on flexible metamaterial absorbers and near-field wireless power transfer in the GHz and MHz regions. Firstly, a dual-band, polarization-insensitive, ultrathin and flexible metamaterial absorber (MA), based on high-order magnetic resonance, was demonstrated [1]. By exploiting a flexible polyimide substrate, the thickness of MA came to be  $1/148$  of the working wavelength. The absorption performance of the proposed structure was investigated for both planar and bending models. In the case of the planar model, a single peak was achieved at a frequency of 4.3 GHz, with an absorption of 98%. Furthermore, additional high-order absorption peaks were obtained by the bending structure on a cylindrical surface, while the fundamental peak with a high absorption was maintained well. Secondly, a flexible broadband metamaterial perfect absorber (FBMPA) was proposed by exploiting a pasted conductive-graphene ink on a polyimide substrate [2]. For the flat FBMPA, an absorption over 90% was found to cover a wide frequency range (from 7.88 to 18.01 GHz). The high-absorption feature was polarization-insensitive and regarded as stable with respect to the oblique incidence up to 30 degrees of electromagnetic wave. The high absorption was maintained well even when the absorber was wrapped. That is, the FBMPA was attached to cylindrical surfaces (with the varying radius from 4 to 50 cm). For applications in wireless energy transfer, we investigated the propagation of magneto-inductive waves (MIWs) in ordering magnetic metamaterial (MM) structures [3]. The MIW propagates along with the MM structure through the magnetic coupling of MM unit cells. By exploiting the strong magnetic field confinement in the waveguide, the transmittance after nine elements of the non-homogeneous MM slab can be enhanced up to 5.2 times greater than that of the homogeneous MM slab. Our work might be useful for the realization and the development of future electronic devices, such as filters, emitters, detectors, sensors, low-frequency communication, wireless chargers and energy converters.

### References:

- [1] D. T. Ha et al., *Photonics* 8, 440 (2021).
- [2] L. V. Long et al., *Photonics* 8, 574 (2021).
- [3] L. T. H. Hiep et al., *Phys. Scr.* 97 025504 (2022).

### Keywords:

metamaterial, absorption, wireless power transfer, magneto-inductive wave waveguide

# Au-MoS<sub>2</sub> Nanostructures for Electronic and Optoelectronic Device Applications

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## Abstract:

MoS<sub>2</sub> is one of the most representative 2D semiconductors (SCs), which exhibit unique electrical, optical, and mechanical properties. Understanding the band alignment at metal/SC contacts is crucial for electrical characterizations of SC materials as well as fabrication of high-performance devices. Numerous works have reported experimental and theoretical approaches to optimize the electrical properties of metal/2D SC contacts. In addition to the conventional transport analyses, we have measured contact potential measurements of Au/MoS<sub>2</sub> contacts using Kelvin probe force microscopy (KPFM), which have revealed the distinct features of 2D SC contacts compared with the 3D counterparts. When Au nanostructures, such as nanogratings, nanodots, and nanoholes, are integrated with MoS<sub>2</sub> layers, the plasmonic effects play important roles in the optical characteristics of the Au-MoS<sub>2</sub> nanostructures. Using KPFM, we obtained the surface photovoltage maps of the nanostructures, which could visualize the spatial distribution of net charges under illumination. Plasmon-induced light confinement and potential gradient at Au-MoS<sub>2</sub> contacts can affect creation and drift of the photo-generated charge carriers. Complementary measurements using KPFM and conventional techniques improve our understanding of photon-plasmon-exciton coupling in Au-MoS<sub>2</sub> nanostructures, leading to proposal of novel electronic and optoelectronic devices.

## Keywords:

MoS<sub>2</sub>, metal semiconductor contact, Kelvin probe force microscopy, surface photovoltage

## Efficient ambient ammonia synthesis by Lewis acid pair over cobalt single atom catalyst with suppressed proton reduction

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### Abstract:

Improving the ammonia yield and Faraday efficiency of ambient electrochemical nitrogen fixation is a priority for altering the energy-intensive Haber-Bosch process. In this work, positively charged single cobalt atoms anchored on sponge-like nitrogen-doped mesoporous interconnected hollow carbon nanofibers (serving as a Lewis acid pair) were intentionally designed as catalytic centers that can suppress the side effect of the competing hydrogen evolution reaction and simultaneously boost the electrochemical conversion of nitrogen ( $N_2$ ) to ammonia ( $NH_3$ ). The Lewis acid pair catalyst exhibits an  $NH_3$  production rate of  $67.6 \mu g h^{-1} mg^{-1}$  and a maximum Faraday efficiency of 56.9 % at a peak potential of -0.1 V vs. RHE, which outperforms previously reported nitrogen reduction reaction (NRR) catalysts. First-principles DFT calculations suggest the regulation of the local electronic structure that induces Lewis acid pair formation upon charge transfer between the single Co atom and substrate, confirming a high intrinsic NRR by both experiments and theoretical calculations.

### Keywords:

Lewis pair, single atom catalyst, ammonia synthesis, nitrogen reduction reaction, electrocatalytic

## STM investigation on layered chalcogenide materials

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### Abstract:

Layered chalcogenide materials (LCMs) have been intensively studied due to their versatile physical properties and potential applications. In this presentation, I would like to introduce our recent progress of scanning tunneling microscopy (STM) investigations on layered chalcogenide materials. First, heterointerface effect will be discussed for two-dimensional junction of monolayer (ML) ReSe<sub>2</sub> grown on bilayer graphene (BLG) [1]. ML ReSe<sub>2</sub> shows an energy gap of 1.7 eV with the conduction and valance band edges of 0.5 eV and -1.2 eV, respectively. Interestingly, STM image obtained within the band gap (i.e., at in-gap bias voltages) reveals unexpected structure, which is attributed to ReSe<sub>2</sub> – graphene heterointerface effect. Density functional theory (DFT) calculations confirm that the observed in-gap topography shows trapped charge distribution at the heterointerface. Secondly, I will briefly discuss about Fe-Ge ordering leading to helimagnetism in Fe<sub>5-x</sub>GeTe<sub>2</sub> [2]. Fe<sub>5-x</sub>GeTe<sub>2</sub> system is suggested as a promising van der Waals ferromagnet due to its high Curries temperature of ~ 317 K. STM analysis reveals that two symmetric orderings of Fe-Ge pairs give rise to  $\sqrt{3}\times\sqrt{3}$  superstructures in Fe<sub>5-x</sub>GeTe<sub>2</sub>. Interestingly, the orderings of Fe-Ge pairs break the inversion symmetry which results in helimagnetism in Fe<sub>5</sub>GeTe<sub>2</sub>. Analytic study also supports that the observed ordering can induce the helimagnetism.

### References

- [1] Trinh Thi Ly *et al.*, Appl. Surf. Sci. **12**, 2490 (2022)
- [2] Trinh Thi Ly *et al.*, Adv. Funct. Mater. **31**, 2009758 (2021)

### Keywords:

STM, ReSe<sub>2</sub>, Fe<sub>5-x</sub>GeTe<sub>2</sub>, Heterointerface effect, Helimagnetism

## Recent Progress on the Black Hole Information Problem

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### **Abstract:**

The black hole information problem — whether information escapes an evaporating black hole — is one of the most longstanding problems in theoretical physics. Recent years have seen a leap in progress on many facets of the subject, from entropy to complexity. I will review this progress and describe some open questions.

## Wormholes and Black Holes

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### **Abstract:**

I will give a review of the recent progress on understanding the physics of black holes using wormholes.

### **Keywords:**

Wormholes, Black Holes

## Quantum circuit picture of black hole interior

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### **Abstract:**

I will give an overview about the quantum circuit picture of black hole interior. I will discuss how this picture is connected to the recent development on holographic complexity, information retrieval from black hole, and Python's lunch.

## **WIMPs interpretations with NaI detectors: DAMA/Libra and beyond**

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### **Abstract:**

I will show that analyzing the data with the smallest set of theoretical assumptions it is possible to reconcile a phenomenological interpretations of the DAMA/Libra excess in terms of a WIMP signal with the constraints from detectors using targets different from sodium iodide. I will also stress the importance of complementarity among different target nuclei and of the role of sodium iodide scintillators when analyzing direct detection data in model-independent ways.

### **Keywords:**

Weakly Interacting Massive Particles, Dark Matter, Direct Detection

## Testing DAMA/LIBRA at three-sigma with ANAIS–112 experiment

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### Abstract:

DAMA/LIBRA observation of an annual modulation in the detection rate compatible with that expected for dark matter is one of the most puzzling results in the present particle physics scenario. In this talk I will review the performance, present status and prospects of ANAIS-112 experiment. ANAIS-112 experiment, using 112.5 kg of NaI(Tl) as target, is taking data at the Canfranc Underground Laboratory in Spain since August 2017. Results corresponding to 3 years were presented in 2021. These results are compatible with the absence of modulation and in tension with DAMA/LIBRA result. Moreover, they support our goal of reaching a  $3\sigma$  sensitivity to the DAMA/LIBRA result with 5 years of data that will be accomplished along 2022.

## COSINE experiment

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### **Abstract:**

Astrophysical observations give overwhelming evidence for the existence of dark matter. Several theoretical particles have been proposed as dark matter candidates, including weakly interacting massive particles (WIMPs), axions, and more recently, their much lighter counterparts. However there has not yet been a definitive detection of dark matter. One group, the DAMA collaboration, has asserted for years that they observe a dark matter-induced annual modulation signal in their NaI(Tl)-based detectors. Their observations seem to be inconsistent with those from other direct detection dark matter experiments under most assumptions of dark matter. In this talk I will discuss the COSINE-100 and COSINE-200 experiments and our progress toward resolving the current stalemate in the field.

## Neutrino mean free path within neutron star with the KIDS-EDF model

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### Abstract:

The Korea-IBS-Daegu-SKKU energy density functional (KIDS-EDF) model has been widely and successfully applied to describe the properties of finite nuclei and infinite nuclear matter. In the present work we extend the application of the KIDS-EDF model to neutrino mean free path and its interaction with neutron star matter constituents using the linear response approach. The roles of neutron and proton effective masses and symmetry energy on neutrino interaction in neutron star will be investigated. Our remarkable results on neutrino mean free path in neutron star will be presented and their implications to the properties of neutron star (M-R relations) and neutron star cooling will be also discussed.

### Keywords:

KIDS-EDF model, Neutrino mean free path, symmetry energy, Neutron star, nucleon effective mass

## The electromagnetic fluctuation in the astrophysical plasma.

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### Abstract:

본 연구는 천체 플라스마 내부에서 발생하는 전자기 요동이 핵반응에 미치는 영향에 대해 논의한다. 천체 플라스마 내부에는 열적으로 평형을 이루고 있는 상황에서도 전기장과 자기장의 요동이 발생할 수 있다. 이러한 전자기 요동은 플라스마 환경의 수직 유전율(transverse permittivity)을 변화시킨다. 그 결과 광자의 분포가 달라지게 되며 이는 천체 플라스마 내부의 열 핵반응에 영향을 미칠 수 있다. 또한 별 내부에서는 광자에 의한 복사압이 달라지는 결과를 얻게 된다. 본 연구에서는 초기우주와 태양의 환경에서 전자기 요동에 의해 달라진 광자의 분포를 비교하고 해당 변화로 인해 각 환경에서 달라지는 핵반응과 태양 중성미자의 변화를 논의한다.

### Keywords:

electromagnetic fluctuation, astrophysical plasma, solar neutrino, thermonuclear reactionrate

## The effect of the magnetized electron to neutrino process in core-collapse supernova

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<sup>2</sup>Center for Relativistic Laser Science, IBS

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### Abstract:

초신성 폭발 시 나오는 다량의 중성미자들은 별 내부에서 다른 입자들과 상호작용하면서 초신성 밖으로 나오게 됩니다. 이때 초신성 내부 전자들 뿐만 아니라 중성미자들과의 상호작용으로 인해 중성미자 진동이 영향을 받습니다. 이번 연구에서는 이전 연구에서 고려했던 상호작용에 더해 초신성 내부에 매우 강한 자기장이 존재 할 때 중성미자와 전자들의 상호작용에 대해 논의합니다. 자기장으로 인해 전자들이 정렬하게 되고 전자와 전자 중성미자의 상호작용이 달라지게 됩니다. 이는 초신성 폭발시 중심으로부터 나오게 되는 중성미자와 핵 사이의 열핵반응들을 바꿀 수 있다는 것을 의미합니다. 이로 인해 초신성 폭발시 중성미자가 유도하는 핵반응(neutrino-process)을 계산해서 원소들의 생성양을 바꿀 수 있는 가능성에 대해 소개를 하려고 합니다.

## Stellar Nucleosynthesis Studies with the COREA Detector

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<sup>1</sup>Department of Physics, Korea University  
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### Abstract:

The COREA (**C**arbon **O**xygen **R**eaction **E**xperiment with **A**ctive-target TPC) is an experiment to measure the precise cross-section of the  $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$  reaction in stellar nucleosynthesis. We constructed a conduction-cooled superconducting magnet with a maximum field of 3 T. We tested the cooling performance and mapped out the field strengths over the AT-TPC volume. We also tested LaBr<sub>3</sub> detectors with a Am/<sup>13</sup>C neutron source and a Ni disc for the energy calibration in the range up to 10 MeV. Furthermore, Geant4 simulation was performed to study the performance of the TPC with the superconducting magnet. We will present the performance of the 3-T superconducting magnet and LaBr<sub>3</sub> gamma-ray detectors, and the simulation results.

### Keywords:

Stellar nucleosynthesis, Superconducting magnet, Active-target TPC, Gamma-ray detector

## Oxygen isotopes in Nuclear Lattice Effective Field Theory

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### **Abstract:**

For the non-perturbative calculation of nuclear  $N^3\text{LO}$  interaction in Nuclear Lattice Effective Field Theory, new wave function matching method is developed. We discuss the results of preliminary calculation of wave function matching method for Oxygen isotopes and its implications.

## Hint of shape evolution in $^{110}\text{Sn}$ from Coulomb excitation

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### Abstract:

The structure of semi-magic Sn isotopes has been brought to focus by a recent theoretical work using Monte Carlo Shell Model (MCSM). Explanations for the trends of experimental  $B(E2; 0_1^+ \rightarrow 2_1^+)$  values of Sn isotopes, deviating away from the simple seniority scheme, were accompanied by shape evolution from spherical to either prolate or oblate shapes of excited states. From the analysis of Doppler-shifted gamma-ray data from a Coulomb excitation experiment on  $^{110}\text{Sn}$  at HIE-ISOLDE, the lifetime of the  $2_1^+$  state was extracted for the first time. In conjunction with the obtained Coulomb excitation cross section, the direct conversion of the lifetime to the  $B(E2)$  value hints at a non-zero intrinsic quadrupole moment of the  $2_1^+$  state in  $^{110}\text{Sn}$ . This result is consistent with the MCSM, and challenges the historical assumption of spherical excited states in semi-magic Sn isotopes when determining  $B(E2)$  values from Coulomb excitation experiments.

### Keywords:

Nuclear deformation, Coulomb excitation, Lifetime measurement, Gamma-ray spectroscopy

# Energy Correction Methods for High Resolution Prompt and Delayed Gamma-ray Spectroscopy Using AGATA and EXOGAM Ge Detector Array

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## Abstract:

Studying the nuclear structure of neutron-rich nuclides near N=126 major shell closure is important to understand nuclear interactions, nuclear shell evolution and relevant to the nuclear-astrophysical r-process. We used multi-nucleon transfer reactions of 7MeV/u  $^{136}\text{Xe}$  beam on  $^{198}\text{Pt}$  target to access these nuclei. VAMOS++ spectrometer [1] at GANIL was used to detect and identify the projectile-like fragments at 40° angle, and the complementary target-like fragments were detected by a newly constructed second arm which was installed in the relevant angle range. The prompt and delayed gamma rays from nuclei of interest was measured by AGATA HPGe tracking array with 13 triple clusters [2] placed around the target position and 4 EXOGAM HPGe clover detectors [3] placed at the end of the second arm, respectively.

In order to measure the energy of low-lying states of the nuclide we are interested in, precision measurement using gamma-ray spectroscopy of AGATA and EXOGAM array is essential. The initial calibration and efficiency of AGATA and EXOGAM detectors were obtained using known radioactive sources such as  $^{152}\text{Eu}$ . In this presentation, we will mainly discuss the way to improve the calibration using iterative correction for gain changes over time with on-line data. We will also discuss the method for checking and correcting the crosstalk of crystals in each EXOGAM detector, for better add-back procedures.

## References

- [1] M. Rejmund et al., Nucl. Instr. And Meth. A, 646, 184-191 (2011)
- [2] S. Akkoyun et al., Nucl. Instr. And Meth. A, 668, 26-58 (2012)
- [3] J. Simpson et al., Acta Phys. Hung. New Ser. Heavy Ion Phys. 11, 159 (2000)

## Keywords:

AGATA, EXOGAM, Gamma-ray spectroscopy

## Particle identification of VAMOS++ spectrometer data using artificial neural network

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### Abstract:

The evolution of low-lying nuclear states of the neutron-rich nuclides near  $N=126$  magicity in the south of  $^{208}\text{Pb}$  is important for studying the evolution of nuclear shell and interaction. Especially the evolution of  $\pi 1h_{11/2}$  single-particle state is crucial for providing constraints to astrophysical r-process predictions.

We used multi-nucleon transfer reactions of  $7\text{MeV/u } ^{136}\text{Xe}$  beam and  $^{198}\text{Pt}$  target to study these nuclei at GANIL G1 hall. The projectile-like fragments were identified by VAMOS++ magnetic spectrometer [1]. The target-like fragments were detected by newly installed second arm which is composed of a vacuum chamber and multi-wire proportional counter to measure the velocity vector. The prompt and delayed gamma rays from the excited states of the produced nuclei were measured by the AGATA HPGe tracking array [2] at the target position and the EXOGAM HPGe clover array [3] at the end of second arm, respectively.

Before studying the nuclear structure by gamma rays, unambiguous particle identification of the nuclei is essential. Multi-parameter analysis is used for particle identification of VAMOS++ spectrometer due to the complexity of detector setup and reconstruction method. We present the conventional method and the new method using deep neural network (DNN) to determine mass and charge states. The mass and charge state resolution shows similar value as reported from the literature [4] using the conventional analysis technique.

### Reference

- [1] M. Rejmund et al., Nucl. Instr. And Meth. A, 646, 184-191 (2011)
- [2] S. Akkoyun et al., Nucl. Instr. And Meth. A, 668, 26-58 (2012)
- [3] J. Simpson et al., Acta Phys. Hung. New Ser. Heavy Ion Phys. 11, 159 (2000)
- [4] Y. H. Kim et al., Eur. Phys. J A, 53, 162 (2017)

### Keywords:

VAMOS, AGATA, machine learning, neural network, shell evolution

## Exact-exchange functional in relativistic nuclear density functional theory: study for neutron drops

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### Abstract:

The exchange terms can play an important role in describing the ground state and excited state properties of finite nuclei.

We apply the relativistic optimized potential method to take into account the exchange energy in the relativistic nuclear density functional theory. This method is applied to solve the ideal neutron drop systems and very close agreement with the relativistic Hartree-Fock (RHF) calculation is found. It is the first time that this method is extended to describe not only with the vector potential but also the scalar potential. By using this method, the RHF equation, which is not easy to solve, is replaced by the relativistic local Kohn-Sham equation. It is hopeful to further apply the exchange terms to the cases where the RHF cannot be applied currently due to its complexity, e.g., triaxial deformed nuclei.

### Keywords:

Nuclear density functional theory, Relativistic density functional theory, Relativistic optimized potential method, Relativistic Hartree-Fock, Neutron drop

## Tolman temperature in general relativity

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### **Abstract:**

We examine Tolman temperature due to gravity by using Carter's variational formalism of thermodynamics. We restrict our interests to fluids in dynamical thermal equilibrium that the heat does not propagate, but chemical and mechanical changes can happen. We show that the condition presents a general formula for the local temperature gradient. This condition allows defining a temperature for fluids in a time-dependent spacetime. We also address a resolution for the recently addressed conflict in Tolman temperature when a chemical potential does not vanish.

### **Keywords:**

Tolman temperature, general relativity

## The meaning of the speed of light in the FLRW universe.

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### **Abstract:**

We review the speed of light both in Minkowski spacetime and in the Friedmann- Lemaître- Robertson-Walker (FLRW) universe. The local Lorentz frame is defined simply as a lattice of space and time coordinates. This is done for the homogeneous and isotropic Universe (i.e., FLRW universe). We show that the new interpretation of the speed of light is required in order to satisfy the cosmological principle.

### **Keywords:**

speed of light, FLRW universe, adiabatic expansion

## Classicality revisited via Wheeler-DeWitt equation

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### **Abstract:**

We study the Hartle-Hawking wave function in the light of the Wheeler-DeWitt equation. The classicality notion from the instanton computations might be extended if we study the global structure of the wave function of the universe. We discuss possible conceptual issues.

### **Keywords:**

quantum cosmology, Wheeler-DeWitt equation, Hartle-Hawking wave function

## Gravitational Waves by the Perturbation of a Rotating Axisymmetric Rigid Body

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### **Abstract:**

Precession is one of the important mechanisms of gravitational wave generation in astrophysics. In general, free precession of a rigid body can be caused by the rotation of a triaxial body. In the case of symmetric body, if only the principal axis does not coincide with the axis of rotation, then there is the precession. When a symmetric body rotates around one of its principal axes, the body cannot move with precession. However, when there is a perturbation in angular velocity of the symmetric body spinning around the largest of the principal axes, the body can have a precession motion. In this presentation, the wave forms and their characteristics of gravitational waves by the perturbation of a rotating axisymmetric rigid body are studied.

### **Keywords:**

gravitational waves, rigid body, precession, perturbation

## Detection of Gravitational Waves by Electromagnetic Waves without Acceleration Noise

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### **Abstract:**

All detectors have motions with velocities and accelerations that affect measurements. Because electric and magnetic fields rely on 4-velocities of observers, their measurements also depends on the motions. Moreover, when we detect a gravitational wave (GW), the motions are under the influence of GW. Even if we set a stationary observer that does not oscillating along GW, the spatial direction in which the measurement is performed has an unpredictable rotational mode. To avoid these complexities, we propose a gauge-invariant quantity of electromagnetic waves to detect GWs without acceleration noise. We discuss a thought experiment to measure the quantity.

### **Keywords:**

gravitational waves, electromagnetic waves

## Binary neutron star mergers as a probe of quark-hadron crossover equations of state

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### Abstract:

We simulate binary NS mergers which adopt various quark-hadron crossover (QHC) EOSs which are constructed from combinations of a hadronic EOS ( $n_{\{b\}} < 2 \sim n_0$ ) and a quark-matter EOS ( $n_{\{b\}} > 5 \sim n_0$ ), where  $n_{\{b\}}$  and  $n_0$  are the baryon number density and the nuclear saturation density, respectively. At the crossover densities ( $2 \sim n_0 < n_{\{b\}} < 5 \sim n_0$ ), the QHC EOSs have a gradually increasing stiffness reaching to the stiffness of the strongly correlated quark matter. This enhanced stiffness leads to much longer lifetimes of the hypermassive NS than that for a pure hadronic EOS. We find a dual nature of these EOSs such that their maximum chirp GW frequencies  $f_{\{max\}}$  fall into the category of a soft EOS while the dominant peak frequencies ( $f_{\{peak\}}$ ) of the postmerger stage falls in between that of a soft and stiff hadronic EOSs. An observation of this kind of dual nature in the characteristic GW frequencies will provide crucial evidence for the existence of strongly interacting quark matter at the crossover densities for QCD.

# Gapless Electronic Topology Driven by Strong Correlations

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## Abstract:

In insulators, correlations can drive topological states, as exemplified by the fractional quantum Hall effect. Whether and how that happens in gapless matter is an outstanding and pressing question. I will describe a concrete route that has been taken from the canonical correlation physics of quantum criticality to electronic topology in strongly correlated metallic systems. This has been done in the context of heavy fermion metals, where there is well-defined input about the effective degrees of freedom that describe the low-energy physics. I will present the theoretical concept and salient properties of Weyl-Kondo semimetal [1,2]. They set the stage for a general approach of utilizing the cooperation between interactions and crystalline symmetry to produce correlated topological phases and design the corresponding materials [3], as well as for the identification of an electronic topological state without any free-electron counterpart [4]. Some general implications about topology and correlation physics will be discussed.

[1] H.-H. Lai, S.E. Grefe et al., PNAS115, 93 (2018)(<https://doi.org/10.1073/pnas.1715851115>)

[2] S. Dzsaber et al., PNAS 118,e2013386118(2021) (<https://doi.org/10.1073/pnas.1715851115>)

[3] L. Chen et al, arXiv:2107.10837 ( <https://arxiv.org/abs/2107.10837> )

[4] H. Hu et al., arXiv:2110.06182 ( <https://arxiv.org/abs/2110.06182> )

## Keywords:

Electronic topology, Strong correlations, Kondo-driven topological semimetal

# Giant signatures and genuine control of topology in Kondo systems

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## Abstract:

Heavy fermion compounds – intermetallics governed by the Kondo effect – initially attracted attention because of their unusual Fermi liquid behavior, with effective mass renormalizations by orders of magnitude [1,2]. Since they respond strongly to external control parameters, they then became model systems for the study of quantum criticality [3]. In this talk, I will discuss the most recent advance: the discovery of exceptional properties of Kondo systems with nontrivial electronic topology. As evidenced for the noncentrosymmetric and nonsymmorphic heavy fermion material Ce<sub>3</sub>Bi<sub>4</sub>Pd<sub>3</sub> [4,5], strong electron correlations can lead to giant signatures of topology [4-6], as well as the genuine topology control by only moderate magnetic fields [7]. I will also discuss how quantum criticality and correlation-driven topology may interplay [8], and close with an outlook.

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- [2] S. Paschen, and Q. Si, The many faces (phases) of strong correlations, Europhys. News 52/4, 30 (2021).
- [3] S. Paschen and Q. Si, Quantum phases driven by strong correlations, Nat. Rev. Phys. 3, 9 (2021).
- [4] S. Dzsaber, L. Prochaska, A. Sidorenko, G. Eguchi, R. Svagera, M. Waas, A. Prokofiev, Q. Si, and S. Paschen, Kondo insulator to semimetal transformation tuned by spin-orbit coupling, Phys. Rev. Lett. 118, 246601 (2017).
- [5] S. Dzsaber, X. Yan, M. Taupin, G. Eguchi, A. Prokofiev, T. Shiroka, P. Blaha, O. Rubel, S.E. Grefe, H.-H. Lai, Q. Si, and S. Paschen, Giant spontaneous Hall effect in a nonmagnetic Weyl-Kondo semimetal, PNAS 118, e2013386118 (2021).
- [6] H.-H. Lai, S.E. Grefe, S. Paschen, and Q. Si, Weyl-Kondo semimetal in heavy-fermion systems, PNAS 115, 93 (2018).
- [7] S. Dzsaber, D.A. Zocco, A. McCollam, F. Weickert, R. McDonald, M. Taupin, X. Yan, A. Prokofiev, L.M.K. Tang, B. Vlaar, L. E. Winter, M. Jaime, Q. Si, and S. Paschen, Controlling correlation-driven electronic topology, arXiv:1906.01182.
- [8] W. T. Fuhrman, A. Sidorenko, J. Hänel, H. Winkler, A. Prokofiev, J. A. Rodriguez-Rivera, Y. Qiu, P. Blaha, Q. Si, C. L. Broholm, and S. Paschen, Pristine quantum criticality in a Kondo semimetal, Sci. Adv. 7/21, eabf9134 (2021).

## Keywords:

Kondo systems, Weyl-Kondo semimetal, giant topological response, topology control

## Quantum spin liquid in a nearly disorder-free Kagome antiferromagnet $YCu_3(OH)_{6+x}Br_{3-x}$

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### Abstract:

Quantum kagome Heisenberg antiferromagnets (QKHA) have been hailed as one of the most promising platforms to realize quantum spin liquid (QSL)- a highly entangled quantum state featuring strong temporal and spatial spin correlations without any symmetry breaking. To date, only a handful of  $S=1/2$  kagome systems have been reported to host fractionalized spin excitations in the absence of long-range magnetic order, including the herbertsmithite  $ZnCu_3(OH)_6Cl_2$ , the kapellasite  $Cu_3Zn(OH)_6Cl_2$ , and Zn-barlowite  $Cu_3Zn(OH)_6FBr$ . Nevertheless, the Zn-Cu intersite disorder in such kagome materials hinders the experimental identification of a ground state inherent to QKHA, namely, resonating valence bond, gapped  $Z_2$ , and gapless  $U(1)$  spin liquids. In this vein, a newly discovered QKHA  $YCu_3(OH)_{6+x}Br_{3-x}$  ( $x \approx 0.3$ ) can shine a light on elucidating the nature of QSLs as it is nearly free from intersite disorders. In this talk, we present magnetization, specific heat, thermal conductivity, and Raman scattering measurements of  $YCu_3(OH)_{6+x}Br_{3-x}$  ( $x \approx 0.3$ ) and discuss their ramifications in view of the well-established theory.

### Keywords:

Quantum spin liquid, long-range entanglement, Kagome lattice

## Glassy behavior in quantum spin liquids

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### Abstract:

In quantum spin liquids, fractionalized excitation and massive entanglement are uniquely characterized with an emergent gauge structure. In particular, interaction between fractionalized particles and disorder effect may give rise to additional phase transitions at low temperature. In this talk, we introduce generic scalar fields and their interactions to characterize fractionalization and discuss the glassy behavior and relevant phase transitions. Our theory is widely applicable to U(1) quantum spin liquids in the presence of long range interaction between fractionalized particles.

### Keywords:

spin liquids, glass, fractionalization, gauge structure

## Measurements of nanosecond dynamics in ferroelectric oxides using synchrotron x-ray radiation from PAL

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### Abstract:

The nanosecond response of ferroic materials to the external stimuli is closely linked to the dynamics of ferroelectric polarization, domain, and phase. The order of hundreds picosecond time resolution of x-ray pulse generated from single-bunch mode at 3rd generation synchrotron radiation facility allows the nanosecond structural dynamics to be measured. We have measured electric-field-driven nanosecond dynamics in ferroelectric and dielectric materials using the recently developed hybrid bunch mode at Pohang Accelerator Laboratory (PAL). In this presentation, we will discuss how to synchronize the reference clock signal provided from PAL with the nanosecond electric pulse and detection. Then, we will discuss the nanosecond electric pulse-driven electromechanical response of ferroelectric relaxer Sn-doped BaTiO<sub>3</sub> thin film and non-polar to polar phase transformation of dielectric SrTiO<sub>3</sub> thin film.

### Keywords:

Ferroelectric, XRD, synchrotron radiation

## Open-loop non-raster scanning in high-speed atomic force microscope

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### Abstract:

Lateral non-raster scan can reduce the time used to acquire images in atomic force microscopy (AFM) by 1) a targeted scan of features in a sample, and/or 2) redesign of the scan trajectory to produce more natural scanner movement during scanning. Scanners installed with position displacement sensors are typically used in either case to match measured features to corresponding lateral positions. In this work, we present an open-loop approach to acquiring high-speed AFM (HS-AFM) images using non-raster scan trajectories. We use a custom HS-AFM setup to acquire images using Lissajous, cycloidal, spiral, and rosette scan patterns. The images obtained using the non-raster scan trajectories are comparable to those acquired using the widely employed raster scan approaches.

### Keywords:

Atomic force microscopy, non-raster scanning

## Anisotropic metamagnetic transition and intrinsic Berry curvature in magnetic Weyl semimetal NdAlGe

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### Abstract:

Single crystalline NdAlGe was synthesized and measured its anisotropic magnetism and magnetotransport property. NdAlGe shares same structure of  $I4_1md$  with neighboring RAX group PrAlGe and NdAlSi, so that has possible type-II Weyl semimetal(WSM) property invoked from inversion symmetry(IS) breaking with  $m_z$  mirror plane missing and time reversal symmetry(TRS) breaking from native magnetic  $Nd^{3+}$  ion. It was examined again by the density functional theory result, suggesting highly similar energy band structure that has multiple Weyl nodes lying on ab plane like other RAX materials.

NdAlGe has ferromagnetism on c-axis and metamagnetic transition, thought to be from same reason of collective magnetism like NdAlSi. We found it has  $607 \text{ (Ohm cm)}^{-1}$  of large anomalous Hall conductivity(AHC) and longitudinal magnetoresistivity(LMR) is located on moderately dirty metal regime, concluding the origin of large anomalous Hall effect(AHE) in NdAlGe is from intrinsic Berry curvature of WSM. Therefore, NdAlGe has both of properties of two neighboring WSM materials together, constitutently meaning the collective magnetism and correlation is making this material as special WSM.

### Keywords:

Weyl semimetal, Anomalous Hall effect

## Direct determination of quantum decoherence with high-harmonic spectroscopy

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### Abstract:

Ultrafast dynamics incorporating the quantum mechanical decoherence in graphene is explored through the high-harmonic spectroscopy. When Dirac electrons are exposed to the elliptically polarized laser pulse, the elliptically polarized high-harmonic generation (HHG) is produced and exhibits a rotation of the major axis of its polarization ellipse with respect to the pump pulse, which is found to sensitively depend on the quantum decoherence time,  $T_2$ , corresponding to an actual lifetime of the electric polarization scattered by hot electrons. Furthermore, it is found from the theoretical model that  $T_2$  could be in a wide range of subfemtoseconds under several optical conditions and eventually reach fs, the extreme ultrafast time scale in solids, which perfectly reproduces the experiment of the sub-laser-cycle high-harmonic spectroscopy. Providing a direct determination for the nonequilibrium response enables the dynamics of hot electrons toward an access to the controllable petahertz frequency domain.

### Keywords:

High-harmonic spectroscopy, electric polarization lifetime, graphene, quantum decoherence

## Current-driven modulation of magnetic interlayer coupling in $\text{Fe}_5\text{GeTe}_2$ van der Waals magnet

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### Abstract:

Magnetization control is principal issues in spintronics for proposing next generation memory devices. Particularly, there are increasing demands for versatile manipulation of magnetic state in van der Waals (vdW) magnets for spintronic devices with their unconventional functionalities. The control has been achieved by an external field and spin torque, which can switch the magnetization but yet modify the exchange coupling. Here, we report the current induced magnetic exchange transition from ferromagnetic to antiferromagnetic state in vdW ferromagnet  $\text{Fe}_5\text{GeTe}_2$ . Based on the current dependent magnetoresistance, we found that the transition occurs at a critical current, driven by the tunnelling current across the vdW gap. The current-tunability in  $\text{Fe}_5\text{GeTe}_2$  opens a path for electric control of the magnetic properties, expanding our ability to use the vdW magnets.

### Keywords:

2D ferromagnet, Magnetic exchange,  $\text{Fe}_5\text{GeTe}_2$

## Steady Floquet-Andreev States in graphene Josephson junctions

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### Abstract:

Engineering quantum states through light-matter interaction has created a new paradigm in condensed matter physics. A representative example is the Floquet-Bloch state, which is generated by time-periodically driving the Bloch wavefunctions in crystals. Previous attempts to realise such states in condensed matter systems have been limited by the transient nature of the Floquet states produced by optical pulses, which masks the universal properties of non-equilibrium physics. Here, we report the generation of steady Floquet Andreev (F-A) states in graphene Josephson junctions by continuous microwave application and direct measurement of their spectra by superconducting tunnelling spectroscopy. We present quantitative analysis of the spectral characteristics of the F-A states while varying the phase difference of superconductors, temperature, microwave frequency and power. The oscillations of the F-A state spectrum with phase difference agreed with our theoretical calculations. Moreover, we confirmed the steady nature of the F-A states by establishing a sum rule of tunnelling conductance, and analysed the spectral density of Floquet states depending on Floquet interaction strength. This study provides a basis for understanding and engineering non-equilibrium quantum states in nano-devices.

### Keywords:

Steady Floquet Andreev bound states, Josephson junctions, superconductor, Tunnelling spectroscopy

## Absence of supercurrent in edge-free Corbino graphene Josephson junction in the quantum Hall regime

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### Abstract:

The first observation of the supercurrent in graphene Josephson junction in the quantum Hall regime has attracted considerable attention, which demonstrated the hybridization of two seemingly incompatible phases: quantum Hall state and superconducting state. However, the mechanism of the quantum Hall supercurrent is still controversial due to not exactly quantized resistance at quantum Hall plateau. This suggests that the supercurrent may flow through not perfectly insulating bulk state instead of quantum Hall edge states. In order to specify this issue, we fabricated and measured graphene Josephson junction both in conventional rectangular geometry with edges and Corbino geometry without any edge. Highly transparent molybdenum/rhenium superconducting contacts are realized to achieve Josephson coupling as high as  $I_C R_N \sim 350 \mu V$  at zero magnetic field in both rectangular and Corbino geometry. In the quantum Hall regime, supercurrent was observed in rectangular graphene Josephson junction with edges, however, supercurrent was absent in edge-free Corbino graphene Josephson junction. Our results strongly support that the supercurrent observed in quantum Hall regime flows along the edges of graphene.

### Keywords:

Josephson Junction, Graphene, Quantum Hall, Corbino

## Thermal entanglement of the pseudogap Kondo model

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### Abstract:

Many-body spin-singlet entanglement is at the heart of the Kondo spin screening. In the phase diagram of the pseudogap Kondo model, there appears a quantum critical regime between the strong coupling regime and the local moment regime. We study the thermal entanglement in those regimes of the pseudogap Kondo model, by using the numerical renormalization group method. We find that in the strong coupling and quantum critical regimes, the entanglement has maximum value at zero temperature. In the local moment regime, the entanglement has a smaller non-zero value at zero temperature. The entanglement shows a power-law scaling behavior of thermal decay. The value of the scaling exponent depends on the regimes. The entanglement shows how the quantum coherence of the Kondo effect is thermally suppressed when conduction electrons show the pseudogap behavior.

### Keywords:

Kondo effect, Entanglement, Pseudogap

## Theoretical study of spin-valley polarized electronic structures of twisted bilayer graphene

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### Abstract:

Magic-angle twisted bilayer graphene (MA-TBG) has tunable flat bands by the twist angle. Its electronic structures can be characterized with spin-valley degrees of freedom. Here, we present spin-valley polarized electronic structures based on the density functional theory (DFT). We perform self-consistent DFT calculations of undoped unpolarized MA-TBG, and obtain doped unpolarized electronic structures by estimating the Hartree interaction of doped electrons or holes. Then we estimate the exchange-correlation potential of electrons in the flat bands and search for spin-valley polarized phases as a function of doping. We consider limiting cases and intermediate ones for the valley dependence of the exchange-correlation potential and discuss spin-valley polarized electronic structure in MA-TBG. This work was supported by NRF of Korea (Grant No. 2020R1A2C3013673) and KISTI supercomputing center (Project No. KSC-2021-CRE-0384).

### Keywords:

twisted bilayer graphene, magic angle, spin-valley polarization

## Diffusive density response of electrons in anisotropic multiband systems

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### Abstract:

We explicitly calculate the density-density response function with conserving vertex corrections for anisotropic multiband systems in the presence of impurities including long-range disorder. The direction-dependence of the vertex corrections is correctly considered to obtain the diffusion constant which is given by the combination of the componentwise transport relaxation times and velocities on the Fermi surface. We also investigate the diffusive density response of various anisotropic systems, propose some empirical rules for the diffusive response of anisotropic systems, and demonstrate that it is crucial to consider the component-dependence of the transport relaxation times to correctly interpret the transport properties of anisotropic systems, especially various topological materials with a different power-law dispersion in each direction.

### Keywords:

density response, diffusion, vertex correction, anisotropic system

## Water evaporation inside hexagonal micropillars

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### Abstract:

Micropillar arrays are good templates for electronic devices or solar cells. Appropriate design of micropillar arrays is essential for feasible applications, particularly by increasing droplet mobility and solute deposition through droplet evaporation inside micropillar arrays. Here we explore water droplet behaviors floating between hexagonal micropillar arrays by controlling micropillar's width, spacing, and wettability. We compare evaporation dynamics for a water droplet suspending between the micropillars and a water droplet wetting on the micropillar bottom. We find that the evaporation rates of wetted droplets are faster than suspended droplets, as determined by X-ray imaging and mass tracking. In-situ, high-resolution, high-penetration X-ray imaging would be used to identify water droplet behaviors inside hexagonal micropillar arrays, which helps the understanding of the interplay between evaporation and water-substrate interfaces. Our results may be used to improve the designs of micropillar arrays in future applications.

### Keywords:

water droplets, micropillar arrays, evaporation, contact line, X-ray tomography

## The interplay between spin-orbit coupling, Hund's coupling and van-Hove singularity in BaOsO<sub>3</sub>

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### Abstract:

BaOsO<sub>3</sub> is a 5d transition metal oxide with four electrons in the t<sub>2g</sub> orbitals, and is a heavier analogue of the ruthenate compounds. The spin-orbit coupling (SOC) is accordingly large 0.3eV but insufficient to drive the compound to a van-Vleck regime. I will describe how moderate correlations in this compound arise due to SOC : 1. SOC competes with the Hund's rule coupling and 2. it splits the van-Hove singularity. The results were obtained by the DFT+DMFT calculation using matrix-product state solver [1]. I will also discuss the interplay between SOC and Hund's coupling in a more general setting [2].

[1] Max Bramberger, Jernej Mravlje, Martin Grundner, Ulrich Schollwöck, and Manuel Zingl, Phys. Rev. B 103, 165133 (2021).

[2] Robert Triebl, Gernot J. Kraberger, Jernej Mravlje, and Markus Aichhorn, Phys. Rev. B 98, 205128 (2018).

### Keywords:

Hund's metals, spin-orbit coupling, van-Hove singularity, BaOsO<sub>3</sub>

## Vertex-based diagrammatic impurity solver

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### Abstract:

We present a new diagrammatic Monte Carlo impurity solver based on the strong-coupling expansion of the vertex functions. By directly sampling the four-point pseudo-particle vertex diagrams and applying the self-consistency equation at the level of the triangular vertex, we significantly improve the traditional schemes such as non-crossing and two-crossing approximations, and eventually achieve numerically exact results. We analyze the performance and the convergence rate of the impurity solver using exactly solvable models and observe that the efficiency of the vertex self-consistent scheme strongly depends on the particle statistics of the bath degrees of freedom. As an example, we discuss the physics of strong light-matter coupling in the spin-boson model representing an emitter in an optical waveguide.

### Keywords:

Hund's coupling, Mottness, Coulomb repulsion, diagrammatic Monte Carlo

## How to differentiate Hund from Mott physics?

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### **Abstract:**

Strong correlations in multiorbital metals are induced by the Coulomb repulsion through Mott physics, or by the Hund's-rule coupling through Hund physics. Though these two mechanisms are distinct, it was an open problem to determine whether a system has more "Hundness" than "Mottness" or vice versa. In this talk, I will summarize our recent study, where we identified numerous fingerprints distinguishing Hundness from Mottness in the temperature dependence of various physical quantities.

### **Keywords:**

Mott physics, Hund's coupling, dynamical mean-field theory, numerical renormalization group

## How are crystal structures and superconductivity affected by Hund's coupling?

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### Abstract:

Correlation effects in solids were long believed to arise primarily due to on-site Hubbard interaction, which blocks the charge fluctuations. Recently it became clear that strong correlations are even more often caused by the Hund's interaction, which does not block charge fluctuations, rather it tends to align electrons with the same spin when they find themselves on the same atom. This effect is strongest in compounds which have orbital configuration close to half-filling, or one unit charge away from half-filling, such as iron-pnictides and ruthenates.

The coherence in these systems is achieved in stages, with orbital and spin coherence temperature being substantially different, and giving rise to orbital differentiation or selective Mottness in the temperature range between the two temperature scales. The anomalous metallicity in this temperature range gives rise to large mass enhancement even though no clear Hubbard bands exist in the one-particle spectra. Moreover, the electron-phonon coupling in certain channels is substantially enhanced boosting tendency to superconductivity, which is already favored in the bad metallic regime near the point of strong short range spin fluctuations, where long range magnetic order fails to develop.

### Keywords:

Hund's coupling, Mottness, Coulomb repulsion

## Kondo interaction in FeTe and its potential role in the magnetic order

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### Abstract:

Finding *d*-electron heavy fermion (HF) states has been an important topic as the diversity in *d*-electron materials can lead to many exotic Kondo effect-related phenomena or new states of matter such as correlation-driven topological Kondo insulator. Yet, obtaining direct spectroscopic evidence for a *d*-electron HF system has been elusive to date. Here, we report the observation of Kondo lattice behavior in an antiferromagnetic metal, FeTe, via angle-resolved photoemission spectroscopy (ARPES), scanning tunneling spectroscopy and transport property measurements. The Kondo lattice behavior is represented by the emergence of a sharp quasiparticle and Fano-type tunneling spectra at low temperatures. The transport property measurements confirm the low-temperature Fermi liquid behavior and reveal successive coherent-incoherent crossover upon increasing temperature. We interpret the Kondo lattice behavior as a result of hybridization between localized Fe 3d<sub>xy</sub> and itinerant Te 5p<sub>z</sub> orbitals. Our observations strongly suggest unusual cooperation between Kondo lattice behavior and long-range magnetic order.

### Keywords:

Superconductivity, Heavy fermion, Kondo effect, Magnetism, Iron-based superconductors

## Coexistence of Kondo effect and Weyl semimetallic states in Mn-doped $\text{Mn}_x\text{VAl}_3$ compounds

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### Abstract:

The strong correlation effect in Weyl semimetal is a critical issue in condensed matter physics. Recently, the Kondo effect in Weyl semimetal was theoretically proposed but not yet experimentally realized. Here we suggest a coexistence of the Weyl semimetal and Kondo effect in disordered Mn-doped  $\text{Mn}_x\text{VAl}_3$ . Dilute Mn-doping in type-II Dirac semimetal  $\text{VAl}_3$  increases the chemical potential so that Dirac point is close to the Fermi energy and lifts band degeneracy, leading to the Weyl semimetal phase transition. We observed a Kondo effect, confirmed by the resistivity minimum at  $T_K = 40$  K, and logarithmic increase of electrical resistivity, magnetic susceptibility, and specific heat divided by temperature with a significant Sommerfeld coefficient at low temperature. The angle-resolved magnetoresistance has revealed the negative longitudinal magnetoresistance below Kondo temperature due to chiral anomaly in Mn-doped  $\text{Mn}_x\text{VAl}_3$ . At low temperature below Kondo temperature ( $T \leq T_K$ ), the exchange interaction by RKKY interaction in  $\text{Mn}_x\text{VAl}_3$  breaks time-reversal symmetry even in Kondo screening, resulting in the topological phase transition from Dirac to Weyl semimetal. This research shows the coexistence of the Kondo effect and Weyl semimetallic state as well as the temperature-induced topological phase transition.

### Keywords:

Kondo effect, Weyl semimetal, topological phase transition,  $\text{VAl}_3$ , Dirac semimetal

## La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>/NdNiO<sub>3</sub> 이중층의 전기적 상전이 과정에서 나타나는 전자구조 분석

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### Abstract:

강자성/비자성층 접합으로 이루어진 이중층 계면에서는 라쉬바-에델스타인 효과 혹은 스핀 홀 효과로 인해 전하전류가 스핀전류로 전환될 수 있다. 비자성층 물질이 금속-절연체 전이를 가지는 경우, 상전이에 따라 전하에서 스핀으로 전환되는 효율을 제어할 수 있기 때문에 이러한 소재는 스핀 전류에 의한 자화제어 연구분야에서 중요성이 높아지고 있다. 본 연구에서는 La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>(LSMO)/NdNiO<sub>3</sub>(NNO)를 강자성층/비자성층 구조를 가진 강상관계 전자 시스템으로 구성하여 NNO 두께에 따른 전자기적 상전이 특성에 대해 연구하였다. NNO는 전자 사이의 강한 결합 및 상호작용으로 인해 상자성-반강자성 자기상전이 및 금속-절연체 전이를 함께 가지는 니켈산염이다.

상전이 과정에 대한 연-X선 흡수 분광법 관찰을 통하여, 시료가 저온의 절연상에서 상온의 금속상으로 전이할 때 527.6 eV 근처에서 Ni<sup>2+</sup> 피크가 새로이 생성되는 것이 관찰되었다. 이는 LSMO의 Mn에서 NNO의 Ni로 국부적인 전하이동이 발생했다는 증거이며, 해당 피크의 출현 여부는 상전이 과정에 대한 I-V 실험 결과와 일치한다. 이는 LSMO/NNO 이중층 계면에서 전하이동에 의해 라쉬바-에델스타인 효과가 온도에 따라 제어될 수 있음을 의미한다.

### Keywords:

Rashba-Edelstein Effect, Metal-Insulator Transition, X-ray absorption spectroscopy, Rare-earth nickelate, Charge to Spin conversion

## Symmetry-preserving strain engineering of Hundness and Mottness in a two-dimensional correlated system

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### Abstract:

The Electronic states of materials with partially filled  $d$ - or  $f$ -orbitals are governed by strong correlations. The electron correlation due to strong on-site Coulomb repulsion ( $U$ ) has been a central paradigm in physics since the 1940s. Recently, the correlation due to Hund's rule coupling ( $J$ ) has been studied extensively to describe the novel quantum phases of matter. Here, we developed a unique strain engineering method to investigate the roles of  $J$  in the energetics of the Mott gap. By growing SrRuO<sub>3</sub> monolayers on various substrates with a symmetry-preserving interlayer, we gradually tuned the crystal field. This lifts the degeneracy of the Ru  $t_{2g}$  orbitals and effectively varies the numbers of involved orbitals and electrons. We used *in-situ* angle-resolved photoemission spectroscopy to observe a metal-to-Mott insulator transition. This study shows that monolayer transition metal oxides will be good material systems for exploring the physics of Hundness and Mottness, particularly in two dimensions.

### Keywords:

SrRuO<sub>3</sub>, Hund coupling, Symmetry-preserving strain engineering, two-dimensional correlated system

## Fine details of sixfold Dirac fermions in a pyrite-structured PdSb<sub>2</sub>

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### Abstract:

We report detailed angle-resolved photoemission measurements on the electronic structure of an unconventional multi-fold Dirac fermionic semimetal PdSb<sub>2</sub> with a pyrite structure. By exploiting the photon energy and polarization dependence of the matrix element in photoemission intensity and by comparing photoemission data with ab-initio band calculations, we can experimentally identify the exact structure including the orbital characters of the electron pockets at the R point in the Brillouin zone of PdSb<sub>2</sub>. Each electron pocket and hole pocket-like structure consists of three doubly degenerate parabolic bands respectively, which cross one another at the R point, forming a sixfold Dirac fermion. The overall electronic structure is consistent with the band calculation results, but the gap size between two sextuple points is very sensitive to the Wyckoff position of Sb atoms.

### Keywords:

PdSb<sub>2</sub>, Six-fold Dirac fermion, ARPES

## Acoustic and Optic Phonons in Lead Halide Perovskite MAPbX<sub>3</sub> (MA = methylammonium and X = Br, Cl) Single Crystals

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### Abstract:

Hybrid Halides Perovskites are an intriguing family of materials with attractive properties in various study areas, especially perovskite solar cells with a certified photovoltaic efficiency of 25.5% and 29.5% (perovskite-silicon tandem solar cells) as of 2022 [1,2]. For practical use of these mixed perovskites, a reliable understanding of structural changes upon composition change is necessary, for which Raman and Brillouin spectroscopy are a useful approach. In this research, we synthesized seven different compositions of MAPbBr<sub>3-x</sub>Cl<sub>x</sub> with x= 0,0.5,1,1.5,2,2.5, and 3. X-ray diffraction and Brillouin spectroscopic measurements were performed on all compositions at room temperature. However, Raman measurements were performed at both low and room temperature. The diffraction patterns of mixed perovskites reveal that when the Cl content increases, the diffraction peaks move to higher 2 $\theta$  angles. Br has a greater ionic radius than Cl (1.81Å), hence interplanar spacing reduces when the bigger Br atom is substituted in the lattice, causing the diffraction peaks to move to higher diffraction angles. The lattice constants were computed which exhibit almost linear behavior as a function of halide composition, approximately following Vegard's law. The MA (methylammonium) torsional mode is most influenced by the substitution of halides among other modes, with a change from 485 cm<sup>-1</sup> in MAPbCl<sub>3</sub> to 325 cm<sup>-1</sup> in MAPbBr<sub>3</sub>. The C-N stretching and MA rocking modes exhibit a blue shift from cubic to orthorhombic phase, associated with a change in hydrogen bonding from NH<sub>3</sub> to CH<sub>3</sub> as the temperature is lowered. The most captivating outcome of this research is that the torsional mode, which is known to be sensitive to the local environment of the MA cations, particularly the condition of the NH<sub>3</sub>-X bonding, has a significant nonlinear dependence on the halide composition, whereas the lattice constant has a nearly linear dependence. At intermediate compositions, the frequency of the torsional mode displays a significant spike, as well as mode splitting at low temperatures. The linear change in lattice constant implies that the blue shift of the torsional mode with Cl composition is not only due to cage shrinking. Taken together, these findings show the importance of halides in changing numerous aspects of perovskites that are linked to chemical interplay. The dependence of the elastic properties on the composition, investigated by Brillouin scattering, will be reported in this study.

Acknowledgments: This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. 2020R1A2C101083111, 2019R1A6A1A11053838)

References:

- [1] N.G. Park, Organometal perovskite light absorbers toward a 20% efficiency low-cost solid-state mesoscopic solar cell, J. Phys. Chem. Lett. 4 (2013) 2423–2429
- [2] NREL Efficiency Chart, [http://www.nrel.gov/ncpv/images/efficiency\\_chart.jpg](http://www.nrel.gov/ncpv/images/efficiency_chart.jpg)

### Keywords:

Raman spectroscopy, Halide perovskites, Brillouin spectroscopy, phase transitions

# Data-Efficient Iterative Training of Gaussian Approximation Potentials: Application to Surface Structure Determination of Rutile IrO<sub>2</sub> and RuO<sub>2</sub>

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## Abstract:

Machine-learning Gaussian Approximation Potentials (GAPs) have recently evolved as a powerful class of surrogate models to computationally demanding first-principles calculations. Along with structure exploration techniques, they enable us to examine the potential energy surface of interest with a hitherto unforeseen combination of physical accuracy and computational efficiency and to achieve global surface structure determination (SSD) for increasingly complex systems. This can be leveraged e.g. to discover novel surface motifs which are critical in understanding the "living" state of heterogeneous catalysts and their degradation under dynamic operating conditions. In our preceding study, this versatility could be leveraged by a general and data-efficient iterative training protocol that allows for the on-the-fly generation of GAPs via the actual surface exploration process. The iterative refinement of GAPs identifies plenty of unknown low energy terminations of RuO<sub>2</sub> even within the restricted sub-space of (1 × 1) surface unit-cells. Moreover, by extending the protocol to larger surface unit-cells, we discovered new surface structures, which provide solutions to longstanding questions in heterogeneous catalysis.

[1] *Phys. Rev. Lett.* **125**, 206101 (2020)

[2] *J. Chem. Phys.* **155**, 244107 (2021)

## Keywords:

Gaussian Approximation Potentials, first-principles calculations

## Nano structure prediction using the first-principles data based machine learning force field

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### Abstract:

Machine learning (ML) accurately analyzes and predicts the physical/chemical properties of materials using the accumulated big database. As nanoscale control has become important in most material science and engineering, the need for predicting atomic-level phenomenon using ML is emerging. Among the widely used methods for predicting nanophysical properties, the first principle density functional theory (DFT) predicts nanostructure characteristics only under limited simple conditions with high computational and time cost. However, the DFT results revealed that physicochemical properties can be predicted by accurately knowing structural information such as atomic arrangement and coordination number. Therefore, it is important to develop a force field (FF) that can quickly and accurately predict structural changes at the nano level. In this presentation, I demonstrates the effective development of ML-FFs for nanomaterials using high-dimensional neural network potentials (NNPs) and a Gaussian process (GP) with a database accumulated by DFT calculations and ab-initio molecular dynamics (AIMD) simulations. The computationally efficient and precise ML-FF approach proposes the physical properties and design principles for high-performance nanomaterials.

### Keywords:

Density functional theory, Machine learning, Nanomaterials

# Efficient electronic passivation schemes for surface calculations of semiconductors exhibiting spontaneous polarization: Thermodynamic and electronic properties of GaN surfaces

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## Abstract:

Semiconductor surfaces play a central role in modern technology related to catalysis, electronics, and energy applications. The most widespread approach to study surfaces with density-functional theory calculations is to use slab geometries with periodic boundary conditions. A common strategy employed to avoid artificial charge transfer from one side of the slab to another is to passivate the dangling bonds at its backside. Using the examples of wurtzite polar and semipolar surfaces, we demonstrate that the conventional passivation scheme using pseudo-H atoms fails to describe the electronic structure of low-symmetry semiconductors. We, therefore, developed an improved passivation method [npj Comp. Mater. 7, 58, 2021 and PR Mater. 5, 044605, 2021] that takes the polarization effect and the concept of surface reconstructions into account. It accurately describes surface electronic properties and enables computationally efficient surface energy calculations. This approach is generic and robust and can be straightforwardly implemented in DFT investigations of low-symmetry surfaces as well as in high-throughput and machine learning studies. We applied this novel approach to calculate the energies and electronic properties of several hundred GaN surface phases as function of the growth conditions. Based on these calculations, we construct the Wulff diagram and identify the role of surface and strain energies in the formation of technologically important interface defects such as V-pits.

## Keywords:

Polar surface calculations, density-functional theory, high-throughput calculations, surface thermodynamics, surface electronic properties

## 자기 이방성 방향의 분포를 적용한 Stoner-Wohlfarth 모델을 이용하여 입상 박막의 보자력 분석

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### Abstract:

FePt-C와 같은 입상 자성 박막은 초고밀도 기록 매체 (Ultra-high-density recording media)를 구현하기 위한 대표적인 시스템이다. 이 물질 시스템은 일반적으로 수 나노미터 두께의 경계로 분리된 수 나노미터 규모의 작은 알갱이들로 구성되어 있다. MgO (100) 위에서 FePt는 L1<sub>0</sub> 구조로 증착 될 수 있으며, [1] C는 L1<sub>0</sub> 구조의 FePt 알갱이를 둘러싸고 있다. 서술한 바와 같이, 한 박막 내에서 열안정성이 우수한 자성체를 나노 사이즈의 알갱이로 분리할 수 있다. 한 알갱이의 지름은 7 – 20 nm까지 다양하게 가질 수 있다. Stoner-Wohlfarth 모델 (SW 모델)은 단일 입자의 자기장과 자화 방향 사이의 관계를 설명하는 적합한 모델로 알려져 있다. FePt 알갱이는 L1<sub>0</sub> 구조로 인해 매우 높은 자기 이방성 상수를 가져 열 안정성이 매우 높고, 15 nm 미만의 작은 크기로 인해 단일 자화 영역 (magnetic domain)을 가져 단일 입자의 자화 반전 거동이 가능하다. 하지만 다수의 알갱이로 구성된 입상 자성 박막은 스위칭 필드의 각도 의존성은 단일 입자에 대한 SW 모델과 일치하지 않는다.

본 발표에서는 입상 자성 박막과 같은 불 균일한 자성 박막의 자화 반전 거동을 이해하기 위해 자화 용이축의 표준 편차를 갖는 SW모델을 제안한다. 우리 모델에서는 FePt-C 입상 자성 박막에서 자화 용이축의 편차 정도를 정량화 하는 것이 가능하다.

[1] Wanjiao Zhu et al, J. Phys.: Condens. Matter, 25, 396001 (2013)

[2] H. Pandey et al., IEEE Trans. Magn., 52, 3200108 (2016)

### Keywords:

Stoner-Wohlfarth model, granular film, FePt

## Colossal THz emission by Spin-to-Charge Conversion in topologically non-trivial $\text{Bi}_{1-x}\text{Sb}_x$

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### Abstract:

$\text{Bi}_{1-x}\text{Sb}_x$  alloy which is first reported 3D topological insulator (TI) is the most promising material in spintronics owing to its giant spin Hall angle and large conductivity. Compared to other TIs,  $\text{Bi}_{1-x}\text{Sb}_x$  has about ten times larger spin Hall angle ( $\sim 52$  in  $\text{Bi}_{0.9}\text{Sb}_{0.1}$ ) and one order larger conductivity ( $\sim 10^5 \Omega^{-1} \text{m}^{-1}$ ). Nevertheless, there have been few efforts to figure out its spintronic phenomena due to its difficulty (e.g., the origin of giant spin Hall angle). While  $\text{Bi}_{1-x}\text{Sb}_x$  undergoes topological phase transition with respect to  $x$ , multiple states that could contribute to spin-to-charge conversion are mixed in each phase and their contributions are hard to differentiate. In this study, we successfully grow  $c$ -axis aligned epitaxial  $\text{Bi}_{1-x}\text{Sb}_x$  with various Sb concentrations by Molecular Beam Epitaxy (MBE). Also, to measure the spin-to-charge conversion efficiency of  $\text{Bi}_{1-x}\text{Sb}_x$ , we made Ferromagnet (FM)/ $\text{Bi}_{1-x}\text{Sb}_x$  heterostructure and conducted THz emission spectroscopy. We observed much larger spintronic THz emission than Pt. What we are demonstrating is that noticeable spin-to-charge conversion is occurring in different phases of  $\text{Bi}_{1-x}\text{Sb}_x$  and this research could expand to developing efficient spintronic devices.

### Keywords:

Topological insulator, THz emission, Bismuth, Antimony, Spintronics

## High-power heat generation from ferrite nanoparticles for hyperthermia application

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### Abstract:

Magnetic hyperthermia has been studied to convert magnetostatic energy to heat for therapeutic usage [1-3]. However, due to limited heat-generation power from magnetic nanoparticles, its practical application is still challenging. Here, we explored a new paradigm of magneto-thermal modality using resonantly excited spin dynamics followed by consequent energy dissipation, which has yet to be realized for hyperthermia applications. We experimentally demonstrated that distinctly efficient heat-dissipation power is available from ferrimagnetic  $MFe_2O_4$  ( $M = Fe, Mn, Ni$ ) nanoparticles by applying extremely low strengths of microwave oscillating magnetic fields at resonance. The amount of heat generated from those particles is significantly enhanced by about two orders of magnitude compared to those obtained by conventional mechanisms such as the Néel-Brownian model. From micromagnetic simulations and analytical derivations, we found that the temperature increment can be determined by the intrinsic material parameters of the damping constant and saturation magnetizations of the nanoparticles' constituent materials; the heat-dissipation power is proportional to the saturation magnetization and inversely proportional to the damping parameter. Our experimental results and theoretical formulations lead to a better understanding of spin-dynamics driven high-power heat generation as well as offer a straightforward guidance for the design of advanced materials for control of highly localized incrementation of targeted temperatures using magnetic particles for magnetic hyperthermia bio-applications.

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### Keywords:

Magnetic Hyperthermia, Ferromagnetic resonance

## The relationship between contact resistance and transistor performance of negative capacitance field effect transistors

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### Abstract:

Subthreshold swing (SS) in conventional metal-oxide-semiconductor field-effect transistors (MOSFETs) have been limited to the 60 mV/dec by "Boltzmann tyranny". To overcome the limitation, The negative capacitance (NC) field effect transistor with thin film based on a doped HfO<sub>2</sub> ferroelectrics has been attracting attentions due to the compatibility of CMOS process, maintaining ferroelectricity under 10 nm thickness, high retention and endurance. In addition, Molybdenum disulfide (MoS<sub>2</sub>) of transition metal dichalcogenides has been extensively studied for low-power and high performance transistors as a channel layer due to high carrier mobility, thickness dependence of band structure and no surface roughness.

Here, we fabricated a negative capacitance ferroelectric field effect transistor (NC-FET) using a HfZrO<sub>2</sub> ferroelectric and Al<sub>2</sub>O<sub>3</sub> dielectric in series, and a monolayer MoS<sub>2</sub> as a channel layer. 10 nm and 4 nm of HfZrO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> respectively were deposited by thermal atomic layer deposition (ALD). Then monolayer MoS<sub>2</sub> grown by chemical vapor deposition (CVD) was transferred by wet transfer. Finally In and Au were deposited as a source and drain electrode by e-beam evaporation. It showed over 10<sup>7</sup> I<sub>on</sub>/I<sub>off</sub> ratio and less than 60 mV/dec subthreshold swing without hysteresis behavior at the low voltage driving (1 V<sub>g</sub>), and compared the transistor performance depending on contact electrode such as In/Au, Ni, Ti/Au and TiN.

### Keywords:

Negative capacitance, Ferroelectrics, Transistor, Supersteep

## Microwave absorption properties of multi-phase TiO<sub>x</sub> thin films

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### Abstract:

Multi-phase titanium oxide thin films were deposited on the soda-lime glass using reactive DC magnetron sputtering method. By controlling sputtering gas flow and plasma power, the impedance of plasma discharge was adjusted in order to manipulate the phase and compositions of the as-grown films. The crystal structure and phase of the films were characterized by x-ray diffraction, x-ray photoelectron spectroscopy as well as transmission electron microscopy. The microwave absorption (MA) properties were monitored using grounded coplanar waveguide with a vector network analyzer. The thin films having higher population of Ti and TiO phases turned out to be effective MA absorber. The mechanism of observed MA properties was studied with respect to the localized surface plasmon resonance and induced local polarization in the multi-phase boundary.

### Keywords:

microwave absorption, plasma impedance, titanium oxide

## Anomalous domain switching dynamics in Si:HfO<sub>2</sub> thin film capacitors.

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### Abstract:

The HfO<sub>2</sub>-based ferroelectric thin films have attracted a great of attention due to their potential applications, such as nonvolatile memories and negative capacitance field effect transistors. Especially, compared to conventional ferroelectrics, the HfO<sub>2</sub>-based ferroelectrics have many advantages, including full CMOS compatibility, large bandgap, and very small critical thickness. The operation principle of ferroelectric-based memories is the polarization switching induced by the application of external electric field. Therefore, understanding ferroelectric domain switching dynamics is one of the most important prerequisites for the realization of HfO<sub>2</sub>-based memories. In particular, it is highly required to directly observe how ferroelectric domain nucleates and grows at the nanoscale in real capacitor geometry. Here, we present our recent efforts to study ferroelectric domain switching dynamics in Si-doped HfO<sub>2</sub> thin film capacitors using piezoresponse force microscopy (PFM). In most regions, we observed normal domain switching; namely, the domains aligned along the applied electric field by domain nucleation and growth. However, in some regions, the domains aligned against the applied electric field, the-so-called "anomalous domain switching". Using the stroboscopic PFM imaging and local PFM spectroscopy, we investigated the difference between normal and anomalous domains. We discuss the possible origin of the anomalous domain switching in the Si:HfO<sub>2</sub> capacitors.

### Keywords:

ferroelectrics, HfO<sub>2</sub>, PFM, Domain switching, nonvolatile memories

## Strain control of oxygen sublattice structures in epitaxial SrCuO<sub>2</sub> thin films

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### Abstract:

Infinite-layer cuprate SrCuO<sub>2</sub> has attracted great attention to lots of researchers in the fields of condensed-matter physics and materials science, because electron- or hole-doped SrCuO<sub>2</sub> can exhibit superconductivity [1]. Intriguingly, the SrCuO<sub>2</sub> incorporates CuO<sub>2</sub> sublattice planes where the  $d_{x^2-y^2}$   $e_g$  orbitals partially occupied with electron-hole pairs play a key role in the superconducting transition [2]. It is further interesting that the oxygen sublattice configuration is controllable in epitaxial SrTiO<sub>3</sub>/SrCuO<sub>2</sub> superlattice heterostructures via an interfacial proximity effect [3]. Note that two types of oxygen sublattice structures are possible in SrCuO<sub>2</sub> (001) thin films [3, 4]. Namely, for the planar type, SrO and CuO sublayers are alternatively piled up in the [001] direction, whereas the stacking sequence in the chain type is Sr-CuO<sub>2</sub>-Sr-CuO<sub>2</sub>. Since the orbital configuration of Cu ions in SrCuO<sub>2</sub> is very susceptible to the oxygen sublattice structures, it is plausible for us to manipulate the  $e_g$  orbital occupancy by modifying the oxygen sublattice coordination [3, 4]. In this work, we found that the oxygen sublattice structures in epitaxial SrCuO<sub>2</sub> (001) thin films were changeable relying on misfit strain arising from the lattice mismatch between the SrCuO<sub>2</sub> layer and the underlying substrate. Using various experimental techniques, the physical properties of the as-grown SrCuO<sub>2</sub> thin films were systematically characterized. Based on the obtained results, we will discuss how the electronic structures in our SrCuO<sub>2</sub> thin films evolve depending on the controlled oxygen sublattice structures (i.e., planar and chain types)

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### Keywords:

Oxide, Thin film, Epitaxy

## On-chip transferrable light source and its electrification in photonic circuit

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### Abstract:

The full potential of high-index dielectrics and Si photonics platforms to realize compact integrated photonic circuits has been limited by the long-standing challenge related to the on-demand and efficient integration of high-quality light sources. Although some strategies (e.g., Si-compatible materials, wafer-bonding, hybrid integration, etc.) has been developed, they are only partly successful resulting in an inefficient light generation, inaccurate integration, and waste of gain materials. Here, we report on on-chip transferrable micro-/nano-scale light sources by utilizing the micro-structured polymer-assisted transfer printing technique. We separately fabricated III-V semiconductor light sources and successfully transfer these single devices onto the targeted sites on Si<sub>3</sub>N<sub>4</sub> and/or Si receiving substrates. With the help of the micro-transfer method, we have also developed an 'all-graphene-contact' approach capable of defining electrical contacts on nanomaterials and nanostructures that were extremely challenging to be electrified using the conventional methodology. Optical characterizations of single device exhibit the successful light generation, confirming stable contact formation and electrical operation. Lastly, we accurately couple these sources to single photonic waveguide and demonstrate the electrically pumped light generation, light coupling and waveguiding. We believe that micro-transfer technique and all-graphene-contact approach is readily applicable to various micro/nanostructures and devices, which facilitates stable electrical operations and thus extends their practical applicability in compact integrated circuits.

### Keywords:

photonic integrated circuits, nanoscale light sources, micro-transfer technique, graphene contact, electrical pumping

## Ultrasound sensor on silicon photonic MEMS

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### Abstract:

초음파 영상은 뛰어난 해부학적 공간 분해능, 실시간 기능, 안전성 및 환자에 대한 접근성으로 인해 가장 널리 사용되는 진단 영상 기술 중 하나이다. 기존의 초음파 transducer는 압전기를 기반으로 압력 에너지를 전기 신호로 변환한다. 그러나 이러한 압전기반 변환기는 좁은 대역폭, 작은 감도, 작은 수용각, 큰 크기 및 고가의 비용과 같은 한계가 있다. 이러한 단점을 극복하기 위해 광학 공진기를 기반으로 한 광학 초음파 감지 기술이 개발되어왔다. 최근 광자 집적 회로(PIC) 기반 광학 초음파 센서는 초고감도 초음파 감지 및 다기능 폼 팩터에서 뛰어난 성능으로 인해 많은 관심을 받고 있다. 그러나 이것의 구조적 한계로 인해 디자인 자유도가 제한되고 있다. 지금까지 PIC 기반 초음파 센서는 외부 멤브레인(예: 공진기 자체 진동)을 사용하지 않거나 매우 좁은 설계 공간을 제공하는 non-conventional한 제조 기술(예: 웨이퍼 본딩)로 만든 멤브레인을 사용한다. 초음파 센서의 성능(예: 대역폭, 공진 주파수, 감도)은 멤브레인의 설계(예: 두께, 길이, 모양)에 크게 의존하기 때문에 지금의 방법에서 벗어난 설계 자유도가 높은 새로운 멤브레인 구조의 개발이 필요한 상황이다. 또한, 초음파 센서의 감도는 필름의 두께와 직접적인 관련이 있으므로 가능한 한 얇은 필름을 사용하는 것이 바람직하다. 본 발표에서는 매우 얇은 멤브레인 구조를 가지면서 쉽게 제작할 수 있는 새로운 광학 초음파 센서 설계에 대해 얘기할 예정이다. 본 구조는 멤브레인의 치수와 모양이 리소그래피 및 에칭에 의해 정해지기 때문에 기존에 비해 훨씬 큰 설계 자유도를 갖는다. 해당 구조로 이루어진 6.5MHz의 공진 주파수를 갖는 70nm 두께의 멤브레인만으로 센서를 구현한 결과도 보여줄 예정이다. 장치의 감도와 fractional bandwidth는 각각 0.41 $\mu$ V/Pa 및 62%이다.

### Keywords:

Silicon photonics, ultrasound, array

## Resource-saving photonic quantum memory based on integrated photonics

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### Abstract:

Optical quantum memory is an essential building block for universal quantum computing based on linear optics. In spite of limited lifetime of photon, on-chip delay lines are considered a very practical solution compared to other matter-based ones because the insertion loss can be engineered to a tolerable level.

Simple delay lines, however, take up a large space since photons run at the speed of light. Large footprint devices are extremely undesirable for linear optics quantum computing, since its architecture is largely dependent on multiplexing scheme.

In this work, we theoretically investigate the application of multi-mode light converting devices to recycle the same physical waveguide without having bandwidth-limiting interference. We point out the weakness of current mode converter design and propose a new solution that can improve the performance in many aspects. Thorough theoretical analysis is followed to verify the validity of our design.

### Keywords:

quantum memory, linear optics quantum computing, optical delay lines, integrated photonics, silicon photonics, multi-mode photonics

## 빛의 굴절에 대한 2015 개정 초등과학 교육과정 및 교과서 분석

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### Abstract:

초등에서 광학, 특히 빛의 굴절은 중요하게 다루어지나 학생과 교사가 이해에 어려움을 갖는다는 보고가 많다. 내용 자체의 난이도 때문인지, 제시방법, 구성, 표현 등이 어려움을 유발하는 것인지 분석할 필요가 있다. 2015 초등 과학과 교육과정을 중심으로 빛의 굴절이 어떻게 다루어지고 있는지 살펴보고, 개정 교육과정을 위한 시사점을 도출하고자 한다.

### Keywords:

초등, 광학, 굴절, 과학 교육과정

## 2015 개정 초등학교 과학 검정교과서에는 '무게' 개념을 어떻게 설명하고 있는가?

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### Abstract:

'질량'은 중학교 교육과정 '힘과 운동' 및 '에너지' 단원 학습에 기본이 되는 개념이지만, 초등학교 수준에서는 질량을 정의하고 측정하기 어렵기 때문에 '무게'로 물체의 양을 나타낸다(교육부, 2015). 그런데 초등학교 학생들은 무게 개념 학습에서도 많은 어려움을 겪고 있다. 본 연구에서는 무게 개념 설명 방식, 무게와 질량의 관계, 무게 단위 도입과 활용, 수평잡기의 원리와 무게 측정의 관계 설명 과정의 4가지 관점에 따라 2015 개정 초등 과학 검정교과서 7종과 국정교과서의 '물체의 무게' 단원 내용을 비교하였다. 이 4가지 관점은 국정교과서 개발과정에서 집필진, 연구검토진, 심의진 사이에서 논쟁이 되었으나 해법을 찾지 못했던 것들이다. 연구 결과, 모든 검정교과서에서 무게 개념을 '지구가 물체를 끌어당기는 힘의 크기'로 직접 설명하고 있었고, 무게와 질량 개념을 연결시키지 않았으며, 무게 단위를 'g중', 'kg중'으로 사용하고 용수철 저울에 표기된 질량 단위와 밀접하게 연결시키지 않았으며, 일부 교과서에서 '수평잡기 원리'를 하나의 개념으로 서술하였으나 수평잡기 원리와 무게 측정과의 관계를 매끄럽게 연결시키지는 않았다. 결론적으로 새로 개발된 초등 과학 검정교과서를 통해 국정교과서 개발과정에서 해소하지 못했던 무게 개념 설명 과정에서의 쟁점이 충분히 해소되었다고 판단하기 힘들었다.

### Keywords:

초등학교, 과학 검정교과서, 무게, 개념 설명과정

## 초등학생을 위한 양자물리 교수학습의 사례와 가능성 탐색

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### Abstract:

현대 사회에서 양자역학의 중요성은 더 언급할 필요가 없을 정도로 지대하다. 양자역학이 실생활에 미치는 영향은 최근에는 양자 기술(quantum technology)이라는 이름으로 더욱 확장되고 있다. 양자 기술은 국가의 핵심 전략기술로 간주되기 시작하면서 정부는 2021년에 '양자 기술 연구개발 투자 전략'을 발표했으며 국회에서는 2022년 초에 '양자 기술 개발 및 산업화 촉진에 관한 법률'을 입법하였다. 이 법률안에는 초중등학교 수준에서 양자 기술 관련 교육을 포함할 것이 포함되어있기도 하다. 그러나 당장의 현실은 초중등학교 수준에서 양자 기술 교육에 대한 사회적 수요에 대응하기가 어려운 실정이다. 이 연구에서는 초중등학교 수준에서 양자 기술을 포함하는 양자물리 교육을 도입하기 위한 기초 논의로서, 초중등학교에서의 양자물리 교육에 대한 현황을 검토하고 그 가능성을 탐색하고자 한다. 이를 위해 첫째, 초중등학생을 대상으로 하는 관련 연구 동향을 분석하고, 둘째, 특히 초등학생을 위한 양자물리 관련 대중 과학도서들의 내용과 접근 전략을 분석한다. 이를 바탕으로 초등학생을 위한 양자물리 교수학습 전략에 대한 시사점을 도출하고 학교 과학교육에서의 실천 가능성을 논의한다.

### Keywords:

양자물리, 양자 기술, 초등학생, 교수학습, 대중 과학도서

## 고등학교 과학과 서·논술형 학생평가의 운영 실태 및 쟁점

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### Abstract:

최근 미래교육을 위한 일련의 교육혁신이 추진됨에 따라, 학교 평가 패러다임의 전환에 대한 요구도 커지고 있다. 이에 따라 학습과 평가와의 관계는 전통적으로 강조되어 온 '학습 결과의 평가'에서 '학습을 위한 평가', '학습 과정으로서의 평가'로 변화되어 왔다. 특히, 학생들의 미래역량의 성장을 확인하기 이 평가 패러다임으로 '서·논술형 평가'가 주목받고 있다. 따라서 서·논술형 평가가 현장의 교사들이 어떻게 해석하여 실천하고 있는 지 파악하고 이에 대한 지원방안을 모색할 필요가 있다.

본 연구는 고등학교 국어, 영어, 수학, 과학 교과에서의 서·논술형 평가에 관한 정책 연구의 일환으로 진행된 것으로 그 중 과학과를 중심으로 논하고자 한다. 이를 위해 과학교사 13명 포함한 고등학교 교사 56명을 대상으로 개방형 설문조사를 실시하였다. 분석결과 4개 과목 공통으로 드러나는 특징이 있었고, 과학과 특이적인 쟁점이 있었다. 그 특징을 보다 살펴보기 위해 서·논술형 평가에 대한 경험이 많은 IB DP 교사와 과학고 근무 경험이 있는 교사들을 대상으로 초점집단면담(FGI) 실시하였다. 이를 바탕으로 서·논술형 평가에 관한 쟁점을 파악하고 지속 및 확장 방안을 모색하였다. 설문과 면담의 응답 결과는 전사하여 범주화하는 과정을 거쳐 범주별로 나타나는 특징을 도출하였다.

분석 결과, 4개 교과 공통적 쟁점은 다음과 같다. 첫째, 수능 시험과 대입 체제는 여전히 고교 교육의 현실을 결정하는 가장 중요한 요소임을 확인하였다. 교사들은 평가의 목표에 대해 본인의 신념인 '학생들의 성취와 성장 파악'과 달리 '변별'과 '공정성' 등의 사항들에 더욱 무게를 두고 있었다. 둘째, 채점에 대한 부담감으로 인해 실제 지필평가에 사용되는 문항들은 정답이 정해져 있는 서술형 문항이나 단답형을 주로 사용하고 있었다. 한편, 변별에 대한 부담감이 적은 수행평가에서는 논술형이 많이 활용되고 있었다.

과학과만이 겪는 특이적 쟁점은 먼저, 과학교사들은 '서·논술형 평가'에 대해 일관되지 않는 해석을 하였다. 과학과 서·논술형 평가는 과학적 글쓰기, 토론 등으로 유형이 다양한데, 일부 교사는 실험보고서 작성을 서·논술형 평가로 분류하고 어떤 교사는 기타 유형의 평가로 분류하였다. 게다가 서·논술형 평가의 실천에 있어서 과학교사는 담당하고 있는 교과(예: 과학탐구실험, 과학사 등)의 수가 상대적으로 많아 평가 관련 업무 부담이 컸다. 특히, 과학 교사는 실험 탐구보고서를 수행평가로 많이 활용하는데 이를 일일이 채점하고 피드백하기 위한 시간이 매우 부족했다. 본 연구에서 주목하고자 하는 점은 과학의 서·논술형 평가는 학생들에게 창의성과 다양성을 추구하고 장려하지만, 이를 결국 변별해야하는 상대평가 체제에서 학생들의 창의성에 점수의 선을 그어야 하는 현실에 처해 있다는 것이었다. 이와 같은 배경에서 교사들은 서·논술 평가를 실시하더라도 평가는 후하게 채점할 수 있는 수행평가로 제한적으로 활용하고 있었다.

이를 바탕으로 본 연구는 고등학교 서·논술형 평가의 확장을 위해 실질적 지원 방안을 제안하였다. 특히, 채점의 신뢰성을 높이고 교사 개인의 부담을 완화하기 위해 지역교육청 수준의 <교육과정평가지원센터>의 설립 및 운영을 제안하고자 한다. 그러나 교사들은 외부에서 자신의 평가를 모니터링(monitoring)이나 조정(moderation)하기보다는 지원과 자료 제공을 희망하였다.

### Keywords:

과학교사, 서·논술형 평가, 평가 실태, 평가 지원 방안, 채점 변별

## 예비교사의 온라인 기반 물리 교수자료 개발 역량 향상을 위한 학습조력 프로그램의 개발과 적용

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### Abstract:

COVID-19로 인한 온라인 수업으로의 급격한 전환이 이루어짐에 따라, 예비교사들 또한 온라인 수업에 대한 이해를 높이고 수업을 설계하고 시행할 수 있는 역량이 요구된다. 이 연구에서는 예비교사들의 온라인 기반 물리 교수자료 개발 역량을 향상시키기 위한 학습조력 프로그램을 개발하고 이를 적용하였다. 프로그램에 참여한 13명의 예비 물리교사들은 온라인으로 진행되는 수업에서 Desmos를 통해 기하광학 개념 이해를 돕는 교수자료와 소리파동 개념 이해를 돕는 실험 동영상을 제작하였고, 전문가 및 동료 피드백을 통해 교수자료를 수정하였다. 예비교사들은 타전공 학생들의 물리 수업에 학습조력자로서 참여하여 수정된 교수자료를 활용하여 조력활동을 진행하였다. 예비교사들의 교수자료 개발 역량을 확인하기 위해 테크놀로지 교수 내용 지식(TPACK) 사전-사후 검사를 시행하여 향상 정도를 확인하였다. 이를 통해 예비교사의 온라인 수업실행역량 향상에 대한 시사점을 도출하고자 한다.

## Comparison of competency models for graduate students of Korean research-oriented universities

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### **Abstract:**

The Korean government has supported the BK21 project to enhance the international competitiveness of Korean universities. In particular, from 2020, the graduate school innovation project was carried out to reorganize the graduate school governance to enhance research competitiveness at the global level. Major Korean universities participating in this project have developed competency models for graduate students and innovated their curricula. This study compared the competency models for graduate students of major research-oriented universities participating in the innovation of the graduate school of BK21(4th) and discuss the implications given the competencies required for future science and engineering professionals.

### **Keywords:**

BK21, Competitiveness model, Innovation of universities, STEM education, STEM professionals

## E x B Shear Flow Dynamics in a Magnetic Island

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### Abstract:

This presentation is dedicated to the memory of Prof. Duk In Choi who made numerous pioneering contributions to theory of plasma instabilities and turbulence. Significance of his high impact contributions will be discussed at the beginning. E x B shearing rate associated with vortex flow inside a macroscopic magnetic island has been investigated. Due to the elongation of the MI and incompressibility of the E x B flow, the shearing rate near X-points is much lower than that near the mid-plane (x-axis of the local Cartesian coordinate) of the MI on the same flux surface. This result of E x B shearing profile and minimal E x B shear near the X-points [1] is consistent with the recent experimental finding that turbulence tends to spread into an MI through regions around the X-points [2]. In addition, the vortex tends to be better sustained in a large MI, while toroidicity induced precession can break up the quasi-helical symmetry of the vortex, leading to more complicated flow pattern in a long term around a relatively thin MI [3]. Work supported by National R&D Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and Future Planning (NRF-2019M1A7A1A02088355) and by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. 2021R1A2C1094634).

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### Keywords:

Shear flow, Turbulence, Magnetic island

## Linear gyrokinetic simulation of TAE with turbulence in KSTAR

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### Abstract:

Understanding of energetic particle (EP) confinement is a crucial issue for high-performance operation of present-day fusion devices, ITER and future fusion reactor. It is widely recognized that EP-driven Alfvén eigenmodes (AEs) make a significant influence on the EP transport [1]. Moreover, recent simulation studies have revealed that AE-turbulence interactions significantly change EP and thermal plasma transport in a qualitative sense [2,3]. In this presentation, we show early linear simulation results of an on-going gyrokinetic study of EP effect on toroidal Alfvén eigenmode (TAE) and turbulence and their impact on confinement in KSTAR tokamak plasmas [4]. For a detailed physics study, we run both global gyrokinetic code GTC [5] and local gyrokinetic code GWK [6] and compare their results to characterize non-local physics.

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### Keywords:

Alfvén eigenmode, Gyrokinetics, Turbulence, Energetic particle, KSTAR

## Gyrokinetic simulation studies of ExB staircase in KSTAR L-mode plasmas

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### Abstract:

It was found that turbulence in hot magnetized plasmas generates a self-organized flow structure which is called ExB staircase [1]. To study the role of ExB staircase, we investigate KSTAR L-mode plasmas using global nonlinear gyrokinetic code gyroKinetic Plasma Simulation Program (gKPSP) [2]. Nonlinear simulations comparing Linear Ohmic Confinement (LOC) and Saturated Ohmic Confinement (SOC) plasmas with KSTAR parameters have been performed. ExB Staircase structure has been found as observed in KSTAR experiments [3] and other gKPSP simulations [4,5]. Staircase structure is only found in SOC plasma, which is consistent with the experimental results of Tore Supra [6]. Non-diffusive avalanche events and intermittent bursts are observed for both cases but they show different properties. These turbulence transport properties and the role of ExB staircase are being investigated.

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### Keywords:

ExB staircase, Gyrokinetic simulation, KSTAR, plasma turbulence

## Transport events and $E \times B$ staircase in gyrokinetic flux-driven ion temperature gradient (ITG) turbulence simulation

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### Abstract:

In tokamak plasmas, transport frequently accompanies non-local and non-diffusive intermittent phenomena such as turbulent spreading and avalanches [1]. Recent studies using flux-driven gyrokinetic simulations have shown that self-organized structure named  $E \times B$  staircase arise near marginality and regulate non-diffusive transport events [2, 3]. In this talk, we investigate non-diffusive transport events in flux-driven GKNET gyrokinetic simulations with ion temperature gradient (ITG) turbulence and study their properties in the presence of  $E \times B$  staircase. We use statistical approaches such as the recently developed size probability distribution function (size-PDF) method [4]. We find that  $E \times B$  staircase acts as wave packet traps when it is quasi-stationary, consistent with the wave-kinetic description of the staircase [5]. On the other hand, results also show that bursty transport events can happen across the staircase correlated with abrupt changes in staircase structure. Work supported by the National R&D Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (NRF-2019M1A7A1A02088355)

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### Keywords:

$E \times B$  Staircase, Turbulence, Gyrokinetic Simulation, Avalanches, Flux-driven Simulation

## Evidence of turbulence generated by localized current drive in the core of tokamak plasma

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### Abstract:

Electron cyclotron current drive (ECCD) is considered as one of the notable techniques to control sawtooth instabilities. Dynamics of electron temperature fluctuations measured by electron cyclotron emission imaging system (ECEI) installed on KSTAR tokamak suggests that multiple current-carrying flux tubes can be generated during ECCD blip [1,2]. These flux tubes can be generated as the electrons gain kinetic energy from RF waves within few passages of resonance position and sustain longer than current dissipation time when the q profile is flat inside sawtooth inversion radius [3]. Furthermore, we performed multichannel correlation analysis to understand turbulent fluctuations associated with filaments of flux tubes [4]. During the ECCD pulse, the coherence spectrum shows broadband fluctuations localized to the ECCD deposition radius, in contrary to the narrow-band features (MHD modes) observed during ECCD inter-pulse. In addition, the relation of wavenumber and energy conforms with Kolmogorov's power law relation, which explains the energy transfer from macro- to microscales which constitute eddies of turbulent fluctuations. This suggests the energy transfer and dissipation induced by localized current drive. We investigate the mechanism for driving turbulence in such conditions and compare with theories explaining the power law for collisionless plasmas driven by high guide field ( $B_{\perp} \ll B_{\parallel}$ ) [5]. This work is supported by NRF of Korea under grant no. NRF-2019M1A7A1A03088456.

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### Keywords:

KSTAR, ECEI, ECCD, Plasma turbulence, Transport

## Experimental analysis on the effect of the plasma current overshoot in KSTAR

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### Abstract:

In this study, we report the effect of plasma current overshoot in KSTAR. In the 2020 KSTAR experiment, plasma current overshoot (CuOv) discharges have improved performance of  $\beta N \geq 2.45$ ,  $H_{89} \geq 2.1$  and  $H_{98} \geq 1.2$  during the main heating phase compared to the intermediate performance of the conventional H-mode discharges without plasma current overshoot ( $\beta N \sim 2.0$ ,  $H_{89} \sim 1.8$  and  $H_{98} \sim 0.95$ ). We analyzed the representative CuOv discharge #25464 in plasma performance, 1D profiles, core-edge interplay, and linear gyro-kinetic analysis. In the plasma performance, it was found that the increase of the fast particle content compensates for the decrease of the thermal ion and leads to the enhancement of the plasma confinement. In the 1D profiles, the q profile of #25464 becomes broader, and an s/q value becomes larger than the conventional case. However, these q- and s/q profile differences soon disappear as the current diffuses. In the core-edge interplay, the plasma edge mode affects the core fast ion content, related to transport suppression based on thermal ions dilution [1]. Numerical analyses using a linear gyro-kinetic code [2] reveal that the core confinement enhances due to the favorable magnetic shear configuration and the increased fast particle content. Based on these findings, we conclude that the confinement enhancement results from the core and edge regions. Furthermore, the enhancement by the favorable magnetic shear disappears, and the enhancement by fast particle content maintains.

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### Keywords:

plasma current overshoot, KSTAR

## Discovering nanophotonic structures exhibiting asymmetric optical transmission with factorization machine-quantum annealing interfaces

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### Abstract:

Discovering an optimal design of the nanophotonic structure for specific optical properties (*i.e.*, asymmetric light transmission) has been challenging. In this talk, we propose that a Factorization Machine (FM) – quantum annealing (QA) interface can efficiently discover an optimal photonic structure. FM as a surrogate model needs a sparse training dataset for accurate prediction, while QA can find the optimal design from FM with hardware acceleration. For a demonstration, we use the FM to find the optimal optical diode structure, which lets light transmission in the forward direction but prevents the transmission in the backward direction (*i.e.*, asymmetric transmission). In the optimization, we divide a unit cell of structure into ' $n$ ' number of pixels and assign them with a binary vector. For example, we map '1' to a metal pixel or '0' to a dielectric pixel. We perform Fourier modal method (FMM) to evaluate the energy isolation factor and transmission efficiency at a given binary vector. In this way, we prepare a dataset to train the FM and use QA to predict the optimal binary vector to maximize the figure-of-merit. In a benchmark study, we observe that the FM can find the optimal binary vector with the dataset, which is less than 1 % of the total number ( $N$ ) of binary vector states (*i.e.*,  $N = 2^n$ ). In addition, we perform the designing process by increasing the number of pixels up to  $n = 40$  and successfully identify the optimal plasmonic structure, which has transmission efficiencies of 81 % in the forward direction and 0.4 % in the backward direction at visible frequency.

### Keywords:

Asymmetric Transmission, Factorization Machine, Quantum Annealing, Optical Diode, Plasmonics

## Moiré excitons and correlated states in 2D transition metal dichalcogenide heterostructures

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### Abstract:

Van der Waals heterostructures can be designed to confine electrons and holes in unique ways. One remarkable approach is to vertically stack two atomically thin layers of transition metal dichalcogenide (TMD) semiconductors. The relative twist or lattice mismatch between the two layers leads to moiré pattern formation, which modulates the electronic band structure according to the atomic registry. Single-particle wave packets can be trapped in the moiré-induced potential pockets with three-fold symmetry, leading to the formation of trapped interlayer excitons and correlated states. In this talk, I will explain photoluminescence emission of moiré confined excitons in MoSe<sub>2</sub>/WSe<sub>2</sub>. Interesting properties of moiré excitons like antibunching, large Stark shift, and doping dependence will be presented. Furthermore, correlated states, such as Mott insulating states and Wigner crystals, observed from moiré heterostructures will be presented.

### Keywords:

moiré, excitons, TMD

# Spatio-spectral decomposition of complex eigenmodes in subwavelength nanostructures through transmission matrix analysis

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## Abstract:

Exploiting multiple near-field optical eigenmodes is an effective means of designing, engineering, and extending the functionalities of optical devices. However, the near-field optical eigenmodes of subwavelength plasmonic nanostructures are often highly multiplexed in both spectral and spatial distributions, making it extremely difficult to extract individual eigenmodes. We propose a novel mode analysis method that can resolve individual eigenmodes of subwavelength nanostructures, which are superimposed in conventional methods. A transmission matrix is constructed for each excitation wavelength by obtaining the near-field distributions for various incident angles, and through singular value decomposition, near-field profiles and energy spectra of individual eigenmodes are effectively resolved. By applying transmission matrix analysis to conventional electromagnetic simulations, we clearly resolved a set of orthogonal eigenmodes of single- and double-slot nanoantennas with a slot width of 20 nm. In addition, transmission matrix analysis leads to solutions that can selectively excite specific eigenmodes of nanostructures, allowing selective use of individual eigenmodes.

## Keywords:

mode analysis, nano optics, transmission matrix

## Surface plasmon mediated emission and lasing in InGaAs semiconductor with periodic metal grating

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### Abstract:

Surface plasmons (SPs) are collective and quantized electric charge oscillation at the interface between the metal and dielectric. By compensating the momentum mismatch with the geometrical factor, metal gratings on a semiconductor can induce strong light-matter interactions mediated by SPs called the surface plasmon resonance (SPR).

In order to investigate the interaction of excited charge carriers in a semiconductor with SPs, we fabricated Au gratings on InGaAs with a period around 400 nanometers to locate the SPR position near the semiconductor energy gap for efficient energy transfer. An InGaAs layer with relatively broad photoluminescence (PL) in near-infrared region of ~1500 nm was used in this study.

Grating period dependence of the PL enhancement in the Au/InGaAs/InP structure confirms the SPR effect with a good correspondence to the transmission spectrum and to the numerical simulation of the FDTD method. Moreover, by optically pumping with an ultrafast laser we could enable SP lasing at specific wavelengths satisfying the SPR conditions. We expect that our work will contribute to the development of SP based high-speed photonic devices.

### Keywords:

Surface plasmon, Metal grating, InGaAs, FDTD, SP lasing

## 높은 개구수와 적절한 시야를 가지는 새로운 위상 방식의 메타렌즈

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### Abstract:

메타렌즈는 휴대전화 카메라, 내시경 및 초박형 현미경 대물렌즈를 포함한 기존 광학 시스템을 대체하거나 개선할 수 있는 가능성으로 많은 주목을 받고 있다. 단일층 메타렌즈는 기존 광학 장비보다 훨씬 작은 크기를 가지기 때문에 다양한 장비에 결합이 용이하다는 장점이 있지만, 수차로 인해 높은 조리개수와 적절한 시야를 가지는 것이 어렵다는 한계가 존재한다. 일반적으로 많이 사용되는 쌍곡선 위상 방식은 높은 조리개수를 달성할 수 있지만 시야가 매우 좁고, 이차 위상 방식은 넓은 시야를 가지지만 큰 구면 수차로 인해 높은 조리개수를 달성하기 어렵다. 수차로 발생하는 이런 한계들은 적절한 시야와 높은 조리개수를 동시에 요구하는 고급 광학 현미경이나 광축집에서의 응용에 한계를 가져온다. 이러한 문제를 해결하기 위해 곡면 메타렌즈나 다층 메타렌즈가 개발되었지만, 복잡한 공정과 큰 부피가 요구된다. 이번 연구를 통해 단일층 메타렌즈에서 사용되는 새로운 위상 방식을 개발하였고, 계산과 실험을 통해 높은 조리개수와 적절한 주사 범위를 동시에 가지는 것을 확인하였다. 이러한 특성을 가지는 메타렌즈는 고급 광학 현미경과 광축집계 등의 응용에 활용될 수 있을 것으로 기대된다.

### Keywords:

메타렌즈, 높은 개구수, 넓은 시야, 비축수차, 구면수차

## Nuclear spin-wave quantum register for a solid state qubit

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### Abstract:

Solid-state nuclear spins surrounding individual, optically addressable qubits provide a crucial resource for quantum networks, computation and simulation. While hosts with sparse nuclear spin baths are typically chosen to mitigate qubit decoherence, developing coherent quantum systems in nuclear spin-rich hosts enables exploration of a much broader range of materials for quantum information applications. The collective modes of these dense nuclear spin ensembles provide a natural basis for quantum storage, however, utilizing them as a resource for single spin qubits has thus far remained elusive. Here, by using a highly coherent, optically addressed  $^{171}\text{Yb}^{3+}$  qubit doped into a nuclear spin-rich yttrium orthovanadate crystal, we develop a robust quantum control protocol to manipulate the multi-level nuclear spin states of neighbouring  $^{51}\text{V}^{5+}$  lattice ions. Via a dynamically-engineered spin exchange interaction, we polarise this nuclear spin ensemble, generate collective spin excitations, and subsequently use them to implement a long-lived quantum memory. We additionally demonstrate preparation and measurement of maximally entangled  $^{171}\text{Yb}$ -- $^{51}\text{V}$  Bell states. Unlike conventional, disordered nuclear spin based quantum memories, our platform is deterministic and reproducible, ensuring identical quantum registers for all  $^{171}\text{Yb}$  qubits. Our approach provides a framework for utilising the complex structure of dense nuclear spin baths, paving the way for building large-scale quantum networks using single rare-earth ion qubits.

[1] A. Ruskuc et al., "Nuclear spin-wave quantum register for a solid-state qubit", Nature 602, 408 (2022)

### Keywords:

solid-state qubit, nuclear spin, quantum register, spin wave, Bell state

# High fidelity control and measurement of semiconductor quantum dot spin qubits

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## Abstract:

The electron spin degree of freedom in solids form natural basis for constructing quantum two level systems, or qubits. The electron spin qubit offers a route for fast manipulation of spins using magnetic resonance or field gradient induced electric control, but generally suffers from dephasing due to strong coupling to the environment, especially nuclear spin bath, where decoherence dynamics is often non-Markovian. We report energy-selective tunneling readout-based Hamiltonian parameter estimation of a two-electron spin qubit in a GaAs quantum dot array. Optimization of readout fidelity enables a single-shot measurement time of 16 ns on average, with adaptive initialization and unambiguous qubit frequency estimation based on real-time Bayesian inference. We demonstrate quantum oscillation visibility, single-shot measurement fidelity, and state initialization fidelity of 97.7%, 99%, and over 99.9%, respectively. By pushing the sensitivity of the energy-selective tunneling-based spin-to-charge conversion to the limit, the technique is useful for advanced quantum control protocols such as error mitigation schemes, where fast qubit parameter calibration with a large signal-to-noise ratio is crucial.

## Keywords:

Solid-state quantum computing, cryogenic quantum transport, coherent manipulation, Hamiltonian estimation

## Multiplexed sensing of magnetic field and temperature using a quantum diamond sensor

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### Abstract:

The nitrogen-vacancy (NV) color center in diamond is a versatile quantum sensor, being able to measure physical quantities such as magnetic field, electric field, temperature, and pressure. In this talk, I will be talking about multiplexed sensing of magnetic field and temperature using a NV ensemble in diamond. The dual-frequency-driving technique employed here is based on frequency-division multiplexing, which enables the sensing of both measurables in real time. The pair of N-V resonance frequencies for dual-frequency driving must be selected to avoid coherent population trapping of NV spin states. With enhanced optical collection efficiency higher than 50% and a type 1b diamond crystal with a natural abundance of  $^{13}\text{C}$  spins, the sensitivities of about  $70 \text{ pT/Hz}^{1/2}$  and  $25 \text{ } \mu\text{K/Hz}^{1/2}$  are achieved simultaneously. A high isolation factor of 34 dB in the N-V thermometry signal against the magnetic field is demonstrated; and a theoretical description for the isolation factor is provided. This work paves the way for extending the application of N-V diamond sensors into more demanding conditions.

### Keywords:

Quantum sensor, Nitrogen-Vacancy color center, Multiplexed sensing

## Epitaxial graphene based biosensor for rapid detection of COVID-19

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### Abstract:

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the virus responsible for Coronavirus disease 2019 (COVID-19), was classified as a pandemic in March 2020 by the World Health Organization (WHO), with over 300 million cases and 5.5 million deaths worldwide as of January 2022. The total deaths in the USA are expected to reach over 1,000,000 by May 2022. COVID-19 causes respiratory illnesses of varying severity from the common cold to fatal pneumonia in both humans and animals. The current primary diagnosis of COVID-19 is real-time reverse transcription-polymerase chain reaction (RT-PCR), which is the fastest and most reliable method, for detection and pandemic containment. However, RT-PCR needs an RNA preparation process, which decreases the accuracy and sensitivity of the test, and takes over three hours to confirm the diagnosis. Thus, the direct detection of viral antigens from human to environmental conditions without the RNA sample preparation process is required for future ultra-fast and highly accurate immunological diagnostic methods. Two-dimensional (2D) materials such as graphene are promising for the next generation of electronics, i.e., biological and chemical sensors in environmental and safety monitoring and medical health care systems. In addition, atomically thin 2D graphene has an extremely high surface-to-volume ratio, the most vital parameter for sensing applications. Here we fabricated a heterostructure of SARS-CoV-2 S1 spike antibodies and epitaxial graphene (EG) on 6H silicon carbide (SiC) substrate for SARS-CoV-2 detection. We have combined the advantages of high sensitivity and fast response time of graphene with the high selectivity of antibodies to develop an ultrasensitive SARS-CoV-2 screening platform. The prepared sensor was tested with SARS-CoV-2 S1 spike protein and clinical samples (i.e., mid-turbinate swabs, saliva, and exhaled breath aerosol) and clearly distinguished between blank and SARS-CoV-2 at room temperature. In addition, the sensor demonstrated as a practical application of the portable sensor to detect the SARS-CoV-2 B.1.1.7 variant and the portable unit clearly distinguished variant positive saliva samples in 0.6 s at room temperature. Hence, this sensor has great potential as an ultrasensitive SARS-CoV-2 screening platform.

### Keywords:

2D material, Graphene, SiC, COVID-19, Heterostructure, Biosensor

## Reactant/polymer hybrid films on pn junction photodetectors for self-powered, non-invasive glucose biosensors

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### Abstract:

The portability of electronic-based biosensors is limited because of the use of batteries and/or solutions containing reactants such as enzymes for assay, which limits the utility of such biosensors in point-of-care (POC) testing. In this study, we report on the development of a self-powered biosensor composed of only portable components: a reactant-containing poly (ethylene glycol) (PEG) film for the colorimetric assay, and a self-powered n-InGaZnO/p-Si photodetector. The PEG film containing enzymes and color-developing agents was formed on a glass slide by spin coating. The self-powered biosensor was fabricated by placing the hybrid film on the p-n junction photodetector, and applied in non-invasive glucose detection (salivary glucose). Injection of the target-containing solution dissolved the PEG that led to the release of enzymes and color-developing agents, resulting in a colorimetric assay. The colorimetric assay could attenuate the light reaching the photodetector, thus facilitating target concentration verification by measuring the photocurrent. Our self-powered biosensor has two main advantages: (i) all components of the biosensor are portable and (ii) dilution of target concentration is avoided as the reagents are in the PEG film. Therefore, the self-powered biosensor, without solution-phase components, could be highly beneficial for creating portable, sensitive biosensors for POC testing.

### References

[1] K. Kim et al, *Biosensors and Bioelectronics*, 175, 112855 (2021).

### Keywords:

self-powered biosensor, p-n junction photodetector, glucose

## Probing Pathways of Conductive Filaments of FAMAPbI<sub>3</sub> WORM Device Using Conductive Atomic Force Microscopy

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### Abstract:

Formamidinium (FA) cation-based perovskite resistive switching (RS) memory devices have emerged as the most promising candidates for non-volatile memory devices. However, there is a lack of systematic study on the effect of FA cations on the RS memory device characteristics. Herein The properties of FAMAPbI<sub>3</sub>-based write-once-read-many (WORM) devices were controlled by a cation exchange process as part of a technique to change the FA composition in FAMAPbI<sub>3</sub> films. Interestingly, it was found that an increase in the FA composition in FAMAPbI<sub>3</sub> films resulted in a completely inactive WORM device. Such a memory characteristic of a WORM device was attributed to the high iodine vacancy ( $V_I$ ) ion migration energy that prevented the formation of  $V_I$  conductive filaments (CFs) with the increase in the FA composition in FAMAPbI<sub>3</sub> film.

By comparing the active and inactive FAMAPbI<sub>3</sub> WORM devices, the pathways of CFs within FAMAPbI<sub>3</sub> WORM devices were investigated using conductive atomic force microscopy. Our results showed that the CFs were dominantly formed around grain boundaries, while some grain interior regions showed very low conductivity. These studies on the CF formation mechanism provide a better understanding of RS memory characteristics in multi-cation perovskite materials.

### Keywords:

resistive switching (RS), write-once read-many (WORM), iodine vacancy (VI), Formamidinium (FA)

## Controllable Surface Oxidation and Doping Effect of Indium Selenide (InSe) Using Polymer Passivation

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### Abstract:

InSe, one of the van der Waals crystal structures, is a metal chalcogenide III-VI compound that can be exfoliated and has stable semiconductor properties. It has attracted considerable attention due to its low effective electron mass (0.14 $m_0$ ), direct bandgap in bulk form (1.26 eV), and high charge mobility (300 cm<sup>2</sup>/Vs). However, unlike TMDC, it is susceptible to moisture, so when exposed to air, it gradually oxidizes and degrades the device's performance. In an effort to overcome this, passivation is attempted using PMMA or h-BN, but the oxidation that occurs on the InSe surface itself is still unresolved. In this study, we tried two different types of polymer doping to control the surface oxidation of InSe and improve the device's performance. First, Benzyl Viologen (BV) as an n-type dopant injects electrons into the InSe layer to improve charge mobility. A CYTOP used as a p-type dopant injects holes, resulting in a p-doping effect.

To confirm that these two types of polymers act as passivation to prevent oxidation of the InSe surface, the polymers were covered the surface of the InSe FET. Then, the electrical characteristics of the InSe according to the concentration of the polymer were measured. This study makes the development of high-performance InSe devices useful by controlling InSe surface oxidation with polymers.

### Keywords:

InSe, polymer passivation, doping effect

## Ultra-high photoresponsivity of photodiode based on integrated freestanding two-dimensional transition metal dichalcogenide

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### Abstract:

Two-dimensional transition metal dichalcogenides are attracting attention because of their unprecedented properties, such as high transparency, good flexibility, atomically thin structure, and predictable electron transport. Nevertheless, the current state of device performance in monolayer transition metal dichalcogenide-based optoelectronics is still far from practical for commercialization due to its substantial strain on the heterogeneous planar substrate and its robust metal deposition, which causes crystalline damage. Here, we show that strain-relaxed and non-damaged monolayer WSe<sub>2</sub> results in remarkably improved device performance. We propose a new kind of photodiode (i.e. a point-cell photodiode consisting of a monolayer WSe<sub>2</sub>) simply transferred onto core-shell silicon-gold nanopillars. The maximum photoresponsivity of the device is found to be 23.16 A/W, which is a significantly high value for monolayer WSe<sub>2</sub>-based photodiodes. Such new point-cell photodiodes can resolve critical issues of 2D materials, leading to tremendous improvements in device performance.

### Keywords:

Monolayer WSe<sub>2</sub>, Photodiode, Charge transfer, Nanopillars, Point-cell

# Large-Area MoS<sub>2</sub> via Colloidal Nanosheet Ink for Integrated Memtransistor

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## Abstract:

2D transition metal dichalcogenides (TMDs) exhibit intriguing properties for applications in optoelectronics and electronics, among which memtransistors received extensive attention as multifunctional devices. For practical applications of 2D TMDs, large-area fabrication of the materials via reliable processes, which is in trade-off with their quality, has been a long-standing issue. Here, a simple and effective way is proposed to fabricate large-area and high-quality molybdenum disulfide (MoS<sub>2</sub>) thin films using MoS<sub>2</sub> colloidal ink through a spray coating, followed by a postsulfurization process. High-quality MoS<sub>2</sub> thin films exhibits excellent optical and electrical properties that can be utilized in field-effect transistors (FETs) and memtransistor arrays. The MoS<sub>2</sub> FETs show an average on/off ratio of  $5 \times 10^6$  and a high electron mobility of  $10.34 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , which can be understood by the healing of sulfur vacancies, recrystallization, and the removal of the carbon contamination of the MoS<sub>2</sub>. These MoS<sub>2</sub>-based memtransistors present stable operations with a high switching ratio tuned by back gate and light illumination, which is promising for multiple-levels memory and complex neuromorphic computing. This study demonstrates a new strategy to fabricate 2D TMDs with large-area and high quality for integrated optoelectronic and memory device applications.

## Keywords:

Colloidal synthesis, Memtransistor, TMDs, MoS<sub>2</sub>, large area

## Fabrication of narrow bandgap CuInSe<sub>2</sub> (CIS) solar cell via solution-based spray deposition

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### Abstract:

We fabricated narrow bandgap CIS solar cell with small Ga back graded and alkali treatment, where both absorber and alkali treatment were made by non-vacuum aqueous spray pyrolysis. For spray deposition, we utilized water based solution, which is eco-friendly non-hazardous solvent. The fabricated absorber exhibits energy band gap around ~1.04 eV. We found that power conversion efficiency (PCE) is much improved due to the small Ga back grading and alkali treatment. We characterized systematically the effect of alkali treatment on solar cell performance. Admittance spectroscopy (AS), electrochemical impedance spectroscopy (EIS) and photoluminescence (PL) measurements revealed that defect states are much passivated via the alkali treatment. With the defect passivation, PCE more than ~15 % was achieved.

### Keywords:

Narrow bandgap, CuInSe<sub>2</sub>, Solar cell, Spray pyrolysis, Alkali treatment

## Degradation Mechanism by Moisture of Quasi-2D Halide Perovskite

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### Abstract:

Organic-inorganic metal halide perovskite (OHP) has been recognized for its potential in electrical and optical applications due to its innate properties and simple low-temperature synthesis process. In particular, OHPs-based solar cells have reached the power conversion efficiency (PCE) of currently commercialized silicon solar cells. However, OHP solar cells have reached the commercialization level of PCE, but have limitations due to stability issues. In particular, OHP is very sensitive to moisture due to the hygroscopic properties of MA<sup>+</sup> and FA<sup>+</sup>. Therefore, high water stability was achieved by replacing small cations with bulky cations. Here, a quasi-2D (RNH<sub>3</sub>)<sub>2</sub>(FA)<sub>1</sub>Pb<sub>2</sub>Br<sub>7</sub> film was synthesized with a dual ligand reacting with oleylamine and oleic acid. As the concentration of binary ligands in this film increased, the contact angle increased to 90 degrees at 8 Vol% and the surface free energy was 28.06 mJ/m<sup>2</sup>, which was slightly higher than that of the 2D halide perovskite. In addition, it shows stable photoluminescence even in water and has strong resistance to moisture. In particular, when the PL spectra were compared with the quasi-2D film exposed to moisture for 3 min, the bulky PL peak blue-shifted and the 2D PL peak red-shifted. Moisture simultaneously affects both 2D and bulky perovskite, and 2D perovskite occurs aggregation whereas the bulky perovskite is completely decomposed by water.

### Keywords:

quasi-2d halide perovskite, Degradation mechanism, perovskite solar cell

## 웨어러블 슈퍼커패시터를 위한 전기화학적 양극산화법에 의한 수산화 구리 나노선의 합성 및 특성

EDUGULLA Girija Shankar <sup>2</sup>, AMIT Kumar Das <sup>1</sup>, YU Jae Su <sup>\*2,1</sup>

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### Abstract:

급속한 세계화로 인해 회로 기판, 오래된 전자 케이블, 히터, 팬 등의 금속성 전자 폐기물이 쓰레기 매립장에 쌓여 증가하고 있다. 전자 폐기물을 에너지 저장 장치로 변환하면 화석 연료에 대한 의존도가 더욱 낮아져 경제적 가치가 향상된다. 이와 관련하여, 본 발표에서는 폐케이블에서 구리 와이어를 추출하고 고체 상태의 웨어러블 슈퍼커패시터를 제조하기 위한 집전체(기판)로 사용됨을 보고한다. 편조된 구리 와이어는 chronoamperometry를 사용하여 추가로 양극산화(anodizing)되었다. 다음은 전기화학증착방법을 통해 니켈-코발트-셀레나이드를 성장시키기 위한 기판으로 사용되었다. 다음과 같이 준비된 전극 화학적 성능을 3전극 시스템에서 측정했다. 니켈-코발트-셀레나이드 전극은 Faradaic type 에너지 저장 거동을 보여주었다. 얻어진 결과는 니켈-코발트-셀레나이드 전극이 전자 장치의 에너지 저장 시스템으로 사용될 수 있음을 나타낸다.

### Keywords:

웨어러블, 슈퍼커패시터, 수산화구리, 나노선, 전기화학적 특성

# Interface Engineering for Scalable Fabrication of Planar Perovskite Solar Cells

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## Abstract:

Despite the recent unprecedented increase in the power conversion efficiencies (PCEs) of small-area devices ( $\leq 0.1 \text{ cm}^2$ ), perovskite solar cells (PSCs) still face serious drawbacks in their printability and scalability. The formation of pinhole-free perovskite photoactive films with full surface coverage has been a tremendous challenge for up-scaling planar perovskite solar cells (PSCs) while maintaining their high power conversion efficiencies (PCEs). Particularly, a significant mismatch between the surface energies of a hydrophilic perovskite precursor solution and a hydrophobic organic charge transport layer (CTL) has been a major cause for the incomplete surface coverage of perovskite photoactive films, which drastically reduces the scalability and reproducibility of PSCs. Here, we report a universal method to create extremely compact perovskite photoactive films on a variety of hydrophobic CTLs. By introducing an amphiphilic conjugated polyelectrolyte as an interfacial compatibilizer, we succeed in improving the wettability of perovskite precursor solutions on hydrophobic CTLs and fabricating perovskite photoactive films over large areas. Our approach enables the scalable fabrication of planar PSCs with large areas ( $1 \text{ cm}^2$ , PCE of 17%) while preserving nearly 90% of the PCEs of the corresponding small-area devices (PCE of 19%).

## Keywords:

perovskite solar cells, interfacial compatibilizer, conjugated polyelectrolytes, large-area, printing

# Quantum Computing for High Energy Physics

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## **Abstract:**

The technology of quantum computers and related systems is advancing rapidly, and powerful programmable quantum processors are already being made available by various companies. Long before we reach the promised land of fully fault tolerant large scale quantum computers, we expect unambiguous "quantum advantage" will be demonstrated for problems of interest to physicists. At the same time, advances in the technology of quantum processors are also enabling advances in quantum sensing, enabling new kinds of experiments for fundamental physics, including dark matter and quantum gravity.

## **Keywords:**

Quantum Computing, High Energy Physics

## Quantum Networking and High Energy Physics

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### **Abstract:**

The first quantum key distribution network in the U.S. was the result of a collaboration between NIST, industry, and academic researchers circa 2000. In the past five years, through the U.S. national quantum initiative and our quantum internet blueprint, the Dept. of Energy and other federal agencies have promoted research on advanced quantum networks for scientific research in high energy physics and beyond. I will discuss recent and upcoming results from our quantum teleportation network testbeds, and prospects for the future.

### **Keywords:**

Quantum Networking, High Energy Physics

## Tabletop Flying Plasma Mirrors to Investigate Black Hole Information Loss Paradox

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### **Abstract:**

The question of whether Hawking evaporation violates unitarity, and therefore results in the loss of information, has remained unresolved since Hawking's seminal discovery. To date, the investigations have remained mostly theoretical since it is almost impossible to settle this paradox through direct astrophysical black hole observations. In 2017, Chen and Mourou pointed out that relativistic plasma mirrors can be accelerated drastically and stopped abruptly by impinging intense x-ray pulses on solid plasma targets with a density gradient. This is analogous to the late time evolution of black hole Hawking evaporation. Critical issues, such as how the black hole unitarity may be preserved, can be addressed through the entanglement between the analog Hawking radiation photons and their partner modes. An international AnaBHEL (Analog Black Hole Evaporation via Lasers) collaboration has been formed with the objective to observe the analog Hawking radiation and to shed some lights on the information loss paradox. In this talk, I will give an overview on information loss paradox and the proposed solutions, and various analog black holes concepts. Then I will focus on the concept of flying plasma mirror and the AnaBHEL experiment and its current status.

### **Keywords:**

Black hole, Hawking evaporation, information loss paradox, analog black holes, flying plasma mirror

## Python's lunch geometries in Jackiw-Teitelboim gravity with matter

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### Abstract:

We introduce Python's lunch geometries in the two-dimensional Jackiw-Teitelboim model coupled to a massless scalar field in the semiclassical limit and obtain fully back-reacted general bulk solutions with a massless scalar field, which can be understood as deformations of two-sided black holes. We provide information-theoretic interpretation of deformed geometries including Python's lunches, minimal quantum extremal surface and appetizers according to the entanglement wedge reconstruction hypothesis and show that the observational probability of Python's lunch degrees of freedom from the boundary is exponentially suppressed.

### Keywords:

2D gravity, quantum extremal surface, entanglement wedge reconstruction, quantum complexity

## Page curve from Euclidean path integral

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### **Abstract:**

In this presentation, we revisit the entanglement entropy via the Euclidean path integral of the quantum state and allow for the branching of semi-classical histories along with the Lorentzian evolution. We posit that there exist at least two histories that contribute to the path integral, where one is an information-losing history while the other is information-preserving. At early times, the former dominates, while at late times the latter becomes dominant. By so doing we recover the essence of the Page curve and thus the unitarity, albeit with the turning point, i.e., the Page time, much shifted toward the late time. We finally comment on the possible implications of this approach.

### **Keywords:**

information loss paradox, entanglement entropy, Euclidean path integral

# Black hole information paradox and island prescription

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## **Abstract:**

I will give a brief overview of the black hole information paradox and the recent progress. I will describe the island prescription and discuss problems for the future.

## **Keywords:**

Information loss problem, Island prescription

## The COHERENT Experimental Program

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### **Abstract:**

Coherent elastic neutrino-nucleus scattering (CEvNS) is a process in which a neutrino scatters off an entire nucleus at low momentum transfer, and for which the observable signature is a low-energy nuclear recoil. It represents a background for direct dark matter detection experiments, as well as a possible signal for astrophysical neutrinos. Furthermore, because the process is cleanly predicted in the Standard Model, a measurement is sensitive to beyond-the-Standard-Model physics, such as non-standard interactions of neutrinos. The process was first predicted in 1973. It was measured for the first time in 2017 by the COHERENT collaboration using the high-quality source of pion-decay-at-rest neutrinos from the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory and a CsI[Na] scintillator detector; a second measurement on argon followed in 2020. This talk will describe COHERENT's CEvNS measurements, the status and plans of COHERENT's current suite of detectors, and the future physics reach of the program with upgraded beams and detectors at the SNS first and second target stations.

## Search for Light New Particles

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### **Abstract:**

Recently, light new particle searches are receiving more rising attention as alternatives to conventional weak-scale new-physics searches. First, I focus on new directions in light particle searches at low-energy but high-intensity neutrino facilities that will exploit both the high intensity source of photons (and therefore, possible production of low-mass new particles such as dark photon, axion-like particle, and dark matter) and low-energy capabilities of the current detector technology. For the direct detection of super-light dark matter, a handful of detection schemes have been proposed thus far, based on new technologies measuring small energy depositions in the detector. Among them, I introduce a new super-light dark-matter direct-detection experiment adopting recently invented graphene-based Josephson-junction technology, and show the current status of the experiment.

### **Keywords:**

Light new particle, Neutrino, Dark matter, Axion, Graphene-based Josephson junction

## NaI(Tl) detector development and the NEON experiment

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### Abstract:

Thallium-doped sodium iodide crystals are widely used in radiation detection from gamma-ray spectroscopies to rare event searches such as neutrino and dark matter particle interactions because of their high light yield above 15 photoelectrons per keV electron equivalent. More recently, we have developed a new design for the crystal detector which improves the light yield further and therefore is useable for the measurement of sub-keV tiny signals.

Taking advantage of this detector development, we installed the NEON (Neutrino Elastic-scattering Observation in NaI) experiment with a 15 kg crystal array at 24 meters away from the reactor core of the Hanbit nuclear power plant. NEON aims at detecting a coherent neutrino-nucleus scattering process for the first time using the reactor antineutrinos.

Current performance and future prospect of the experiment are reviewed.

### Keywords:

NaI, crystal, coherent scattering,

## Checking Non-Flow Assumptions and Results via PHENIX results in small collision systems

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### Abstract:

Recently the PHENIX Collaboration has made available two-particle correlation Fourier coefficients for multiple detector combinations in minimum bias p+p and 0-5% central p+Au, d+Au, <sup>3</sup>He+Au collisions at 200 GeV. Using these coefficients for three sets of two-particle correlations, azimuthal anisotropy coefficients  $v_2$  and  $v_3$  are extracted for midrapidity charged hadrons as a function of transverse momentum. we use the available coefficients to explore various nonflow hypotheses as well as compare the results with theoretical model calculations. The non-flow methods fail basic closure tests with AMPT and PYTHIA/ANGANTYR, particularly when including correlations with particles in the low multiplicity light-projectile going direction. In data, the non-flow adjusted  $v_2$  results are modestly lower in p+Au and the adjusted  $v_3$  results are more significantly higher in p+Au and d+Au. However, the resulting higher values for the ratio  $v_3/v_2$  in p+Au at RHIC compared to p+Pb at the LHC is additional evidence for a significant over-correction. Incorporating these additional checks, the conclusion that these flow coefficients are dominated by initial geometry coupled with final-state interactions (e.g. hydrodynamic expansion of quark-gluon plasma) remains true, and explanations based on initial-state glasma are ruled out. The detailed balance between intrinsic and fluctuation-driven geometry and the exact role of weakly versus strongly-coupled pre-hydrodynamic evolution remains an open question for triangular flow, requiring further theoretical and experimental investigation.

### Keywords:

Collectivity, Nonflow, Small collision system

## Model study on the collectivity in small collision systems of different geometry

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### Abstract:

In recent years, momentum anisotropies of produced particles have been measured in small systems such as p+Au, d+Au, and <sup>3</sup>He+Au collisions. The measurement at PHENIX shows a larger elliptic flow in d+Au and <sup>3</sup>He+Au and a larger triangular flow in <sup>3</sup>He+Au. The results can be well described by hydrodynamic models translating initial collision geometry into final momentum anisotropy. However, there are still details to understand such as a nonflow effect, longitudinal decorrelation, and an effect of sub-nucleonic geometry. A multiphase transport model (AMPT) can also qualitatively describe the collective behavior with scatterings at partonic and hadronic stages. We utilize the AMPT model to further investigate the correlation between initial geometry and final momentum anisotropy, and the impact of the longitudinal decorrelation. In this presentation, we will discuss the simulation study to understand the flow results in small systems of different geometry.

### Keywords:

AMPT, Small System, Collectivity

## **f<sub>0</sub>(980) resonance production in small collision systems with ALICE**

KIM Junlee \*<sup>1</sup>, KIM Eun-Joo <sup>1</sup>, LIM Sanghoon <sup>2</sup>, KIM Beomkyu <sup>3</sup>

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### **Abstract:**

Short-lived resonances are powerful observables to research the hadronic phase in ultra-relativistic heavy-ion collisions, due to their short lifetimes, which are comparable with the timespan between chemical and kinetic freeze-out. f<sub>0</sub>(980) resonance, whose lifetime is about 2–20 fm/c, is one of the good probes to study the hadronic phase. In addition, the internal structure of f<sub>0</sub>(980) is still under discussion, the study of its production will give important information to explore the structure. In this respect, we present the multiplicity dependence of production of f<sub>0</sub>(980) at mid-rapidity in pp and p–Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV. The measurement has been performed with ALICE at the LHC via the f<sub>0</sub>(980)  $\rightarrow \pi^+\pi^-$  decay channel. The presentation will show particle yield ratios and the nuclear modification to discuss late hadronic phase and possible scenario of the structure of f<sub>0</sub>(980).

### **Keywords:**

f<sub>0</sub>(980), resonance, ALICE, small system, scalar meson

## Measurement of electron from beauty-hadron decays in pp collisions at $\sqrt{s} = 13$ TeV with ALICE

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### Abstract:

The measurement of heavy-flavour (charm and beauty) production in proton-proton (pp) collisions at the LHC provides a crucial information about quantum chromodynamics (QCD) in high-energy regime. Due to their large masses, heavy quarks are mainly produced in initial hard scattering processes. Therefore, heavy-flavour production cross section represents a primary benchmark for perturbative QCD (pQCD) calculations. Furthermore, heavy-flavour measurements in pp collisions provide a reference for measuring nuclear modification in nucleus-nucleus collisions.

In this contribution, the  $p_T$ -differential production cross section of electrons from beauty-hadron decays in pp collisions at  $\sqrt{s} = 13$  TeV with ALICE detector at midrapidity will be reported. Electrons from beauty-hadron decays were extracted based on the distance of closest approach (DCA) to the collision vertex. Comparison of the result with the FONLL (Fixed-Order with Next-to-Leading Log) pQCD calculation will also be shown.

### Keywords:

LHC, ALICE, heavy-flavor

## Measurement of the transverse momentum ( $j_T$ ) distribution of jet fragmentation in 5.02 TeV pp collision with ALICE

LIM SangHoon \*1, [RYU Jaehyeok](#) <sup>1</sup>  
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### Abstract:

Jets are a useful probe for the study of the early stage of Quark-Gluon Plasma (QGP) as they're created in the initial hard scatterings. By measuring the jets' yield and substructure, detailed information on how hard partons interact with the medium and formed into hadrons can be studied.

Jet fragment transverse momentum ( $j_T$ ) is calculated with charged particles inside a jet cone. We are analyzing data of proton-proton ( $pp$ ) and proton-lead ( $p$ -Pb) collisions at 5.02 TeV to measure  $j_T$  distributions in various longitudinal fragmentation function ( $z$ ) bins. This analysis can test the current understanding of jet fragmentation and possible nuclear effects in  $p$ -Pb collisions, and the developed analysis framework would be extended to analyses of heavy-ion data. In this presentation, the current status and future plan of the data analysis will be presented

### Keywords:

QGP, Jet, Jet fragment transverse momentum( $j_T$ ), ALICE

## Status of the multiplicity dependent analysis of $X_{ic+}$ production in pp collisions at $\sqrt{s}=13\text{TeV}$ with ALICE

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### Abstract:

Heavy quarks such as charm and beauty are produced in the early stage of the collisions, and they can experience the whole system's evolution thanks to its long lifetime. Therefore we can investigate the initial collision system and harmonization mechanism by measuring the hadrons containing the heavy quarks. One of the interesting observables is the multiplicity dependency of the heavy-flavor hadron production. In proton-proton collisions, different from Pb-Pb collisions, QGP is not expected to exist because the collision system is too small to produce QGP. However, recently It has been reported that in high multiplicity, some results show a similar trend with Pb-Pb collisions even in small systems.

ALICE measured the various charmed baryon recently and showed interesting results. Existing models could not describe the production of charmed baryons, therefore it can give a constraint to models. The multiplicity dependency of the  $X_{ic+}$  yield was studied using the hadronic decay channel of  $X_{ic+}$ . In this presentation, the analysis strategy to get the yield of  $X_{ic+}$  will be introduced, and the plan to take the multiplicity into account will be presented.

### Keywords:

ALICE, QGP,  $X_{ic+}$

## Measurements of light-by-light scattering and lepton pair photoproduction in PbPb collisions with the CMS experiment

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### Abstract:

Ultrapерipheral lead-lead collisions at  $\sqrt{s_{\mathrm{NN}}} = 5.02$  TeV produce very large photon fluxes that provide the conditions to study photon-photon fusion processes in phase space regions inaccessible with proton-proton data. Measurements of light-by-light (LbL) scattering and lepton pair photoproduction in ultraperipheral PbPb collisions will be presented with data collected by the CMS detector during the LHC Run 2. These processes open up a unique window through which to search for physics beyond the standard model, e.g., the LbL study allows for competitive searches for axion-like particles (ALPs) in the 5--100 GeV ALP mass range. The lepton pair photoproduction provides the first data-driven demonstration that the average transverse momentum of photons emitted from relativistic heavy ions has an impact parameter dependence, the latter determined based on the number of neutrons detected in the very forward pseudorapidity. All results are compared with quantum electrodynamics calculations and provide crucial new tests and constraints on models of photon-induced interactions in ultraperipheral collisions.

### Keywords:

UPC, BSM, tau, CMS, Heavy Ion

## Production of molecular configuration hadron

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### Abstract:

We calculate the yields of molecular configuration hadrons produced by heavy ion collision using coalescence model. First, we calculated the transverse momentum distribution of deuteron using the coalescence model from proton transverse momentum distribution in Pb-Pb collisions at 2.76TeV measured by ALICE collaboration. From this, we estimate the parameters required for coalescence model at kinetic freeze-out. We then calculate the transverse momentum distribution of helium-3 using this parameter and compared with the experimental results by ALICE collaboration to confirm that parameterizaion was succesful. After this, we assume that X(3872) is molecular structures and estimate the transverse momentum distributions of X(3872) using coalescence model. Also, we compare yields calculated using coalescence model with statistical hadronization model.

### Keywords:

coalescence, deuteron, helium-3, X(3872)

## Performance study of $\Xi_{cc}^{++}$ via decays into $\pi^+ + \Xi_c^+ (\rightarrow pK^- \pi^+)$ with ALICE 3

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### Abstract:

Multi-charm baryons containing multiple charm quarks provide a unique window on uncovering the hadronisation mechanism in the quark-gluon plasma (QGP). The production yield of multi-charm baryons from single hard scattering is negligible compared to the one by coalescence of charm quarks from multiple hard scatterings. In Pb–Pb collisions, multi-charm baryon can be formed by a combination of charm quarks which are formed in independent hard scatterings, leading to an increase of the yield by up to 3 orders of magnitude compared with that in pp collisions.

ALICE 3, the next-generation heavy-ion programme for LHC Run 5, will offer an advanced opportunity to understand QGP, measuring the multi-charm baryon production from proton-proton to heavy-ion collisions. This contribution will present the performance study of  $\Xi_{cc}^{++}$  via decays into the non-strangeness channel in pp collisions at 14TeV with ALICE 3.

### Keywords:

Multi-charm baryon, ALICE 3, Heavy-flavour

## Seismic Metamaterial and Bandgap Engineering for the Next Generation Terrestrial Gravitational-Wave Observatories

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### **Abstract:**

The wave propagation under a certain complex medium is still not understood well so far even for an electromagnetic wave as well as other waves. A remarkable interesting feature on artificial media structures is opening a new field of fundamental theories of wave mechanics and its application in various fields. In this study, we investigate a novel possibility of providing a new framework of gravitational wave science by using metamaterial physics, improving the ground-based gravitational-wave observatories.

### **Keywords:**

seismic metamaterial, gravitational-wave telescope, wave control, noise mitigation

# Optimizing Parameters of Information-Theoretic Correlation Measurement for Multi-Channel Time Series Datasets in Gravitational-Wave Detectors

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## Abstract:

Data analysis in modern science using extensive experimental and observational facilities, such as a gravitational wave detector, is essential in the search for novel scientific discoveries. Accordingly, various techniques and mathematical principles have been designed and developed to date. A recently proposed approximate correlation method based on the information theory is widely adopted in science and engineering. Although the maximal information coefficient (MIC) method remains in the phase of improving its algorithm, it is particularly beneficial in identifying the correlations of multiple noise sources in gravitational-wave detectors including non-linear effects. This study investigates various prospects for determining MIC parameters to improve the reliability of handling multi-channel time-series data, reduce high computing costs, and propose a novel method of determining optimized parameter sets for identifying noise correlations in gravitational wave data.

## Keywords:

maximal information coefficient, gravitational-wave data analysis, detector characterization, parameter optimization

## Neutrinos from Red Super Giants

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### Abstract:

Stars emit neutrinos during their evolutions. Detecting such neutrinos will provide us with valuable information on the physical processes that govern their evolution and structure. So far, neutrinos only from the Sun has been observed, because unlike photons, neutrinos do not interact much with matter due to their extremely small cross-section. However, as the size of neutrino observatories keep increasing and the detector technology keep improving, stellar neutrinos, other than from the Sun, will be eventually observable, opening the era of the neutrino stellar astronomy. In this work, we search for possibilities to observe neutrinos from red supergiant (RSG) stars, which are expected to emit the amount of neutrinos much larger than the Sun. We calculated neutrino luminosities along the evolutionary tracks of massive stars of 12 - 30  $M_{\odot}$  with metallicity 0.01 – 0.02, using MESA, a publicly available stellar evolution code. We then calculated the energy spectra of neutrinos emitted through various production processes. We present the fluxes of such neutrinos from nearby RSGs on the Earth, and discuss the prospect of detecting them in current and future neutrino observatories.

## Cherenkov fluorescence hybrid observatory for astrophysical neutrinos of 1 MeV energies

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### Abstract:

Neutrinos of  $E \sim 1$  MeV are produced at various channels of C, N, and O burnings inside stars. Observation of such neutrinos, hence, would provide us with important knowledge on the structure and evolution of stars. Currently, two types of neutrino observatories are running. One for high energy neutrinos (from several MeV to PeV) utilizes Cherenkov light (e.g. Super Kamiokande and IceCube), and the other for low energy neutrinos ( $<$  several MeV) registers fluorescence light (e.g. Borexino). In the latter, fluorescent materials are used for the production of a large amount of fluorescence photons, so low-energy neutrinos can be observed; however, their directional information is lost. In the former, on the other hand, the number of Cherenkov photons produced by low-energy neutrinos is limited; hence, the background noise from radon contamination and also the dark noise of PMTs make the reliable count of low-energy neutrino events difficult.

In this talk, we introduce a detector based on the Cherenkov and fluorescence hybrid technology, aiming to observe astronomical neutrinos of  $\sim 1$  MeV energies from the Sun and also sources such as red supergiant stars. The hybrid detector consists of a water-based liquid scintillator with fast photodetectors. The water-based liquid scintillator emits both Cherenkov and fluorescence photons at UV, and the fast photodetectors record both kinds of photons with accurate timings. Then, in principle, it could be possible to recode neutrinos of energies **down to** 0.6 MeV, with directional information, although the uncertainty in direction would be rather large. The expected event rate at a 50 kton hybrid tank from a source with  $10^6$  cm<sup>-2</sup> s<sup>-1</sup> flux at 1 MeV would be  $\sim 100$  events/year. We also present events from background noises. Finally, we discuss the prospect of this kind of detectors for studies of astronomical neutrinos.

### Keywords:

Fluorescence , Cherenkov , Astrophysics, Red Super Giant, Neutrino

## Vision Transformer for Gamma-Hadron Classification with the HAWC Observatory

LEE Jason Sang Hun<sup>\*1</sup>, [JO Baeksun](#)<sup>1</sup>, WATSON Ian James<sup>1</sup>, CHOI MyeongHun<sup>1</sup>  
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### Abstract:

The High Altitude Water Cherenkov (HAWC) gamma-ray observatory consists of 300 water Cherenkov detectors, each of which contains four photomultiplier tubes (PMTs). In the atmosphere, both cosmic rays and gamma rays produce air showers containing cascades of ionized particles and electromagnetic radiation. We train a neural network to distinguish gamma-ray events from cosmic ray events using a novel semi-supervised method, which uses real data to train the network. We show that the network trained by our method outperforms a network trained with simulated data.

### Keywords:

ViT, Deep learning, Air shower, HAWC, gamma-ray

## Deep Learning applied to Air Shower Reconstruction with the HAWC Observatory

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### Abstract:

The High-Altitude Water Cherenkov (HAWC) Observatory is a facility for gamma-ray astronomy located in the Sierra Negra mountain in Puebla, Mexico. Air showers are created when a high-energy gamma ray or cosmic ray interact with the atmosphere, producing a cascade of secondary particles that spread out over a large area. HAWC reconstructs the incident angle by using the timing information of the photomultiplier tubes triggered by the air shower particles. Our goal in this study is to use machine learning to reconstruct the air showers created by gamma rays. We apply Deep Learning to this task to try to improve the angular resolution of HAWC. We train a Vision Transformer with simulated data and compare the performance to the current HAWC reconstruction.

### Keywords:

Gamma ray, Reconstruct the air showers, Deep Learning, Angular resolution, Vision Transformer

## Search for Dark Matter Decay in Galaxy Clusters and Galaxies with IceCube

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### Abstract:

The abundance of dark matter in the Universe could be explained by heavy dark matter. Heavy dark matter decay in massive astrophysical objects could produce highly energetic neutrinos that can be detected at neutrino telescopes. The IceCube Neutrino Observatory is a cubic kilometer-scale Cherenkov radiation detector deployed in deep glacial ice at the geographic South Pole. Since its completion in 2010, IceCube has observed a large number of high-energy astrophysical neutrinos, allowing us to probe heavy dark matter hypotheses. We present an analysis that searches for dark matter decay in extragalactic sources, using nine years of IceCube data. The sources considered are galaxy clusters, dwarf galaxies, and the Andromeda galaxy. We use well-established neutrino event selection criteria for neutrino candidate events from the northern hemisphere. We focus on heavy decaying dark matter with masses from 10 TeV to 10 PeV and consider several benchmark decay channels into pairs of Standard Model particles. In this contribution, we present the latest analysis status and sensitivities calculated using the individual sources and by stacking the sources within the same source class.

### Keywords:

dark matter, neutrinos, IceCube

## Anomalous thermodynamics of multiband superconductors near a quantum critical point

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### Abstract:

Recent high-precision measurements employing different experimental techniques have unveiled an anomalous peak in the doping dependence of the London penetration depth which is accompanied by anomalies in the heat capacity in iron-pnictide superconductors at the optimal composition associated with the hidden antiferromagnetic quantum critical point. In my talk I am going to argue that finite temperature effects can be a cause of observed features. Specifically I will present the results of the calculations and interpret them to show that quantum critical magnetic fluctuations under superconducting dome can give rise to a nodal-like temperature dependence of both specific heat and magnetic penetration depth in a fully gaped superconductor. In the presence of line nodes in the superconducting gap fluctuations can lead to the significant renormalization of the relative slope of T-linear penetration depth which is steepest at the quantum critical point. The results that have been obtained are general and can be applied beyond the specific microscopic model that has been adopted.

### Keywords:

Quantum criticality, superconductivity, thermodynamic response functions

## Quantum transition in an integer spin quasi-2D square lattice antiferromagnet $\text{Ba}_2\text{FeSi}_2\text{O}_7$

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<sup>2</sup>Center for Complex Phase Materials, MPK  
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### Abstract:

Quasi 2D Heisenberg antiferromagnets have often been exhibited exotic low-dimensional magnetism involving lattice topology and spin-orbit coupling. Here we introduce a new quasi 2D square lattice antiferromagnet  $\text{Ba}_2\text{FeSi}_2\text{O}_7$  with an integer spin  $S = 2$  ( $\text{Fe}^{2+}$ ), which exhibits a non-trivial magnetic transition with temperatures and external magnetic fields. In this talk, we will present experimental results such as the magnetization ( $\chi$ ,  $M$ ), specific heat ( $C_p$ ), neutron diffraction and inelastic scattering on this new quasi 2D antiferromagnet as well as the theoretical Monte Carlo simulations. We also discuss nature of the ground state and the non-trivial quantum transition.

### Keywords:

low dimensional quantum magnet

## Electric quantum oscillations in Weyl semimetals

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### Abstract:

Electronic transport in Weyl semimetals is quite extraordinary due to the topological property of the chiral anomaly generating the charge pumping between two distant Weyl nodes with opposite chiralities under parallel electric and magnetic fields. Here, we develop a full nonequilibrium quantum transport theory of the chiral anomaly, based on the fact that the chiral charge pumping is essentially nothing but the Bloch oscillation. Specifically, by using the Keldysh nonequilibrium Green function method, it is shown that there is a rich structure in the chiral anomaly transport, including the negative magnetoresistance, the non-Ohmic behavior, the Esaki-Tsu peak, and finally the resonant oscillation of the dc electric current as a function of electric field, called the electric quantum oscillation. We argue that, going beyond the usual behavior of linear response, the non-Ohmic behavior observed in BiSb alloys can be regarded as a precursor to the occurrence of electric quantum oscillation, which is both topologically and energetically protected in Weyl semimetals.

### Keywords:

Weyl semimetal, Chiral anomaly, Quantum transport, Quantum oscillation by electric field

## Pre-thermalization via self-driving and external driving of extensive subsystems

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### Abstract:

We discuss the non-equilibrium states of an interacting multi-component quantum system when only an extensive subsystem is quantum-quenched or driven from the ground state. As a concrete example, we consider a system where two XXZ spin chains are coupled to a transverse field Ising (TFI) chain, and only the transverse field in the TFI chain is quantum-quenched or periodically driven in time, starting from an initially ordered state. This system is studied using density matrix renormalization group (DMRG) simulations and various entanglement entropy diagnostics. In the case of quantum quenching, when the transverse field is suddenly switched on to become the largest energy scale, the resulting internal dynamics leads to a pre-thermal steady state with persistent oscillating magnetization ('self-driving') and emergent conservation laws. Upon applying the time-dependent drive to the TFI chain ('external driving'), sufficiently fast drive gives rise to a pre-thermal steady state with finite magnetization, whereas a slow drive generates a high-temperature disordered state. We briefly discuss the experimental implementation of our protocol in organic materials with quantum-tunneling hydrogen atoms.

### Keywords:

Prethermalization, Quantum quench, MPS, DMRG

# Anisotropic nature and spin-flop transition in antiferromagnetic NiPS<sub>3</sub>

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## Abstract:

The van der Waals (vdW) antiferromagnet NiPS<sub>3</sub> is a proto-type candidate for a realization of two-dimensional XY- or XXZ-like spin models which have continuous in-plane symmetry. However, its in-plane magnetic anisotropy has been highlighted from recent experiments like neutron diffraction or photoluminescence. Nevertheless, its magnetic anisotropy has not been fully unveiled in experiments and theory. Here, we use torque magnetometer, density functional theory, and spin model analysis to understand the full magnetic anisotropy profile in NiPS<sub>3</sub>. Our combined approaches not only reveal the anisotropy but also directly show that the spin-flop transition at around H=9 T which is suggested from recent experiments. Our theoretical calculation indicates that the order of magnetic anisotropic energy is different from the previous XXZ-type prediction and originates from magnetic dipole-dipole interactions. Our results and approach manifest strong merits of magnetic vdW materials and related systems as a demonstration for the pursuit of spintronic or magnetic photo-device functionality.

## Keywords:

NiPS<sub>3</sub>, magnetism, van der Waals, torque magnetometer, magnetic anisotropy

## Conductance study for ultrathin Pt film with roughness

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### Abstract:

Thin Pt films have been widely studied for its spin orbit coupling and spin Hall effect in spintronics field. Most of transport theories are well established for thin films. However, analysis of thin film resistance based on classical transport theories is not well matched for ultrathin Pt film under 10 nm.

Pt and Pt/CoFeB films are deposited on SiO<sub>2</sub> substrate. To analyze the ultrathin film transport based on roughness, Pt films are sputtered at various working pressure. The resistance and roughness are measured by 4-probe method and atomic force microscopy (AFM), respectively.

Quantum mechanical theories are adopted to explain Pt and Pt/CoFeB film sets. Quantum mechanical theories are well explained conductance variation with roughness of film sets.

### Keywords:

Pt, Conductance, Ultrathin film, Roughness

## Mn<sub>3</sub>Sn 박막에서 관찰되는 비 이상적 홀 효과의 결정 의존성 연구

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### Abstract:

비 공선형 반 강자성체(non-collinear antiferromagnet)로 알려져 있는 Mn<sub>3</sub>X (X=Ga, Ge, 그리고 Sn) 화합물은 육각형 구조를 가지며 Kagome 격자라고 불리는 120°의 스핀 구조를 가진다. 특히, Mn<sub>3</sub>Sn은 자화 용이 축인 c-평면을 따라 약 0.002<sub>B</sub>/Mn의 작은 자기모멘트를 가짐에도 불구하고 향상된 베리 곡률에 의해 나타나는 큰 비 이상적인 홀 효과를 관찰할 수 있다 [1]. 여기에서, 베리 곡률은 운동량 공간에서 자기장의 역할과 유사하게 작용한다 [2]. 그러므로 위상학적 물질인 (topological material)인 바일 반금속 (Weyl semimetal)으로 알려져 있는 Mn<sub>3</sub>Sn은 역 삼각형 스핀 구조를 가지는 비 공선형 반 강자성체를 대표하는 물질 중 하나이며, 위상학적 자성물질로서 스핀트로닉스에서 활용도가 매우 높다 [1].

이번 학술대회에서, 본 연구자들은 다양한 방향성을 가진 사파이어 기판에서 성장된 Mn<sub>3</sub>Sn 박막의 비 이상적인 홀 효과에 대한 결정학적 의존성에 대해 발표한다. 다결정 Mn<sub>3</sub>Sn 박막은 마그네트론 스퍼터링 시스템을 이용하여 결정성이 c-와 m-평면을 가지는 사파이어 기판에 증착되었다. 증착된 Mn<sub>3</sub>Sn 박막의 비 이상적 홀 전도도 ( $\sigma_{xy}$ )는 사파이어 기판의 방향성에 따라  $\sim 0.133 \Omega^{-1} \text{cm}^{-1}$  (c 평면 방향)와  $\sim 6.00 \Omega^{-1} \text{cm}^{-1}$  (m 평면 방향)의 값을 가졌으며, 끝으로 TEM (transmission electron microscopy)을 이용한 결정학적 분석을 통해 Mn<sub>3</sub>Sn 박막에서의 비 이상적 홀 전도도의 차이를 설명한다.

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### Keywords:

Mn<sub>3</sub>Sn, 비 이상적 홀 효과, TEM, 박막

## Field-induced easy-axis softening of weak quantum ferromagnet with cubic anisotropy

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### Abstract:

When a ferromagnetic material takes less energy to magnetize along a certain direction, usually related to the principle axes of its lattice structure, it is said to possess the magnetocrystalline anisotropy with some easy axes. In this presentation, we will introduce our latest results studying ferromagnets with  $\langle 111 \rangle$  easy axes under a weak quantum effect by the Heisenberg coupling and an external field. While the mean-field analysis suggests a phase coherence for our reshuffled on-site Hilbert space, leading to the easy axes always along  $|x| = |y|$ , an introduction of quantum entanglement will cause the "leaking" of on-site information and result in a decoherence. The later case has also been studied using the two dimensional tensor network ansatz, the infinite projected entangled-pair states, and an emergent  $U(1)$  symmetry breaking scenario is proposed as a strong enough magnetic field is cast. For real materials, such as the ferromagnetic Mn-doped gallium phosphide (a III-V semiconductor), our discovery suggests a "softening" of magnetic easy axes when the external field strength is strong enough, leading to possible manipulation of magnetic moments without changing its intrinsic properties.

### Keywords:

Quantum ferromagnetism, Tensor network ansatz, Magnetocrystalline anisotropy, Magnetic semiconductors

## The study of helical magnetic state in $\text{Fe}_{5-x}\text{GeTe}_2$ crystals with magnetic force microscopy

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### Abstract:

The van der Waals (vdW) ferromagnet have attracted great interests in two-dimensional spintronics because it provides an ideal platform to explore the spin transport and configuration of magnetic interactions in low-dimensional magnetism with time reversal and inversion symmetry breaking [1]. As a promising vdW ferromagnet, the  $\text{Fe}_n\text{GeTe}_2$  family ( $n = 3, 4, 5$ ) was proposed because of its high  $T_C$  (260 ~ 310 K) and large saturation magnetization [2]. Recently, the helical magnetic state and topological spin configuration of  $\text{Fe}_5\text{GeTe}_2$  have been observed with the presence of Dzyaloshinskii-Moriya interaction (DMI) [3,4].

In this presentation, we show the magnetic helical state of  $\text{Fe}_{5-x}\text{GeTe}_2$  single crystal at low temperature by means of MFM (magnetic force microscopy), and micromagnetic simulation with MUMAX3. Clearly, a commensurate-incommensurate transition just below  $T_C = 310$  K was exhibited on the temperature dependent magnetization of  $\text{Fe}_{5-x}\text{GeTe}_2$ , indicating a typical helimagnetic behavior arising from the DMI. The estimated DMI energy density was  $\sim 0.36\text{mJ/m}^2$  at 140K. And, we observed that the magnetic state of  $\text{Fe}_{5-x}\text{GeTe}_2$  have reached the helical magnetic state without applying magnetic field at 77K using MFM measurement. This result will provide new information to understand magnetic properties of  $\text{Fe}_{5-x}\text{GeTe}_2$  for future topology-based spintronics.

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### Keywords:

Helical magnetic state,  $\text{Fe}_{5-x}\text{GeTe}_2$ , Dzyaloshinskii-Moriya interaction, magnetic force microscopy, micromagnetic simulation

## Effect of impurities and inhomogeneity in magnetic quantum oscillations

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### Abstract:

Magnetic quantum oscillations (MQOs) of material provide useful information about its Fermi surface. Recently, investigating topological and magnetical properties of the Fermi surface by MQOs has drawn much attention [1,2]. In the studies, researchers assume homogeneity for theoretical simplicity. However, depending on the sample synthesis process, the inhomogeneity of the sample can be introduced and give an unexpected effect on the phase and amplitude of MQOs. Here, we measured and analyzed the MQOs of semimetal NbSb<sub>2</sub> with various dopants like Cr, Bi, Fe, Ti. We observed unexpected MQOs violating the Lifshitz-Kosevich (LK) theory in some samples. We found that the unexpected MQOs can be interpreted by inhomogeneity. We interpreted the unexpected MQOs due to the superposition of MQOs from the regions with various chemical potentials. Our MQOs data is successfully fitted with a superposed MQOs model probing our interpretation is reasonable. With this study, we emphasized that the exotic phase and amplitude of MQOs should not be hastily interpreted as a result of exotic topological or magnetical properties.

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### Keywords:

magnetic quantum oscillations, semimetal, inhomogeneity

## First-principles study on phononic, electronic, and optical properties of MoSe<sub>2</sub>/WSe<sub>2</sub> heterobilayer

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### Abstract:

Twistronics is of great interest because of their fascinating physical phenomena that can be tuned by the twist angle between layers of two-dimensional materials. In this study, we report the atomic structures and phononic properties of MoSe<sub>2</sub>/WSe<sub>2</sub> heterobilayer as a function of the twist angle from  $\theta = 0^\circ$  (3R-like) to  $\theta = 60^\circ$  (2H-like). Using the  $\Gamma$ -phonon folding model and atomistic calculations, we discuss the twist-angle dependence of the atomic structure relaxation, low-frequency interlayer phonon modes, and high-frequency intralayer phonon modes. In addition, we also investigate electronic and optical properties of the 3R- and 2H-like system using the density functional theory, the GW method, and the Bethe-Salpeter equation. We discuss the bright exciton spin and valley configuration, the optical band gap, and the exciton binding energy of each system. This work is supported by the NRF of Korea (Grant No. 2020R1A2C3013673). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2021-CRE-0384).

### Keywords:

Twistronics, MoSe<sub>2</sub>, WSe<sub>2</sub>, Phonon, Exciton

## Two dimensional checkerboard charge density wave in NbTe<sub>2</sub>

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### Abstract:

Charge density wave (CDW) is one of the fascinating phenomena in transition metal dichalcogenides (TMDC). The reduced dimensionality from weak van der Waals bonding allows CDWs to occur in orders, even in bulk form. Although the characters of CDWs are widely studied using various measurements methods and theoretical calculation, the origin of lattice instability and the consequence of its relaxation is still controversial since the predicted experimental signatures related to Peierls' model are sometimes missing or confusing. Here, we investigated the surface of bulk NbTe<sub>2</sub>, a TMDC material, with a scanning tunneling microscope (STM) at 2K. The topographic data show a checkerboard-like image constituted of two stripe CDWs: one is commensurate, and the other is incommensurate to the undistorted lattice. The orders of CDWs are explicitly determined by precise Fourier analysis of the STM images. Scanning tunneling spectroscopy captured the energy-dependent density of states suppressions and the phase shifts related to the CDWs. By combining the detailed STM measurements and the simulation, we attribute our observation to multiple CDW gap formations originating from the multiple electronic bands. This detailed information of the CDWs in NbTe<sub>2</sub> can improve the understanding of low dimensional physics in NbTe<sub>2</sub>.

### Keywords:

Charge density wave, Scanning tunneling microscope, Transition metal dichalcogenide

## Band structures and effective Hamiltonian of 90°-twisted few-layer black phosphorus

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### Abstract:

Few-layer black phosphorus (BP) is a gapped two-dimensional (2D) semi-Dirac material which has pseudospin features even in its semiconducting phase [1]. When the band gap is closed, it has a semi-Dirac point [2], and when the band gap is inverted, it has anisotropic Dirac cones [3]. Twisted bilayers of gapped 2D semi-Dirac materials may have interesting emergent phenomena due to directional mismatch of in-plane anisotropy of each layer. The interlayer coupling can be modulated by the twist angle. In our present work, we perform density functional theory (DFT) calculations of 90-degree twisted few-layer BP with different in-plane lattice constants [4]. The band gap of twisted few-layer BP is sensitive to the in-plane lattice constant. When the band gap is closed, two dispersive linear bands and a quadratic band cross at Gamma point, and when the band gap is inverted, band degeneracy is inverted at Gamma point. We construct effective Hamiltonian based on DFT results and obtain relevant pseudospin representations. We also discuss effects of externally applied electric fields. This work was supported by NRF of Korea (Grant No.2020R1A2C3013673) and KISTI supercomputing center (Project No.KSC-2021-CRE-0384).

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### Keywords:

2D anisotropic Dirac material, DFT calculations, model Hamiltonian, Band inversion

## Pseudogap in black phosphorus doped by disordered dopants

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### Abstract:

The band structure of a crystalline solid can be understood based on the periodic order of atoms, but how the effect of disorder modifies this picture remains unknown. In the 1960s, the band structure of disordered systems, such as liquids or glassy solids, was theoretically predicted to exhibit back-bending dispersion and pseudogap<sup>1</sup>. In this talk, I will introduce our recent angle-resolved photoemission spectroscopy study on black phosphorus doped by alkali metals, mainly focusing on the Na case<sup>2</sup>. The alkali metals on black phosphorus are known to have a short-range order. The multiple scattering of doped electrons by the potential of ionized dopants leads to characteristic wavenumber renormalizations, leading to back-bending dispersion and pseudogap, as predicted by theoretical models for the band structure of liquid metals. I will also briefly discuss on our future directions with the use of alkaline earth metals to modulate the scattering potential of disordered dopants.

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### Keywords:

ARPES, Band structure, Liquid metals, Surface-doping, Black phosphorus

## Modulation of surface state hybridization in $\text{Bi}_2\text{Se}_3$ topological Insulator by exchange interaction

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### Abstract:

Topological insulator has unique spin polarized surface Dirac like band due to strong spin orbit coupling. This non-trivial topological nature is robust to non-magnetic disorders. Therefore, it is difficult to modulate of surface state without applying an external magnetic field or magnetic dopant. In this work, we investigated the suppression of surface state in  $\text{Bi}_2\text{Se}_3$  grown on antiferromagnetic NiO by inducing strong exchange coupling between two layers. Measured electrical properties of the film on NiO showed drastic degradation in the thin film  $\text{Bi}_2\text{Se}_3/\text{NiO}$  heterostructure. Also, we could elucidate the origin of surface state suppression by using THz-TDS and optical pump THz probe measurements. As a result, that the extended surface penetration depth accelerates surface state hybridization was found. This unique role of antiferromagnetic material suggests that topological surface nature can be modulated by exchange interaction.

### Keywords:

Topological insulator, Antiferromagnetic insulator, Exchange interaction, THz

## Atomic vacancy induced short-range disorder scattering in a bipolar pseudospin system

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### Abstract:

Impurity states and their scattering processes crucially affect the electronic properties of crystalline solids. However, probing the interplay between impurities and the electronic degrees of freedom is not trivial. Scanning tunneling microscopy (STM) is widely applied to visualize the local electronic states and the electron scattering patterns to elucidate exotic quantum phenomena. We employ STM on Black phosphorus, which serves as an ideal platform to unveil the relation between atomic vacancies and pseudospin scattering since its puckered honeycomb lattice realizes a bipolar pseudospin texture. In this talk, I will present energy-dependent real-space images of anisotropic impurity states and scattering patterns of black phosphorus associated with atomic vacancies. Their fast-Fourier-transformed spectra will be compared with angle-resolved photoemission spectroscopy results and tight-binding calculations to characterize the impurity scattering potential.

### Keywords:

black phosphours, electron scattering , scanning tunneling microscopy

## Anisotropic charge screening in a topological Dirac nodal line semimetal

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### Abstract:

Dirac nodal line semimetals(DNLS) are defined as systems where band crossing lines of the inverted bands are protected by symmetries [1]. The intense theoretical works on these systems have been conducted using a model calculation and ab-initio calculation on candidate materials [2]. However, trivial band structures near the Fermi energy often hinder revealing exotic properties of most DNLS candidates [3]. We investigated SrAs<sub>3</sub> with a low-temperature scanning tunneling microscope and spectroscopy (STM/STS) and found the signature of well isolated Dirac nodal lines in this material. We observed the highly asymmetric charge distribution near the impurity, and this asymmetry is strongly energy-dependent. By combining the model and first-principle calculations, we found this asymmetric charge screening is the distinct signature of DNLS [4].

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### Keywords:

Dirac nodal line semimetals, Anisotropic charge screening, Impurity, STM/STS

# Hund metal and neighboring phases in two and three orbital systems

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## Abstract:

A novel route to the electron correlation, which has attracted a great deal of attention over the last fifteen years, is on-site Hund coupling  $J$ . In multiorbital systems away from half-filling, an intriguing correlated metallic regime dubbed Hund metal emerges, promoted by  $J$  rather than the proximity to a Mott insulator. Accordingly, many related physical phenomena have been uncovered, such as the spin-freezing crossover, the spin-orbital separation, the orbital differentiation, and superconductivity, to name a few.

In this talk, we present two aspects of Hund metal on the periphery of the attention. One is its existence in two orbital systems [1]. By using dynamical mean field theory, we identified  $J$ -promoted correlated metallic phase in two orbital systems, establishing two-orbital Hund metallicity. The other is the effect of non-local interaction ( $V$ ). By using GW+EDMFT approaches, we found that  $V$ -driven charge order instability is significantly enhanced in the Hund metallic regime [2]. Our findings have potential implications for the observed charge-ordered phase in Hund metal  $A\text{Fe}_2\text{As}_2$  ( $A = \text{Rb}, \text{K}, \text{Cs}$ ) and correlated metallic phase in the infinite-layer nickelates.

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## Keywords:

Hund metal, charge order, Dynamical mean field theory, GW+EDMFT

## Electronic structure studies of Hund's metal behavior in $\text{NiS}_{2-x}\text{Se}_x$ and atomic layer of $\text{SrRuO}_3$

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### Abstract:

Understanding characteristic energy scales is a fundamentally important issue in the study of strongly correlated systems. In multiband systems, an energy scale is affected not only by the effective Coulomb interaction but also by the Hund's coupling. Direct observation of such energy scale has been elusive so far in spite of extensive studies.

In this presentation, recent electronic structure study results on  $\text{NiS}_{2-x}\text{Se}_x$  and atomic layer of  $\text{SrRuO}_3$  will be discussed. We observed a kink structure in the low energy dispersion of  $\text{NiS}_{2-x}\text{Se}_x$  and its characteristic evolution with  $x$ , by using angle resolved photoemission spectroscopy (ARPES). Dynamical mean field theory calculation combined with density functional theory confirms that this kink originates from Hund's coupling. We find that the abrupt deviation from the Fermi liquid behavior in the electron self-energy results in the kink feature at low energy scale and that the kink is directly related to the coherence-incoherence crossover temperature scale.

Meanwhile, sharp dispersions are observed on 1 unit cell (UC)  $\text{SrRuO}_3$  film grown on  $\text{BaTiO}_3$  but the spectral function becomes broad and incoherent for  $\text{SrRuO}_3$  grown on  $\text{SrTiO}_3$ . DMFT calculation suggests that the difference stems from the difference in the band width, showing that the incoherent metallic behavior is a result of Hund's coupling. It is found that there is a transition from Hund's metal to a Fermi liquid state upon doping electrons to  $\text{SrRuO}_3$  film on  $\text{SrTiO}_3$ . This indicates the importance of the van Hov singularity in the film.

### Keywords:

Hund's metal

## Tuning of nematicity and spin fluctuations in Fe-based superconductors

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### Abstract:

By means of nuclear magnetic resonance, we investigated the interplay among nematicity, spin fluctuations, and superconductivity in Li-doped NaFeAs [1] and Co/S-doped FeSe [2] by tuning their ground states by doping. Remarkably, the two NMR studies show contrasting results: Namely, in doped FeSe, our NMR data indicate that superconductivity may be driven by spin fluctuations which is enhanced by nematic order, but in Li-doped  $\text{Na}_{1-x}\text{Li}_x\text{FeAs}$  with  $x > 0.03$ , a distinct nematic state which suppresses spin fluctuations emerges above superconducting dome. This may suggest that superconductivity in Fe-based materials is driven not simply by either spin or nematic fluctuations alone, but by a complex combination of the two.

[1] Seung-Ho Baek et al., Nature Communications, 9, 2139 (2018)

[2] Seung-Ho Baek et al., npj Quantum Materials, 5, 8 (2020)

### Keywords:

NMR, spin fluctuations, nematicity

## Strain-Temperature phase diagram of SrRuO<sub>3</sub>-SrTiO<sub>3</sub> : DFT+DMFT study

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### Abstract:

In the current study, we show that the SrRuO<sub>3</sub>-SrTiO<sub>3</sub> heterostructure is an interesting platform to control the various quantum phases, including the Hund metal. Recently, from the density functional theory (DFT) framework, the SrRuO<sub>3</sub>-SrTiO<sub>3</sub> heterostructure, when combined with epitaxial strain, was proposed as a system to study the superconductivity of Sr<sub>2</sub>RuO<sub>4</sub>, a paradigmatic Hund metal [1]. Here, in the framework of the DFT plus dynamical mean-field theory, we show that the SrRuO<sub>3</sub>-SrTiO<sub>3</sub> heterostructure has a correlated electronic structure, which is highly tunable upon the strain. The regime covers in between the orbital selective Mott phase and multi-orbital Mott insulator, including the Hund metal. Also, the strain can tune the competing magnetic instabilities, including ferromagnetism and Neel type antiferromagnetism.

[1] Bongjae Kim et al., Phys. Rev. B 101, 220502(R) (2020)

### Keywords:

Hund Metal, Dynamical Mean Field Theory, Quantum Material

## Holographic Lieb lattice and Gapping its Dirac band.

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### Abstract:

The Lieb lattice is one of the most interesting flat band system due to the location of the flat band at the Fermi surface.

On the other hand, flat band system has 0 fermi velocity so that it is a strongly interacting system.

Therefore the holographic system is ideal to handle

such system. We also need to gap the Dirac band to study the effect of the isolated flat band.

In this talk, we will discuss how to realize the Lieb lattice in the holographic theory and how to introduce a gap in the Dirac band.

### Keywords:

Lieb lattice, holography, Gap, Dirac band

# Attention-based Neural Network Wave Functions for Strongly Correlated Fermions

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## Abstract:

Artificial neural networks have made a great success in condensed matter physics. For instance, neural-network-based variational ansatz accurately approximate ground states in many different models. On the other hand, attention mechanism plays a key role in relating a word to another when a natural language model extracts the meaning of a sentence. Analogously the attention mechanism is expected to find hidden structures in ground states of strongly correlated fermion systems. In this work, we first present a new, simple and clear architecture representing the ground state of non-interacting fermion systems. Then, we add an attention layer to the architecture, which can now simulate the strongly correlated electronic systems. We demonstrate these by extensive numerical simulations on correlated 1,2D fermionic systems which may or may not support superconductivity.

## Keywords:

Machine learning, Neural network, Correlated electrons, Variational wavefunction, BCS superconductor,

## Classification of Non-Unitary MTCs and Topological Phases

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### Abstract:

Unitary modular tensor categories (MTCs) can characterize 2+1D topological phases with their modular data. Due to the rank-finiteness for MTCs, there have been many efforts to classify MTCs by the rank. Recent studies classified unitary MTCs completely up to rank 5, and partially for higher ranks. Meanwhile, modular data of non-unitary MTCs characterize non-unitary conformal field theories, which are relevant for the Yang-Lee singularity or Gaffnian quantum Hall states. We partially classify non-unitary MTCs up to rank 6 computationally by checking consistency conditions of category theory and present the table of non-unitary MTCs for low ranks. Importantly, the consistency conditions for non-unitary MTCs can be obtained from that of unitary MTCs by allowing negative quantum dimensions, or equivalently allowing negative first row entries of the S matrices. Our classification table contains the fusion rules, the central charges, the quantum dimensions, and the modular data of each non-unitary MTC. We believe that our table would be a useful reference for researchers who study category theory or topological phases.

### Keywords:

topological phase, modular tensor category

## Exotic Thermal Transitions with Spontaneous Symmetry Breaking

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### Abstract:

We show that exotic spontaneous symmetry breaking appears in thermal topological phases by perturbing the exact solutions of quantum rotor models coupled to the three-dimensional toric code. The exotic Ising and XY transitions are shown to be in the same universality class in drastic contrast to the conventional Wilson-Fisher classes without topological orders. Our results indicate that topological orders must be included to pin down universality classes of thermal transitions in addition to order parameter symmetry and spatial dimension. We evaluate all the critical exponents and find that the exotic universality class is more stable under the couplings to acoustic phonons and disorder. Applying our results to experiments, we provide a plausible scenario in puzzlings of strongly correlated systems, including the absence of specific heat anomaly in doped  $\text{RbFe}_{1-x}\text{As}_x$ .

### Keywords:

Beyond Landau-Ginzburg theory, Deconfinement, Topological transition

## A reliable parameter-free analytic continuation of imaginary-frequency Green's function

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### Abstract:

Many of practical quantum many-body simulations are conducted in imaginary-time due to computational stability and efficiency. To compare with experiments, one needs to obtain real-frequency Green's function from imaginary-frequency one. This procedure is called as an analytic continuation. In this work, we develop a reliable parameter-free analytic continuation method. Our method is based on a systematic kernel grid, a roughness penalty, and the L-curve criterion. We also develop the L-curve averaged deviation (LAD) to estimate the precision of the analytic continuation. To deal with statistically obtained data, we further develop a bootstrap-averaged analytic continuation. In a test using an exact Green's function with added statistical error, our method produces the spectral function that converges systematically to the exact one as the statistical error decreases. As an application, we simulate the two-orbital Hubbard model for various electron densities with dynamical mean field theory and obtain the real-frequency data with our analytic continuation method. We find that the imaginary part of the real-frequency self-energy splits as the electron density approaches the half-filling from the quarter-filling, inducing a non-Fermi liquid behavior. This work was supported by NRF of Korea (Grant No. 2020R1A2C3013673) and KISTI supercomputing center (Project No. KSC-2021-CRE-0384).

### Keywords:

analytic continuation, DMFT, Dynamical mean field theory, self-energy

## Data-Driven Design of High Entropy Halide Perovskite Alloys

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### Abstract:

Halide perovskites with desirable stability, electronic structure, and optical absorption are sought for solar cells, electronic devices, infrared sensors and quantum computing. Compositional manipulation via alloying at cation or anion sites, or via incorporation of point defects and impurities, can help tune their properties. In this work, we develop a data-driven framework for the on-demand prediction and optimization of the phase stability, band gap, optical absorption spectra, photovoltaic figures of merit, and defect formation energies for a chemical space of ABX<sub>3</sub> halide perovskites with several choices for A, B and X, with mixing allowed at each site. This framework is powered by high-throughput density functional theory (DFT) computations, unique encoding of atom-composition-structure (ACS) information, and rigorous training of advanced neural network (NN) and other regression-based predictive models as well as genetic algorithm (GA)-based multi-objective optimization frameworks. Our models scale robustly well to large system sizes as well as varying amounts of mixing of completely new elements at cation or anion sites. Recommendations from combinatorial screening and GA-based design are synergistically coupled with targeted synthesis and characterization, leading to successful validation and discovery of novel halide perovskite compositions for improved performance in solar cells.

### Keywords:

Perovskite

## Polymer Informatics: Current Status and Critical Next Steps

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### Abstract:

The Materials Genome Initiative (MGI) has heralded a sea change in the philosophy of materials design. In an increasing number of applications, the successful deployment of novel materials has benefited from the use of computational, experimental, and informatics methodologies. Here, we describe the roles played by computational and experimental data generation and capture, polymer fingerprinting, machine-learning-based property prediction models, and algorithms for designing polymers meeting target property requirements. These efforts have culminated in the creation of an online polymer informatics platform ([www.polymergenome.org](http://www.polymergenome.org)) to guide ongoing and future polymer discovery and design. Challenges that remain will be examined, and systematic steps that may be taken to extend the applicability of such informatics efforts to a wide range of technological domains will be discussed. These include strategies to deal with the data bottleneck, new methods to represent polymer morphology and processing conditions, and the applicability of emerging algorithms for design.

### Keywords:

Machine-learning, polymer informatics, data-driven prediction, polymer design

## Nanostructure Self-assembling Peptide Discovery: Overcoming Human Bias Using Machine Learning

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### Abstract:

Peptide materials have a wide array of functions from tissue engineering, surface coatings to catalysis and sensing. This class of biopolymer is composed of a sequence, comprised of 20 naturally occurring amino acids whose arrangement dictate the peptide functionality. While it is highly desirable to tailor the amino acid sequence, a small increase in their sequence length leads to dramatic increase in the possible candidates (e.g., from tripeptide =  $20^3$  or 8,000 peptides to a pentapeptide =  $20^5$  or 3.2 M). Traditionally, peptide design is guided by the use of structural propensity tables, hydrophobicity scales, or other desired properties and typically yields <10 peptides per study, barely scraping the surface of the search space. These approaches, driven by human expertise and intuition, are not easily scalable and are riddled with human bias. Here, we introduce a machine learning workflow that combines Monte Carlo tree search and random forest, with molecular dynamics simulations to develop a fully autonomous computational search engine (named, AI-expert) to discover peptide sequences with high potential for nanostructure self-assembly (as a representative target functionality). We demonstrate the efficacy of the AI-expert to efficiently search large spaces of tripeptides and pentapeptides. Subsequent experiments on the proposed peptide sequences are performed to compare the predictability of the AI-expert with those of human experts. The AI performs on-par or better than human experts and suggests several non-intuitive sequences with high self-assembly propensity, outlining its potential to overcome human bias and accelerate peptide discovery.

## Classification and prediction of hazardous compounds using artificial intelligence

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### Abstract:

Compounds information such as Chemical Abstracts Service (CAS) registry number, hazardous, properties is provided through Globally Harmonized System (GHS) based Material Safety Data Sheet (MSDS). It can protect users from hazardous compounds and helps to safely handle chemicals. GHS that indicates hazardous of compounds is categorized through animal testing (or in vivo testing), in vitro testing, epidemiological surveillance, and clinical trials. In this study, artificial intelligence is used to predict the hazardous of compounds by replacing previous methods. A database of hazardous compounds provided by Ministry of Environment was used as the dataset and, CNN and RNN were used as model of machine learning. As a result, the accuracy of 90% was confirmed in the CNN model using the image data with the structural characteristic of the compound, and the accuracy of 60% was checked in the RNN model using sequence data which is represented as SMILES. We analyzed the training results through various numerical data and visual data. In this study, we expect that artificial intelligence can replace conventional classification methods.

### Keywords:

hazardous compounds, classification, machine learning, GHS, MSDS

## Dual Ag-Graded Structure Engineering for High Efficiency ACZTSSe Solar Cells

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### Abstract:

Kesterite  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  (CZTSSe) solar cell has been considered as the most promising candidate to replace the conventional CIGS and CdTe solar cells. However, CZTSSe solar cells are strongly limited with the large open circuit voltage deficiency ( $V_{\text{oc}}^{\text{def}}$ ) due to its constituent elements of Cu and Zn. To solve the  $V_{\text{oc}}^{\text{def}}$  issues in CZTSSe, we propose dual Ag-graded (front and back) structure engineering. Our experimental results showed that dual Ag-graded structure is beneficial to enhance carrier collection, reduce back contact barrier and minimize Cu/Zn related disorders. Moreover, the final ACZTSSe device exhibited remarkable power conversion efficiency (PCE) of 12.07% with improved device parameters of open circuit voltage ( $V_{\text{oc}}$ ), current density ( $J_{\text{sc}}$ ) and fill factor (FF). To the best of our knowledge, our obtained PCE is the highest among aqueous solution based approach under open air environment.

### Keywords:

Keterite, solar cell, Dual Ag-graded, Defect passivation, Spray pyrolysis

## Crystal structure prediction of mixed-halide perovskites using a machine-learning potential

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### Abstract:

Lead halide perovskites ( $\text{CsPbI}_3$ ) have attracted much attention as a potential candidate for a high-efficiency solar cell. However, they exhibit a very short lifetime since the perovskite phase is unstable at room temperature. One of the engineering techniques is mixing halogen elements to make the perovskite structure more stable. The previous researches have shown that mixing Br alleviates the issue with some loss in power conversion efficiency. In addition, several computational studies investigated the thermodynamic stability of mixed halides with density functional theory (DFT) calculations and showed that mixing can enhance the stability. However, they are based on known prototypes of  $\text{CsPbI}_3$ . This assumption excludes a possibility of finding uncharted phases in mixed-halide perovskites. The heuristic searching methods with ab initio calculations is one of the options to overcome the limitation. However, DFT is computationally too expensive to evaluate the energies of numerous candidates during crystal structure prediction (CSP).

In this study, we conducted CSP in mixed-halide perovskites ( $\text{CsPbI}_x\text{Br}_{3-x}$ ,  $\text{CsPbI}_x\text{Cl}_{3-x}$ ) with SPINNER, a recently developed in-house code for CSP using a neural network potential. With SPINNER, we are able to explore structures beyond prototypes with much less costs compared to the DFT-only based approaches. As a result, we identified the most stable phases at each stoichiometry. The non-perovskite  $\delta$  phases are usually more stable than the  $\gamma$  phases. Nonetheless, the energy difference is reduced and we can observe the crossover in some compositions. We also discovered that the  $\gamma$  phases are expected to have good optical properties even for the mixed-halide perovskites. We anticipate that our findings can contribute to extending the lifespan of solar cells based on lead halide perovskites.

### Keywords:

Lead halide perovskite, Density functional theory, Crystal structure prediction

## Photo-Carrier Dynamics of NH<sub>4</sub>Cl Passivated Interfaces in Efficient Perovskite Solar Cells

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### Abstract:

Owing to unique advantages of SnO<sub>2</sub> including low-temperature solution processability, high optical transmittance and good electrical conductivity, SnO<sub>2</sub> has been traditionally applied as an electron transport layer (ETL) towards the fabrication of highly efficient perovskite solar cells (PSCs). Non-adjusted Sn-dangling bonds of the SnO<sub>2</sub> interfaces are present as traps for arresting the light generation carrier, resulting in hysteresis and device instability. In this report, Ammonium chloride (NH<sub>4</sub>Cl) passivation on the rear and front surface of SnO<sub>2</sub> adjacent to ITO substrates and perovskite interfaces at a low temperature process is reported, following previous studies on SnO<sub>2</sub> surface passivation by ozone and NH<sub>4</sub>Cl treatment [1]. By exploring the interplay between charge transporting and recombination dynamics at the interface passivation of rear and front surface, it is revealed that a rear passivation yields superior interfacial characteristics, in terms of fewer trap densities, lower charge recombination and electron transport efficiency. Furthermore, the reduced non-radiative recombination at the NH<sub>4</sub>Cl passivation interfaces with ITO and perovskite has been observed by photoluminescence (PL) measurement and exhibited enhancement of electron transfer and suppression of the interfacial recombination. Our study circumvents concerns on batch-to-batch inconsistency of perovskite films at the interface due to the interfacial carrier losses by recombination of charge carrier extraction efficiency in conventional time resolved PL-based measurements.

[1] J. H. Kim, Y. S. Kim, H. R. Jung, and W. Jo, "Chlorine-passivation of the ozone-treated SnO<sub>2</sub> thin films: occurrence of oxygen vacancies for manipulation of conducting states and bipolarities in resistive switching", *Applied Surface Science* 555, 149625 (2021).

### Keywords:

NH<sub>4</sub>Cl passivation, Perovskite solar cells, Non-radiative recombination, Photo-carrier, SnO<sub>2</sub> electron transport layer

## Fabrication of Co-Doped Garnet LLZO with Ta<sup>5+</sup> and Ga<sup>3+</sup> by Solid-State Reaction

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### Abstract:

The garnet-type Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> (LLZO) is a promising solid electrolyte for all-solid-state Li-ion batteries due to its outstanding performance, namely, fast ionic conduction, wide electrochemical stability window (against Li/Li<sup>+</sup>) and improved safety. However, LLZO exhibits two polymorph phases, tetragonal and cubic, where the cubic phase exhibits ~ 2 orders of higher Li-ion conductivity but is thermodynamically unstable at ambient temperature. In order to stabilize the cubic phase, doping with aliovalent elements is desirable to induce Li-vacancies and distorted occupations. In this work, we fabricated single and co-doped garnet with Ta<sup>5+</sup> and Ga<sup>3+</sup> (Li<sub>7-3x-z=6.4</sub>Ga<sub>x</sub>La<sub>3</sub>Zr<sub>2-z</sub>Ta<sub>z</sub>O<sub>12</sub>) and characterized by X-ray diffraction, Raman spectroscopy, scanning electron microscopy and electrochemical impedance spectroscopy.

### Keywords:

solid state Li-ion electrolyte, garnet LLZO, ion conductivity, co-doping

## Effect of SnSe<sub>2</sub> formation on CZTSSe thin film solar cells

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### Abstract:

Cu<sub>2</sub>ZnSn(S<sub>1-x</sub>Se<sub>x</sub>)<sub>4</sub> (CZTSSe) has become a promising candidate for the absorber layer of thin solar cells thanks to the advantage of using earth-abundant, non-toxic elements [1]. However, since the stable phase region of CZTSSe is very narrow, secondary phases are easily formed during the thin-film deposition or the post-deposition treatments, and some of the secondary phases are detrimental to the solar conversion efficiency of CZTSSe solar cells [2-4]. Herein, we investigated the influence of secondary phase to the performance of the solar cell device using laser-beam-induced-current (LBIC) measurements and resonant Raman spectroscopy. We found that the SnSe<sub>2</sub> secondary phase has a critical impact on the characteristics of solar cell even with a small amount of the secondary phase. Carrying out LBIC and Raman mapping, we confirmed that the points with the secondary phase had a lower photocurrent. We also performed Raman spectroscopy in a macroscale for all cells on the solar cell device, The existence of the SnSe<sub>2</sub> secondary phase was directly correlated with the low efficiency of the cell. The cells with the secondary phase had lower efficiency about ~3 % than the other cells, whose efficiencies were about ~8 %. Therefore, controlling the formation of the SnSe<sub>2</sub> secondary phase is a crucial factor to obtain CZTSSe solar cells with high efficiencies.

[1] Katagiri, H., Cu<sub>2</sub>ZnSnS<sub>4</sub> thin film solar cells. *Thin Solid Films* **2005**, 480-481, 426-432.

[2] Siebentritt, S., Why are kesterite solar cells not 20% efficient? *Thin Solid Films* **2013**, 535, 1-4.

[3] Dimitrievska, M. *et al.*, Secondary phase and Cu substitutional defect dynamics in kesterite solar cells: Impact on optoelectronic properties. *Solar Energy Materials and Solar Cells* **2016**, 149, 304.

[4] Yoo, H. *et al.*, The formation mechanism of secondary phases in Cu<sub>2</sub>ZnSnSe<sub>4</sub> absorber layer. *Thin Solid Films* **2015**, 582, 245-248.

### Keywords:

CZTSSe, thin film solar cells, secondary phase, resonant Raman spectroscopy, Laser-beam-induced-current

## 내용학 교수가 생각하는 물리교육

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### Abstract:

누구를 대상으로 하던 물리를 잘 가르치는 것은 참 쉽지 않아 보인다. 물리를 잘했던 사람들이 교수나 교사가 되어 어찌면 자신이 공부했던 방식으로 물리를 가르치면서 왜 어려워하고 잘 못하는지 이해를 못하겠다고 하거나 혹은 물리는 원래 어려운 것이니까 소질이 없는 학생들을 포기해 버리는 경우를 종종 볼 수 있다. 이러한 상황은 우리나라 뿐 아니라 세계적인 현상일지도 모른다. 물리교육에 대한 연구가 시작한 이래 얼마나 우리나라 학교 현장은 바뀌었나? 30년간 사범대학교에서 물리학과 물리교육을 연구하면서 물리교육 (과학교육)에서 고려해야 할 만한 점들을 나누고자 한다.

### Keywords:

물리교육, 내용과 교육의 연계

## 물리교사 양성을 위한 물리학(내용학)과목의 운영방안

PARK Jong Won \*1

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### Abstract:

물리교사 양성을 위한 물리학과목의 운영에 대해 다음 3가지 측면을 논의하고자 한다.

첫째, 다음 3가지 내용은 물리학 과목에서 지도될 때 높은 효과를 기대할 수 있다 (1) 물리 오개념: 물리학 과목에서 물리개념을 지도하면서 관련된 오개념을 함께 다루어 주면 초중등학생의 물리개념 지도에 직접적으로 활용될 수 있다. (2) 물리 개념도(concept map): 초중등학생에게 물리개념의 지도는 개념과 개념간 관계를 서술하는 명제 형태로 이루어지기 마련이다. 이러한 개념과 개념과의 관계를 이해하는데 도움을 줄 수 있는 학습전략 중의 하나가 개념도이다. (3) 물리시범: 시범은 가능하면 간단한 도구와 방식으로 직접적이고 두드러지게 현상을 보일 수 있다는 점에서 추상적인 물리개념을 실제 현상으로 경험할 수 있게 하는 효과적인 방안이다.

둘째, 어떤 물리학 지식이든 교사가 많이 알수록 무조건 좋다고 할 수는 없다. 실제로 Abell (2007)은 교사의 내용학 지식과 중등학생 지도와의 관계에 대해 단순한 결론을 내리기 어렵다고 하였다. 예를 들어, 수 학영역이지만, Rockoff *et al.* (2011)는 미국의 수학교사의 대학원 학위 취득 여부와 학생의 수학 성취 사이에 유의한 상관이 없다고 하였다. 이에 박종원 등 (2021)은 교육과정에 명시적으로 제시되어 있어 학생에게 지도해야 할 지식인 '교육과정 지식(Knowledge In Curriculum: 이하 KIC)'과 교육과정을 벗어나는 상위 수준의 지식이지만 교사가 알 필요가 있는 '교육과정 이상의 지식(Knowledge Beyond Curriculum: 이하 KBC)'으로 나누어, 예비 물리교사가 배울 필요가 있는 상위 물리지식의 유형을 [표 1]과 같이 제시하였다.

[표 1] KIC의 유형과 예시      KBC의 선택기준과 예시

현상의 기술	현상의 설명
정성적 설명	정량적 설명
추상적 개념	구체적 사례, 실제 현상
핵심 개념/기본 원리	개념의 시작/발달/변화과정, 개념의 형이상학적/인식론적 의미, 방법론적 규칙,
법칙/공식	법칙/공식의 유도과정

따라서 초중등 물리교육과정에서 어떤 물리내용이 어떤 수준으로 다루어지는지를 고려하고, 그 내용을 지도하는데 관련된/필요한 상위지식을 선정하는 방식으로 물리학 과목의 내용을 결정하는 과정을 고려해 볼 필요가 있다. 즉 현재 지도하고 있는 물리학 과목 내용을 살펴보면, [표 1]에서 제시한 상위지식이 빠진 경우가 있을 수도 있고, [표 1]에서 제시한 상위지식의 수준을 넘는 과도한 상위지식(즉 KIC 지도와 관련짓기 어려운 지식)이 지도되고 있는 경우도 분석될 수 있을 것이다.

셋째, 초중등 물리실험 지도를 고려한 물리학 실험과목 운영에 대해서도 관심을 기울일 필요가 있다. 대학 물리학 실험은 고급 실험장비의 사용과 자료의 정밀한 분석기능에 초점이 맞추어진 경우가 많다. 그러나 최근 초중등 물리실험에는 시뮬레이션, 컴퓨터 센서나 스마트폰 센서, 비디오나 시범관찰을 이용한 다양한 유형의 실험이 포함되어 있다. 또한 탐구문제와 탐구 과정, 그리고 탐구 결과가 정해져 있지 않은 자유 탐구도 포함되어 있다. 따라서 물리교사 양성을 위한 실험과목이라면 다양한 유형의 초중등 실험과 함께, 자유탐구를 직접 수행해 보도록 할 필요가 있다.

**Keywords:** 물리교사 양성과정, 내용학, 초중등 물리교육과정

## 교사양성기관 교과내용학 강의개선을 위한 새로운 방안 모색: '교사를 위한 일반상대성이론'을 중심으로

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### Abstract:

교원양성기관다운 교과내용학 강의의 필요성이 오랫동안 제기되어왔다. 그러나 최근의 연구보고서를 보면 교원양성기관에서 필요로 하는 교과내용학 강의 개발은 여전히 충분히 만족스럽지 못한 것으로 보인다. 이와 관련하여 물리교과내용학 강의의 실태를 파악하고 개선방안을 모색할 필요가 있다. 이에 본 연구에서는 물리교과내용학 강의 개발에서 핵심 쟁점 중 하나인 '물리교과내용의 축소(혹은 부실화) 가능성 문제'의 원인을 파악하고 이에 관한 해소방안을 모색하고자 하였다. 한 가지 해소방안으로서, 본 연구는 물리학의 실천전통에 기반한 물리교과내용학의 필요성을 제안하였고, 구체적인 사례, 즉 '교사를 위한 일반상대성이론' 강의 및 교재개발 내용을 소개할 예정이다.

## Observation of lower-hybrid frequency fluctuations in KAERI divertor plasma simulator

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### Abstract:

KAERI divertor plasma simulator was successfully developed using applied-field magnetoplasdynamic (AF-MPD) thrusters for studying plasma-surface interactions in fusion divertor region [1, 2]. The AF-MPD thruster was adopted because it operates at relatively low gas pressure (<1 mTorr) and produces a high-density plasma in cw mode. We reported that our device can provide the heat flux as high as  $10 \text{ MWm}^{-2}$  and the deuterium ion flux up to  $10^{23} \text{ m}^{-2}\text{s}^{-1}$ . Recently, we found that there is a mode change in deuterium plasmas: the electron density and ion flux abruptly increase several times as the plasma current is increased. In addition, when the plasma is changed from low-density mode to high-density mode, we observed fluctuations of 200-500 kHz in Langmuir probe measurement. This frequency ranges between fast Alfvén and lower-hybrid waves. In the presentation, we will show the details of the measured fluctuations and our plan to identify these fluctuations.

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### Keywords:

MPD thruster, lower-hybrid waves, fast Alfvén waves, divertor simulator, plasma diagnostics

## Collisionless relaxation process of current sheets

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### Abstract:

Current sheets are ubiquitous structures in space, astrophysical, and laboratory plasmas. They serve as crucial localities which store magnetic energy that may be converted to other forms of energy. Although a plethora of current sheet equilibrium solutions have been found, how an initially disequibrated current sheet relaxes has remained a mystery. Here we present the exact collisionless process through which a current sheet equilibrates, namely orbit class transitions. This is done by comprehensively classifying particle orbits in a magnetic field reversal in phase space and then comparing the resultant phase-space morphology with that from particle-in-cell simulations. A useful by-product of this analysis is the prediction of bifurcated current sheets, which have been consistently observed in space without consentaneous explanations. MMS spacecraft data were compared with those from particle-in-cell simulations to demonstrate that the origin of such bifurcation is from the current sheet relaxation process. Guide field effects are also discussed.

### Keywords:

Current Sheets, Magnetic Reconnection, Phase-space Analysis, Particle-in-cell Simulations, Spacecraft Data Analysis

## Evolution of Kinetic and Magnetic Energy in a large magnetic Prandtl number System

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### Abstract:

Many regions of the universe are in the state of hot, magnetized, and ionized X-ray emitting plasmas. We numerically simulated the energy spectrum of this highly viscous and conductive system. Without magnetic field, the fluctuating plasma motion decays in the relatively large viscous scale. However, the magnetic field extends the viscous scale to the magnetic diffusivity one yielding a unique energy spectrum. Numerical simulation shows that kinetic and magnetic energy spectrum are  $E_V \sim k^{-3.7}$  and  $E_M \sim k^{-0.85}$  in the extended viscous scale regime. To explain this extraordinary power law, we set up two simultaneous differential equations for  $E_V$  &  $E_M$  and solved them using Eddy Damped Quasi Normal Markovianized approximation. Focusing on the most dominant terms, we analytically derived the spectrum relation  $E_M^2 \sim k^2 E_V$  consistent with the simulation data. We also simulated the same system with helical energy. The inversely cascaded magnetic energy makes the spectrum steeper. This inverse energy transfer, in addition to the external magnetic field and instabilities, provides us a clue to the diversified spectra characterized  $E_V \sim k^{-3.7} - k^{-3.07}$  and  $E_M \sim k^{-2.17} - k^{-0.27}$  with large magnetic Prandtl number.

### Keywords:

Energy spectrum, magnetic field, dynamo, large magnetic Prandtl number

## Analysis of phase-resolved plasma dynamics in dual-frequency capacitively coupled Ar plasmas

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### Abstract:

이중주파수 용량성결합플라즈마 (capacitively coupled plasma, CCP)는 공간 균일성과 이온 에너지 특성 제어의 장점 때문에 반도체 에칭 및 증착 공정에서 널리 쓰이고 있다. 본 연구에서는 이중 주파수 구동에 의해서 이온 에너지와 이온 flux를 별도로 제어하는 것이 가능한 영역이 존재한다는 것과 그 원리에 대해서 설명하고, 이중 주파수 구동의 고주파 성분과 저주파 성분 전압이 전자 가열에 미치는 영향과 이온 거동에 미치는 영향을 2차원 입자-셀 (particle-in-cell, PIC) 시뮬레이션을 이용하여 관찰하였다. 이온의 transit time 대비 빠르게 변화하는 고주파성분과 느리게 변화하는 저주파 성분의 전압 차이에 따라서 변화하는 이온 에너지 분포를 분석하여 원하는 에너지 분포를 만드는 제어 방법에 대해서 연구하였다. 또한 플라즈마 밀도의 공간 균일성이 달라지는 원인이 되는 전자가열의 원리를 위상별로 분석하여 보다 균일한 플라즈마 분포를 발생시키는 방안에 대해서 제안한다.

### Keywords:

Capacitively coupled plasma, particle-in-cell simulation, ion energy distribution function, electron heating

## Synthetic anti-PT symmetric system in an optical fiber

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### Abstract:

The anti-parity-time (APT) symmetry is associated with various effects beyond fundamental limitations implied in the standard Hermitian-Hamiltonian dynamics. Here, I will show several non-Hermitian dynamics systems and show our recent experimental results of an optical APT-symmetric system in a synthetic frequency domain. Our system is an optical synthetic APT system with negligible gain/loss, providing unique ATP effects, including phase transition, energy-difference conservation, and synchronized power oscillation. We experimentally observed these optical APT behaviors for the first time in excellent agreement with the theory in the key physical aspects, including energy-spectral properties and dynamic responses.

Recent developments of non-Hermitian physics show that carefully designed gain and loss in connection with inter-state coupling strength have produced numerous anomalous effects associated with the parity-time (PT) symmetry [1] and exceptional-point (EP) singularity [2]. These non-Hermitian phenomena have no counterpart in the conventional Hamiltonian systems. Recently, using balanced gain and loss, anti-PT (APT) symmetry systems have been demonstrated in various platforms, whose Hamiltonian has the sign change under PT reversal.

Beyond the geometric dimension, it is possible to explore the APT physics in a new dimension, such as frequency, time, and orbital angular momentum, referred to as the synthetic dimension, and we can achieve phase transition at EP, coherent power oscillation, and energy-difference conservation [3]. The energy-difference conservation effects require a perfectly balanced gain and loss in an APT symmetry system. In that case, the energy of two modes varies in time by an equal amount, which is in contrast to the standard Hermitian dynamics' net-energy conservation.

This presentation will show several recent reports on PT-symmetric and APT-symmetric systems and their unique properties, which are different from that of Hamiltonian systems. In addition, I will present our recent results of the synthetic APT symmetry effects in conventional optical fiber, showing EP, phase transition, coherent power oscillation, and energy-difference conservation. The use of optical fiber as a non-Hermitian system gives us the great advantage of long interaction length, negligible loss, and convenient system construction. The first observation of the energy-difference conservation agrees well with the theory in the non-Hermitian physical dynamics. Our results show a robust synthetic non-Hermitian photonic system in an application-abundant fiber-optic platform. We expect that this exotic property of the fiber-based APT-symmetric system may provide new optical manipulation methods, including anti-adiabatic topological time-asymmetry, quantum optical experiments, EP-related unidirectionality, and diverging parametric sensitivity.

### Acknowledgements

National Research Foundation of Korea (NRF-2019M3E4A1079780); Institute for Information & communications Technology Promotion (IITP) grant funded by the Korea government (MSIT) (No. 2020-0-00947); and Korea Institute of Science and Technology's Open Research Program (2E30620-20-052).

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**Keywords:**

# Organic Hyperbolic Material Assisted Optical Nanoscopy

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## **Abstract:**

Plasmonic enhanced light-matter interactions in dielectric-metal nanostructures and the subwavelength nature of light confinement provide many fascinating possibilities in engineering advanced optical technologies such as nanoscale sensing and super-resolution imaging. As an alternative to these metallic nanostructures, organic hyperbolic materials (OHMs) consisting of self-assembled molecular building blocks have recently been investigated and proven to be a more versatile way to control light at the nanoscale via optical dispersion engineering by supramolecular approaches. In this talk, the significant progress in development of these newly emerging OHMs is reviewed with particular emphasis on their optical applications.

## **Keywords:**

Organic Hyperbolic Material, Super-resolution Imaging

# Scattering Near-field Optical Microscopy for Quantum Interaction Studies

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## Abstract:

Scanning near-field optical microscopy (SNOM) measures optical signals in the near-field zone. Therefore, SNOM can be used as a probe of quantum interactions that mainly occur in the short-range scale beyond the diffraction limit. Here, we present SNOM techniques to study quantum interactions in the near-field zone. In this presentation, we introduce our two recent works; we first show how mid-infrared SNOM can measure quantum interactions in the mixed-dimensional heterostructure composed of graphene and carbon nanotubes. The quantum interaction in the heterostructure allows us to control one-dimensional (1D) plasmon actively, while active plasmon control has been forbidden in bare nanotubes. Secondly, we propose SHG-SNOM (second harmonic generation SNOM) to demonstrate the nonlinear quantum energy transfer between a metallic tip and a noncentrosymmetric sample. Using SHG-SNOM, we experimentally demonstrate that the nonlinear quantum energy transfer enables the measurement of weak SHG signals of non-resonant noncentrosymmetric samples.

## Keywords:

Scattering near-field optical microscopy, Plasmonics, Carbon nanotubes, Graphene, Second harmonic generation

## Engineering real-space optical vortex dynamics in high-dimensional synthetic media

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### Abstract:

Optical vortices, topological textures in electromagnetic waves, received significant attention for quantum optic communication and optical trapping applications. Recently, the demonstration of topological photonic media called gradient-thickness optical cavity brought quasiparticle-like characteristics to optical vortices as the condensed matter counterparts. In this study, we demonstrated the high-dimensional manipulability of real-space optical vortices in topological media, which provides an extra degree of freedom in the design of vortex dynamics. We propose a multiply-stacked gradient thickness optical cavity, which supports a non-trivial topological phase in synthetic dimension consisting of  $N$  layer thicknesses. By selecting the proper combination of  $N$  layer thicknesses, direction and strength of the effective spin-orbit interaction in real-space optical vortices can be tailored drastically. We believe that our study opens new perspectives in topological photonics for the development of active topological photonic devices.

### Keywords:

Topological photonics, Synthetic dimension, Optical vortex

## Nanoscale analyses of EUV and e-beam irradiated photoresists based on near-field infrared spectroscopy

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### Abstract:

As the pattern size of logic devices becomes finer less than 10 nm, the desire for a new investigation tool that can help the development of photoresist materials for the next generation extreme ultraviolet lithography (EUVL) is being raised. In this study, a 10 nm spatial resolution imaging analytic method, scattering-type scanning near-field optical microscopy (s-SNOM), is suggested to evaluate the EUV and e-beam irradiated hydrogen silsesquioxane (HSQ). Taking advantage of the penetrability of the tip-enhanced infrared signal into the films, the spatio-spectral maps of bonding structure are constructed. EUV dose-dependent bonding structures and half-pitch (HP) 100, 200, 300, and 500 nm lines and spaces patterns were evaluated. We calculated the linewidth and line edge roughness (LER) from both pre- and post-developed HSQ. Pattern information which was taken before development can offer new insight and feedback for resist material research.

This work was supported by Samsung Research Funding & Incubation Center of Samsung Electronics (Project Number SRFC-TA1703-051) and the National Research Foundation of Korea (NRF) with a grant funded by the Korean government (MSIT) (NRF-2020M3H4A3081917).

### Keywords:

Photoresist, Pre-development, Pattern inspection, HSQ, Infrared nanoscopy

## Rydberg atoms for quantum simulation and computation

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### Abstract:

Quantum information and quantum computing have drawn significant interest in recent years because of their potentials in solving computational problems which are intractable for non-quantum computational methods. In quantum simulation, quantum adiabatic methods are used to steer a quantum many-body system from one Hamiltonian to the other so that, for example, the complex ground state of the final Hamiltonian can be "calculated" [1]. Such a ground-state finding of the quantum system could be difficult to simulate with a classical device, but it could be natural, thus simple and easy, to implement with a quantum computing system. Rydberg-atom system is one of those programmable quantum many-body system, which has as-many-as a few hundreds of "qubits" and mesoscopic, thus individually controllable, system sizes. Not to mention taking the most advantages of general atom technologies, such as precisions, accuracies, stabilities, identity, Rydberg atoms have strong and short-ranged interactions which are beneficial for fast and high-fidelity operations. In this presentation, we present experiments of Rydberg-atom quantum simulation and discuss the possibilities of Rydberg-atom quantum gate-based computation. Optically induced interactions of neutral atoms can be modelled to, for example, quantum Ising Hamiltonian, and, when the interacting atoms are in an arrangement equivalent to a mathematical graph, finding the ground many-body state of the atoms can be mapped to a certain mathematical problem, for example, the Maximum Independent Set (MIS) problem of the graph [2]. In experiments, Rydberg-atom arrays are implemented for not only planar and but also nonplanar graphs including the Kuratowski subgraphs for MIS problems [3]. With some of the atoms used as ancillary, quantum wires programmed all-to-all arbitrary couplings of the qubits. Furthermore, individual addressing of the Rydberg atom arrays performed small-scale quantum circuit operations.

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### Keywords:

Rydberg atom, quantum simulation, quantum computing, quantum gate

## High sensitivity AlGaAsSb avalanche photodiodes for 1.55 $\mu\text{m}$ applications

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### Abstract:

Currently prevalent Light Detection and Ranging (LiDAR) systems capture 3D images using 905 nm lasers as sources and Si avalanche photodiodes (APDs) as receivers. Silicon APDs are low cost and reliable, but the wavelength range of these LiDAR systems is limited by the band gap of Silicon to less than 1150 nm. LiDAR at longer wavelengths promises significant advantages. In particular, 1550 nm LiDAR is eye-safe and has superior atmospheric transmission. To enable LiDAR at this longer wavelength, a high performance and low-cost receiver APD is needed.

This study focuses on a technology that exploits previously unexplored III-V compound semiconductors to address this APD technology gap. An AlGaAsSb quaternary semiconductor was identified, designed, and demonstrated to be a promising multiplier (gain) material. This material was grown on an InP substrate that supports pairing it with a known light absorber GaAsSb or InGaAs for a cost-effective 1550 nm APD.

Our research on the AlGaAsSb multiplier has advanced the promise of this technology, achieving 2 – 3 times lower avalanche noise than commercial technologies with moderate leakage current [1,2]. Our recent result demonstrated that the avalanche noise of our AlGaAsSb APDs is at the lowest limit which an APD (thicker than 500 nm) can theoretically achieve. The efforts to achieve these characteristics have included modeling this quaternary system; reducing the avalanche noise of the AlGaAsSb by increasing its thickness; and achieving a high purity, single crystalline quaternary by using a digital alloy growth technique. Our next step is the combination of this promising multiplier with a 1550 nm absorber material, a combination we have designed and will grow and characterize. This will demonstrate an APD technology that is predicted to be superior to current commercial technologies and enables eye-safe LiDAR systems.

### Reference

[1] S. Lee et al., Appl. Physics. Lett 118, 081106 (2021).

[2] S. Lee et al., Appl. Physics. Lett 120, 071101 (2022).

### Acknowledgment

This work is supported by the Directed Energy–Joint Transition Office, Award N00014-17-1-2440.

### Keywords:

Avalanche photodiodes, eye-safe LiDAR, High-sensitivity receiver, AlGaAsSb, Molecular beam epitaxy

## GaSb/InGaAsSb and InAs/GaSb based infrared photodetectors

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### Abstract:

We investigated the optical, electrical properties of the infrared photo-detectors through the photoluminescence (PL), photorefectance spectroscopy (PR), current–voltage (I–V) characteristics and photo response measurements. Especially, we investigated the surface leakage current of the InGaAsSb/AlGaSb nBn infrared detector using PR. The Franz-Keldysh oscillations (FKOs) in PR spectra showed that the minority carriers (electrons) mainly affect the surface electric field in the nbn structures. The results show that the electric field increases due to the photovoltaic effect as the temperature increases. However, the increased ratio of the electric field at low temperature is lower than that of high temperature. At low temperatures, when the temperature drops, the generation-recombination (G-R) associated with dark current is eliminated, and the surface electric field variation becomes lower. By increasing the temperature and dark current, the electric field changes more. In addition, the unipolar barrier photodiode exhibits no surface leakage current at low temperatures without blocking the bulk currents.

### References

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[2] Suho Park , Jiyeon Jeon, Vivek Mohan More, Rochelle Safia Lee, Youryang Seo, Minkyung Kim, Phuc Dinh Nguyen, Minkyong Kim, Jong Su Kim, Yeongho Kim, Sang Jun Lee, Applied Surface Science 581, 152421 (2022).

### Keywords:

InAs/GaSb, nBn IR detector

## Effects of flavor SU(3) symmetry breaking on the gravitational form factors of the baryon octet and their stability conditions

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### Abstract:

We investigate the gravitational form factors of the baryon octet within the framework of the chiral quark-soliton model, also known as the pion mean-field approach, emphasizing the effects of flavor SU(3) symmetry breaking on the form factors. The D-term form factors provide information on the stability conditions of the baryon octet in terms of the pressures and shear forces inside them. We show explicitly that the stability conditions are well preserved in the presence of flavor SU(3) symmetry breaking. We also discuss various physical implications of the gravitational form factors of the SU(3) baryon octet.

### Keywords:

Energy-momentum tensor, hadron, gravitational form factors, chiral quark soliton model, baryon octet

## Energy-momentum tensor form-factors and the quark and gluon subsystems inside a large $N_c$ nucleon

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### Abstract:

We investigate the nucleon energy-momentum tensor form factor  $\mathbb{W}(\bar{c})$ , within the instanton model of QCD at the low renormalization point.

The form factor is of particular interest as it corresponds to a higher twist contribution to the mass decomposition of a nucleon. The smallness of the form factor due to the small instanton packing fraction provides an interesting picture inside the nucleon, that the quark and gluon subsystems interact with each other weakly.

### Keywords:

Energy-momentum tensor, Nucleon, Instanton

## The $h_1$ axial-vector meson in the coupled-channel approach

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### Abstract:

We investigate the axial-vector meson  $h_1$ . We coupled 4 channel,  $\pi\rho$ ,  $\eta\omega$ ,  $K\bar{K}^*$  and  $\eta\phi$ , which generate two resonance structure within energy up to 600 MeV above the threshold. Moreover, having reproduced the experimental data of charge exchange reaction ( $\pi p \rightarrow 3\pi n$ ), we extract the pole position and residue of each resonance and identify them as the existing  $h_1(1170)$  and  $h_1(1380)$  resonances. We discuss the nature of these resonances and their internal structures.

### Keywords:

axial-vector meson  $h_1$  , coupled-channel approach

## Axial-vector transition form factors of singly heavy baryons in the pion mean-field approach

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### Abstract:

We present the results of the axial-vector transition form factors of singly heavy baryons within the framework of the chiral quark-soliton model. The chiral quark-soliton model is a pion mean-field approach in the large- $N_c$  limit, which deals with light and heavy baryon on an equal footing. In the limit of the infinitely heavy mass of the heavy quark, a singly heavy baryon can be regarded as  $N_c-1$  valence quarks bound by the pion mean fields with the heavy quark as a color static source. We include the  $1/N_c$  rotational corrections and the effects of SU(3) flavor symmetry breaking. We first compare the results for  $C_5^A(q^2)$  of the heavy baryon transitions with those for the well-known  $\Delta \rightarrow p$  transitions. We also discuss the results for the axial mass for the heavy baryon transitions.

### Keywords:

singly heavy baryon, pion mean-field approach

## Cross-section measurement for $K^-N$ interactions at 1.8 GeV/c with J-PARC E42 detector

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### Abstract:

We report the current status of cross-section measurement for  $K^-N$  reactions at 1.8 GeV/c with the J-PARC E42 detector. We collected approximately  $3 \times 10^5$   $K^-N$  reaction events at forward angles, which include  $K^-p \rightarrow K^+\Xi^-$  and  $K^-n \rightarrow K^-p\pi^-$  reactions. This talk will present preliminary analysis results and discuss physics impacts on the forward cross-section measurements.

### Keywords:

J-PARC E42

## Light-cone distribution amplitude of the nucleon in a pion mean-field approach

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### Abstract:

We present recent results for the light-cone wave function and distribution amplitude of the nucleon based on a pion mean-field approach or the chiral quark-soliton model. We expand the vacuum wave functions in Fock space and consider the five-quark components of the light-quark wavefunction. In addition to the leading-order term from the three-valence-quark state, the five-quark part of the light-quark wave function has sizable effects. We also extract the light-cone distribution amplitude of the nucleon, which contains information on the transition from the nucleon to the vacuum. We compare the current results with those from a recent lattice calculation and QCD sum rules.

### Keywords:

Light-cone wave function, Chiral quark-soliton model, Light-cone distribution amplitude

## Subthreshold Pion Production in pA and AA Reactions with SUPER

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### Abstract:

Subthreshold pion production in pA reactions leads to a low-lying nuclear state so that it involves large momentum transfer even close to the threshold. Therefore, this reaction is sensitive to nuclear dynamics at short distances. However, the existing experimental data sets on the excitation function near 20 MeV are not consistent. An improved excitation function would allow the study of the threshold behavior in more detail, particularly for nuclear structure and the transition from a coherent to an incoherent production mechanism. In AA collisions, pion production at energy per nucleon below the NN threshold is also still a puzzling process. Despite a substantial theoretical effort, no model has globally treated all the involved aspects. The observed cross sections are much larger than predicted by NN collision or statistical models, indicating the presence of a collective production mechanism. We propose a new experimental program on subthreshold pion production envisioned at an early stage of RAON. The KOBRA beam line can deliver  $^{14}\text{N}^{6+}$  in energies up to 43 AMeV and  $^{16}\text{O}^{6+}$  in energies up to 41 AMeV. The beam intensity will be the order of  $10^{12}$  pps. Therefore, we can study neutral pion production from threshold ( $\sim 25$  AMeV) to 41 AMeV with  $^{16}\text{O}^{6+}$  projectiles and various nuclear targets. The new program includes the construction of a neutron-pion spectrometer, the so-called SUPER (subthreshold pion production experiment at RAON). We will report preliminary simulation results on subthreshold pion production in pA and AA reactions.

### Keywords:

Subthreshold production

## Design of Gamma-Ray Detector Array for Nucleosynthesis Reaction Studies

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### Abstract:

We report a preliminary design study of a gamma-ray detector array for nucleosynthesis reaction studies. The so-called HANULball detector was designed for detecting gamma-rays with a superconducting magnet and an active-target time-projection chamber. The detector can accommodate NaI(Tl), BGO, and LaBr<sub>3</sub> crystals, each being with a front face of 50 mm in diameter. The detector is formed as a truncated icosahedron (soccer ball). The scintillation crystals are positioned at every 20 faces (except for the beam entrance and exit faces). We will present a early-stage design of the detector based on Geant4 simulation and preliminary bench test results.

### Keywords:

gamma-ray detector array, nucleosynthesis

## Measurement of $K^*(892)$ mesons and hyperons via $^{12}\text{C}(K^-,p)$ reactions at J-PARC

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### Abstract:

We present the preliminary results on the measurement of  $K^*(892)$  mesons and hyperons via  $^{12}\text{C}(K^-,p)$  reactions at 1.8 GeV/c in J-PARC H-dibaryon search experiment (E42). We have accumulated large amount of  $(K^-,p)$  reaction events during the E42 physics run in 2021. These data set enables us the comprehensive measurement of K-p inelastics scattering with high statistics, especially for  $K^*(892)$  meson and hyperons. In this talk, the preliminary results on  $^{12}\text{C}(K^-,p)$  reaction will be discussed.

### Keywords:

J-PARC, E42

## Viscoelastic instabilities in microfluidic flows

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### **Abstract:**

Microfluidics has emerged in recent years as a versatile platform of manipulating fluids at small length-scales, and in particular, offers a large range of deformation rates and direct visualization of resulting flow fields, providing unique opportunities for capturing the flow instabilities of viscoelastic fluids in real time. By using the subtractive three-dimensional (3D)-printing technique of selective laser-induced etching (SLE), glass microfluidic devices can sustain very high flow rates, provide access to little-explored flow regimes, and enable flow visualization from multiple planes of observation, allowing the quantitative study of 3D flows.

In this talk, I will highlight microfluidic platforms involving microfluidic cylinders to investigate the intricate viscoelastic instabilities of complex fluids. To model synchronized or coupled motions of motile objects (e.g., cilia) translating in biological fluids, we present the first example of viscoelastic fluid-structure interaction in a glass microfluidic device containing free-standing microfluidic circular cylinders. Our studies demonstrate that slender bodies in viscoelastic flow can exhibit complex highly correlated dynamics, which sheds insight on the analogous processes in biological systems. To expand this system, we further study the coupling between the viscoelastic fluid and the micropillar arrays, and discover the spontaneous emergence of metachronal waves in the system. We suggest that the waves originate from pulses of localized high elastic stresses propagating through the elastic wakes that form around the pillars. The occurrence of the wave is chaotic and shows characteristic fingerprints of elastic turbulence.

### **Keywords:**

microfluidics, micropillars, viscoelastic instabilities, elastic turbulence

## Nanorheology of phase changing materials

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### **Abstract:**

At nanoscale common materials such as solid metals, complex liquids or even water strongly depart from what experienced at the macroscale. The need to improve our understanding of matter at smallest confinement pushed the development of advanced investigation techniques based on state of the art force measurements. In this talk we will revisit the advances in the field obtained thanks to a novel class of Scanning Probe Microscopes based on ultrastable mechanical oscillators and we will show how these techniques allow to precisely investigate mechanical phase transition of nanomaterials.

### **Keywords:**

Nanorheology, phase transition, scanning probe microscope, nanomaterials, complex fluids

## Rheology at multi-scales from bulk to micro to nano

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### Abstract:

Conventional rheometers measure bulk-scale properties, which provide average rheological values, thus missing detailed, (sub)micro-scale information on structures and dynamics. At the same time, more emphasis is increasingly given to the characterization and application of smaller volume (micro- and nano-scale) soft materials of high cost, the instrumentation that characterizes quantitative, microscopic mechanical information is in high demand, especially as more stringent regulations are being imposed for the use of bio and soft-matter materials. Here, we present tip-based platform for simultaneous sensitive force measurement and multi-scale strain. It allows to develop novel rheological instrumentation that multi-scale information between macroscale and microscale (and nanoscale) measurements on mechanical and structural properties. Our novel experimental platform, combined with dynamic force spectroscopy as well as optical Raman spectroscopy, not only contributes to open up for multi-scale rheology but expects to further our understanding and applications of nonlinear rheological phenomena in diverse areas of science and engineering. This work represents collaboration with C. Kim, J. Shim, J. Ko, S. An, M. Lee and D. Weitz.

### Keywords:

rheology, multi-scale, atomic force microscopy

## Nano-confined water under high electric fields

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### **Abstract:**

The viscoelectric effect concerns the increase in water viscosity under high electric fields, arising from the interaction of the field with the dipolar water molecules. This was first determined for polar organic liquids more than 80 years ago, but for the case of water, the most common polar liquid, direct measurement of the viscoelectric effect is challenging and has not to date been carried out, despite its importance in a wide range of electrokinetic and flow effects. In consequence, estimates of its magnitude for water have been indirect and vary by more than a thousand-fold. Here we measure the viscoelectric effect in water directly for the first time using a surface force balance (SFB), by measuring the dynamic approach of two molecularly-smooth surfaces with a controlled, uniform transverse electric field between them across highly-purified water. A related study concerns the interaction between lipid-bilayer-coated surfaces across water in the SFB, when a high transverse electric field causes a massive (up to 3 orders of magnitude), reversible change in the frictional dissipation between them as they slide past each other. All-atom molecular dynamics simulations reveal the surprising origin of this.

\*I thank my co-workers Yu Zhang, Nir Kampf, Yongyun Hwang and particularly Di Jin for carrying out these studies

### **Keywords:**

Nano-confined water, viscoelectric effect, hydration lubrication, lipid-bilayer lubrication

## 교육과정 속 전자기 영역의 내용 및 체계 구성에서 고려할 문제들

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### Abstract:

본 발표는 교육과정 개정을 맞이하여, 물리학의 영역 중 전자기 관련 영역에 대한 교육과정 내용 및 체계 구성을 적절성을 검토하고자 한다. 이를 위해 다음과 같은 중심 질문을 선정하여 전자기 영역의 내용 및 체계 구성을 검토하였다. 1) 전자기 영역의 핵심 개념기반 내용 재구성을 위한 고려사항은 무엇인가? 2) 전자기는 역학과 왜, 어떻게 연계되어야 하는가? 3) 미시적인 수준에서의 전자기 효과를 어떻게 다루어야 하는가? 4) 전기, 전자 회로를 어떤 수준에서 어떻게 다루어야 하는가? 이러한 질문들을 바탕으로, 교육과정에서 나타나는 장 개념과 관련된 부적절한 표현 문제, 역선 개념의 삭제, 현 교육과정 속 로렌츠 힘 개념 부재, 물성과 물질을 전자기 영역에서 다루는 문제, 전기 회로, 여러 학년에 걸쳐 큰 변화 없이 반복되는 실험주제와 관련된 문제 등이 논의될 것이다.

### Keywords:

물리교육, 전자기, 교육과정

## 2022 개정 과학과(물리) 교육과정 개발 현황과 쟁점: '힘과 운동' 영역을 중심으로

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### Abstract:

현재 2022 개정 교육과정 시안이 개발되고 있다. 이 발표에서는 현재 개발 중에 있는 2022 개정 과학과 교육과정 중 '힘과 운동' 영역의 개발 현황과 쟁점을 소개하고 이와 관련한 의견 청취 및 논의를 하고자 한다. 현재 '힘과 운동' 영역은 초등학교 '힘과 우리 생활' 단원에서 밀기와 당기기, 무게, 수평잡기, 도구의 이용을, '물체의 운동' 단원에서 위치변화, 속력, 속력과 안전을 다루도록 개발하고 있으며, 중학교 '힘의 작용' 단원에서 힘의 개념 및 여러 가지 힘, 힘의 작용을, '운동과 에너지' 단원에서 등속 운동, 자유 낙하 운동, 일과 에너지, 중력에 의한 위치 에너지, 운동 에너지, 역학적 에너지 보존을 다루도록 개발하고 있다. 이 과정에서 기존의 물체의 무게 단원을 3~4학년군의 첫 단원으로 제시하면서 무게 측정에서 힘에 의한 현상 경험에 좀 더 초점을 두는 변화 등 기존 교육과정에 대한 수정 보완을 시도하고 있다. 아울러 초중고 내용 체계의 연계성 확보 문제, 중복성과 나선형 교육과정 사이의 균형 등 몇몇 쟁점 사항이 논의되고 있다. 끝으로 현재 개발 현황과 쟁점에 관한 여러 의견을 청취하고 논의하고자 한다.

## Real-time volumetric adaptive optical microscopy using compressed time-reversal matrix

YOON Seokchan \*<sup>1</sup>, LEE Hojun <sup>2,3</sup>, HONG Jin-Hee <sup>2,3</sup>, CHOI Wonshik <sup>2,3</sup>

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### Abstract:

Reflection-matrix microscopy provides non-invasive, aberration-free subcellular-resolution optical imaging. It combines the powers of both hardware and computational adaptive optics. It emerges as an appropriate candidate for label-free non-invasive high-resolution optical imaging deep inside biological tissues, which outperforms most conventional adaptive optical microscopes. However, the drawback of the existing reflection matrix microscopy is that measuring the entire reflection matrix is quite time-consuming and vulnerable to external perturbations because a large number of interferometric images needs to be measured for all accessible input illumination fields. It led to practical limitations in its application to biodynamic studies on living samples. In this presentation, we propose a high-throughput volumetric adaptive optical imaging technique which dramatically reduces matrix acquisition time by nearly 100 times. The compressed time-reversal matrix imaging allows for almost real-time aberration-free volumetric imaging over a wide depth range in highly aberrated samples. The new microscope's capabilities were demonstrated by 3D imaging of myelin nerve fibers in a mouse brain over a  $128 \times 128 \times 125 \mu\text{m}^3$  field-of-view with a lateral resolution of  $0.45 \mu\text{m}$  and an axial resolution of  $2 \mu\text{m}$  within the data acquisition time of 3.58 seconds.

### Keywords:

volumetric adaptive optics, optical coherence microscopy, reflection matrix microscopy, deep tissue imaging, digital holography

## Dimensionality reduction adaptive-optical microscopy for in vivo through-skull imaging at visible wavelength

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### Abstract:

Compensation of sample-induced aberrations is crucial for diffraction-limited optical imaging deep within biological tissues. However, strong multiple scattering noise poses a fundamental limitation for identifying and correcting the tissue-induced optical aberrations. Here, we introduce a label-free deep-tissue imaging technique termed dimensionality reduction adaptive-optical microscopy (DReAM) to selectively attenuate multiple scattering noise. We established a theoretical framework in which dimensionality reduction of a time-gated reflection matrix can retain a single scattering signal with a strong wave correlation and attenuate uncorrelated multiple scattering noise, irrespective of sample-induced aberrations. Based on this, we enhanced the single scattering signal to multiple scattering noise ratio (SMR) with minimal impairment to a single scattering signal. This led to the substantial enhancement of the fidelity of aberration correction such that structures initially invisible turned out visible. We performed a mouse brain imaging *in vivo* through the intact skull with the probe beam at the visible wavelength. Image contrast and resolution are higher in the visible wavelength, however, scattering and aberration are much more severe than the previous near-infrared wavelength excitation. In spite of the strong scattering and aberration at the visible wavelength, nevertheless, DREAM offered a 17-fold enhancement of SMR and visualized the neural fibers in the brain cortex under the skull with the diffraction-limited spatial resolution of 412 nm and a 33-fold enhancement of Strehl ratio.

### Keywords:

Adaptive optics, bioimaging

## 고출력 펄스 티타늄사파이어 오실레이터 개발 및 바이오 이미징 응용

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### Abstract:

1991년 티타늄사파이어(Ti:Al<sub>2</sub>O<sub>3</sub>) 펄스 레이저 등장 이후, 해당 펄스 레이저는 30여년동안 이득매질로서, 과학, 산업, 의료분야등에 많이 활용되고 있다. 또한 티타늄사파이어 매질은 넓은 이득 밴드폭을 가지고 있기 때문에 짧은 펄스폭을 생성시키기 유리하여 특히 바이오 이미징, 라만등의 바이의료분야에 필수 광원으로 자리 잡았다. 본 발표에서는 고출력 티타늄 사파이어 오실레이터 제작 방법과 그의 바이오 이미징 활용에 대해서 소개하고자 한다.

### Keywords:

펄스 레이저 , 바이오 이미징

## 투명 다층 센서를 이용한 3차원 위치, 각도 정보 측정

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### Abstract:

3차원 물체는 다양한 방법으로 정의할 수 있지만, 크게 위치 정보 (깊이)와 각도 정보로 정의할 수 있다. 하지만 현재 사용되는 대부분의 3D 카메라들은 대부분 위치 정보를 알아내는 것에 국한되어 있으며, 각도 정보는 2D 이미지 등을 이용하여 유추하는 방식을 사용한다.

본 연구는 다층의 투명 센서 혹은 stack 형태의 다초점 데이터를 이용하여 단일 위치에서 3차원 정보를 획득하는 구조로, 기존 3D 카메라, 스캐너와 달리 연속적인 3차원 각도 정보를 얻어낸다. 기존 3D 카메라 대비 넓은 부피, 각도의 광학 정보를 측정할 수 있을 것으로 보이며, 기존 2D 시스템에 물리적인 추가 요소 없이 데이터 분석을 통하여 3차원 정보를 획득할 수 있는 단초를 제공할 수 있을 것으로 보인다.

### Keywords:

3D sensor, light field, deconvolution, defocus imaging

## High-throughput screening of semiconductor materials for photovoltaic applications

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### Abstract:

First-principles density functional theory (DFT) has been regarded as one of the most popular methods to investigate the physical properties of semiconductors. High-throughput calculations become doable due to the rapid development of computers, and several big databases of the DFT calculations are freely available as a result. However, these databases have some limitations in that the electronic structure is inaccurate, such as the band gap underestimation. More advanced calculation methods such as hybrid DFT are needed to correctly reproduce the experimental band gap, but those methods are typically not suitable for high-throughput calculations due to high computation costs. In this presentation, we discuss how to make hybrid DFT calculations cost-effective and therefore become suitable for high-throughput calculations. Key ideas are the introduction of different k-point meshes for the exact exchange and the other parts of the hybrid functional, and non-self-consistency in obtaining the eigenvalues. Using these methods, the physical properties such as the electronic band gap can be calculated tens of times faster than the conventional hybrid DFT calculation without losing much accuracy. The band gap of about 300 halide perovskite materials was obtained using the proposed method, and two materials were successfully synthesized through experimental collaboration. The former approach can also be utilized to obtain the electronic structure of material more accurately.

### Keywords:

Semiconductor, High-throughput, Hybrid density functional theory, photovoltaic

# Machine-Learning-Guided Prediction models and Materials discovery for high T<sub>c</sub> cuprates

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## Abstract:

Cuprates have been at the center of long debate regarding their superconducting mechanism; therefore, predicting the critical temperatures of cuprates remains elusive. On the other hand, the data-driven machine learning (ML) technique has been developed to predict the properties of materials without demanding a pre-known exact mechanism. Herein, using machine learning and first-principles calculations, we predict the maximum superconducting transition temperature (T<sub>c,max</sub>) of hole-doped cuprates and suggest the functional form for T<sub>c,max</sub> with the root-mean-square-error of 3.705 K and R<sup>2</sup> of 0.969. We have found that the Bader charge of apical oxygen, the bond strength between apical atoms, and the number of superconducting layers are essential to estimate T<sub>c,max</sub>. Furthermore, we predict the T<sub>c,max</sub> of hypothetical cuprates generated by replacing apical cations with other elements. Among the hypothetical structures, the cuprates with Ga show the highest predicted T<sub>c,max</sub> values, which are 71, 117, and 131 K for one, two, and three CuO<sub>2</sub> layers, respectively. These findings suggest that machine learning could guide the design of new high-T<sub>c</sub> superconductors in the future.

## Keywords:

machine learning, superconductor

## Hydrogen Evolution Reaction based on 2D MoS<sub>2</sub> Catalysts

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### Abstract:

Monolayered, semiconducting transition metal dichalcogenides (TMDCs) have attracted significant attention in the field of nanoelectronics, optoelectronics as well as energy conversion and storage systems, due to their outstanding electrical, optical, and mechanical properties. Recently, TMDC monolayers have been considered to be a promising candidate for catalyzing electrochemical hydrogen production from water due to its relatively low cost, its elemental abundance in earth, high catalytic activity, and good electrochemical stability. In this presentation, I introduce recent advances made toward understanding the catalytic behavior of single crystal 2D MoS<sub>2</sub> by fabricating on-chip electrochemical devices. Especially, I will focus on the role of electronic energy levels in hydrogen evolution reaction of 2D MoS<sub>2</sub>. These findings present an important pathway toward designing catalysts based on 2D TMDC monolayers.

### Keywords:

2D materials, energy, hydrogen

## 저차원 나노계면소재를 활용한 고성능 에너지 저장 소자

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### Abstract:

그래핀 및 전이금속 칼코겐물질과 같은 저차원 나노물질은 원자 두께의 제어를 통하여 다양하고 우수한 화학적, 물리적, 기계적 특성을 유발하여 새로운 종류의 계면물질로서 에너지 소자 (리튬이온배터리, 슈퍼커패시터, 수소/산소 생산 촉매 등)에 활용이 가능하다고 알려져 있다. 2차원 나노물질 또는 나노 소재는 두께가 하나 또는 몇 개의 원자 층일 때 나노 구조를 한 형태이며 두께와 크기에 따라서 다양한 도체~부도체 성질이 극대화 되어 에너지 저장 소재로 활용 시 에너지 저장 성능에서 중요한 이온의 흡착도, 윤달 (intercalation) 및 부피 변화에 대한 안정성 등을 제공하여 고 에너지 저장 성능 확보에 도움이 된다. 현재 에너지 저장 소자에 가장 중요한 요소로는 높은 충방전 안정성이 있으며 이는 저차원 나노계면소재를 활용함으로써 고 안정성 확보가 가능하다고 판단된다. 본 발표에서는 다양한 소재의 실용적 저차원 합성법에 대한 고찰과 그래핀, 황화구리, 육각형 질화붕소 등과 같은 저차원 소재를 활용하여 에너지 저장 소자의 전극, 계면 코팅소재 및 분리막 등으로 활용을 하였으며 다음의 소재를 바탕으로 고안정성의 에너지 저장소자 구동이 가능함을 확인하였다. 현재는 Li plating을 비롯하여 10C 이상의 고속충방전의 가능성 여부와 계면소재 활용 및 분석이 필수로 여겨지고 있어 전극 및 계면소재 표면을 in-situ 광학 분석을 통하여 분석 가능하다고 판단된다.

### Keywords:

Li ion battery, Supercapacitor, BN separator, Electrochemistry

## Toward Quantum Force Standard Traceable to Redefined SI

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### **Abstract:**

Redefinition of the international system of units (SI), in effect since 2019, enables the realization of a kilogram from Planck constant, without the need of the international prototype of kilogram whose mass had defined the kilogram for the last 150 years. The historical event also opened up new ways to developing small mechanical quantity standards with radical improvement in precision by directly linking the mechanical quantities to electrical measurands. In this talk, the speaker will present the status and prospect of small mass and force standard candidates traceable to the SI under development in KRISS: a micro-Kibble balance, a radiation-pressure force standard, and a fluxoid-quantum-controlled force standard, covering force range from micronewton to femtonewton. A possible seamless standard system in small force range and future works till its establishment will be also discussed.

### **Keywords:**

SI redefinition, mass standard, small force standard, quantum force standard, micro-Kibble balance

# **$10^{-18}$ Accuracy Optical Clocks: Future Time Standard and Applications**

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## **Abstract:**

The atomic clock has realized the definition of "the SI second-the unit of time" since 1967 and has been utilized in various scientific and technological fields due to its high accuracy. The accuracy of the optical atomic clocks already surpassed the microwave atomic clocks by two orders of magnitude and the SI second will be redefined in the near future. In this talk, we present recent results in Yb optical lattice clock developments at KRISS and introduce current and future applications.

## **Keywords:**

Optical atomic clocks, SI second, International Atomic Time, Ytterbium, Fundamental constant

## Synchrotron X-ray projection imaging and computed tomography at the Pohang Light Source-II

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### Abstract:

Synchrotron X-ray projection imaging implements conventional X-ray imaging techniques using synchrotron radiation. Thanks to the natural collimation, synchrotron X-ray illumination is bright and highly coherent for phase contrast X-ray microscopy. Adopting computed tomography, this extends to three-dimensional microscopy. The illumination is either monochromatized to improve imaging sensitivity or used in whitebeam for high speed imaging.

The Pohang Light Source-II hosts two beamlines for monochromatic and whitebeam X-ray imaging, respectively. The former, Beamline 6C, is tuned to a photon energy between 10 keV and 50 keV for imaging a variety of samples from biology and material sciences. The latter, Beamline 9D, specializes in in-situ observation of high speed phenomena.

### Keywords:

Synchrotron, X-ray, Microscopy, Computed tomography

## Ultrafast X-ray science at PAL-XFEL

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### **Abstract:**

X-ray free electron laser (XFEL) generates ultrashort, extremely bright, and nearly full-coherent X-ray pulses, thus opening new scientific opportunities in physics, material science, chemistry, biology, and various fields. Ultrafast X-ray science is the most studied topic at XFEL.

Pohang Accelerator Laboratory X-ray Free Electron Laser (PAL-XFEL), one of five operating X-ray free electron laser facilities in the world, is open for user operation since 2017. PAL-XFEL has conducted outstanding science projects using spectroscopy, scattering, and imaging techniques in both hard and soft X-ray energy region. At PAL-XFEL, people from various backgrounds, for example X-ray science, laser science, mechanical/electronic engineering, and data/computation, are working together. In this talk, I will briefly introduce the concept of XFEL, and then show how scientists and engineers in PAL-XFEL give their efforts to achieve high-level scientific environments. Finally, several remarkable results in ultrafast X-ray science will be presented.

### **Keywords:**

Ultrafast, X-ray Free Electron Laser, PAL-XFEL, Pohang Accelerator Laboratory

## Neuroscience questions with physics reasoning

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### Abstract:

물리학은 자연계의 물질, 물질의 구성요소, 시공간에서의 물질의 운동과 이를 유발하는 에너지와 힘에 관련된 실체를 연구하는 자연 과학입니다. 이 연구를 하는 인간의 뇌 역시 물질적 구성요소가 있으며, 이 구성요소 간의 상호작용에 따라 인간의 의식과 행동을 만들어냅니다. 뇌과학의 주요 목표는 인간이 어떻게 생각하고 행동하는지를 뇌에서 관측과 교란을 통해 이해하고자 합니다. 뇌도 자연계 중 하나이므로 뇌 역시 물리학자의 연구 대상이라 생각합니다. 다만 우리가 과학적으로 검증할 수 있는 인지와 행동만을 대상으로 한다는 전제하에서입니다. 저는 본 강연에서 21세기 뇌과학에서 가지고 있는 근원적 화두를 여러분들과 공유하고자 합니다. 어떻게 뇌는 그리 빠른지? 도대체 생각의 기본 단위와 구조는 무엇인지? 어떻게 그 복잡한 구성요소 간의 정보교류가 시기적절하고 일관될 수 있는지? 도대체 의식은 무엇이고 무의식은 무엇인지? 이러한 화두를 말씀드리며, 저희 연구실의 장기 목표인 로컬 네트워크의 동역학적 속성이 어떻게 정보 전달 루트를 결정하고 정보를 받는 로컬 네트워크의 동역학적 속성을 변환시켜, 인지와 행동을 유도하는지를 이해하고자 하는 연구를 소개하도록 하겠습니다.

## Algebraic approach to quarkyoniclike configuration and stable diquarks in dense matter

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### Abstract:

We study the color-spin interaction energy of a quark, a diquark and a baryon with their surrounding baryons and/or quark matter.

This is accomplished by classifying all possible flavor and spin states of the resulting multiquark configuration in both the flavor SU(2) and SU(3) symmetric cases. We find that while the baryon has the lowest interaction energy when there is only a single surrounding baryon, the quark has the lowest interaction energy when the surrounding has more than three baryons or becomes a quark gas. As the short range nucleon-nucleon interactions are dominated by the color-spin interactions, our finding suggests that the baryon modes near other baryons are suppressed due to larger repulsive energy compared to that of a quark and thus provides a quark model basis for the quarkyoniclike phase in dense matter. At the same time, when the internal interactions are taken into account, and the matter density is high so that the color-spin interaction becomes the dominant interaction, the diquark becomes the lowest energy configuration and will thus appear in both the dense baryonic and/or quark matter.

### Keywords:

diquark, quarkyoniclike, color-spin interaction

## The mass-radius relations of neutron stars in an pion mean-field approach

KIM Hyun-Chul \*<sup>1</sup>, YANG Ghil-Seok <sup>2</sup>, YAKHSHIEV Ulugbek <sup>1</sup>, GHIM Nam-Yong<sup>1</sup>

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### Abstract:

We investigate the masses and radii of neutron stars within the framework of the in-medium modified chiral soliton model, considering the effects of surrounding baryonic environment on the properties of in-medium baryons. The equation of state describing an infinite and asymmetric nuclear matter are obtained by introducing the density-dependent functions. To extrapolate the high density and highly isospin asymmetric region, we study the masses and radii of neutron stars. The results predict the masses and radii to be  $1.4M_{\odot}$  and  $2M_{\odot}$  respectively. We discuss the physical meaning of the equation of state obtained from the chiral solitonic approach, based on the present results.

### Keywords:

neutron star, pion mean-field approach

## Single transverse spin asymmetry of neutral pion production in the very forward direction

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### Abstract:

We present recent results for the large single transverse spin asymmetries of the pion production in the very forward direction with low  $PT$ . The differential cross section of the  $p + p^\uparrow \rightarrow \pi^0 + X$  can be expressed in terms of hybridized Regge amplitude and inclusive proton-baryon processes  $A_{pB \rightarrow X}$ . The interference of  $p$  and  $\Delta(1700)$  explains very well the experimental data on  $A_N$ . In addition, the inclusive part of the differential cross section can be approximated as a triple-Regge diagram with pion exchange. Our numerical results describe remarkably the RHICf data with both  $x_F$  and  $PT$  dependences considered. The present study indicates that in the low  $PT$  region  $A_N$  is of diffractive nature.

### Keywords:

Diffractive process, Spin asymmetry, Regge phenomenology, Triple-Regge exchange

## $\Lambda_c \rightarrow p K_s \pi^0$ decays at Belle

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### Abstract:

We analyzed  $\Lambda_c \rightarrow p K_s \pi^0$  decays to measure the relative branching ratio of  $\Gamma(\Lambda_c \rightarrow p K_s \pi^0)/\Gamma(\Lambda_c \rightarrow p K^- \pi^+)$  and sub-branching ratios using 980.6 fb<sup>-1</sup> datasets collected in the Belle detector at KEK. This study will test the isospin symmetry in the  $\Lambda_c \rightarrow p K \pi$  decays in a combined analysis with the  $\Lambda_c \rightarrow p K \pi^+$  decay. We will report preliminary results on the branching ratio measurement and sub-channel analysis.

### Keywords:

Belle,  $\Lambda_c$ , Branching ratio

## Current Status of the H-Dibaryon Search with J-PARC E42

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### Abstract:

J-PARC E42 is a dedicated experiment to search for an H-dibaryon using  $^{12}\text{C}(K^-,K^+)$  reactions near  $\Lambda\Lambda$  and  $\Xi^-p$  threshold. The E42 has completed physics runs in 2021. We collected approximately 300k  $(K^-,K^+)$  reaction events in the ranges of  $\theta_{K^+} < 25^\circ$  and  $p_{K^+} > 0.5$  GeV/c. E42 data includes all charged particles from subsequent decays in  $^{12}\text{C}(K^-,K^+)$  reactions. We will report the run summary, current analysis effort, and other physics opportunities with E42 datasets.

### Keywords:

H-dibaryon, J-PARC,  $(K^-,K^+)$  reaction

## Production of $P_c(4312)$ state in electron-proton collisions

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### Abstract:

We compute electro-production of  $P_c(4312)$  in  $e^- + p^+ \rightarrow e^- + P_c$  using Vector Dominance Model

assuming four possible spin parity of  $P_c(4312)$ ,  $J^P = (\frac{1}{2})^\pm, (\frac{3}{2})^\pm$ . Electron Ion Collider which is to be built at Brookhaven National Laboratory, we can collide not only unpolarized beam of electron and proton, but also polarized beam so we can investigate more deeply about the angular distribution of  $P_c(4312)$ . Using high integrated luminosity of Electron Ion Collider, we can predict the yield of  $P_c(4312)$  for each spin-parity. We plot differential scattering cross-section as a function of pseudorapidity of  $P_c(4312)$  in the Lab frame and transverse momentum for polarization set of electron and proton to discriminate spin of  $P_c(4312)$ . To specify parity, we study the effect of transverse and longitudinal polarization of  $J/\psi$  on decay angle in  $P_c \rightarrow p^+ + J/\psi \rightarrow p^+ + e^- + e^+$  channel.

### Keywords:

Vector Meson Dominance, Polarization, Pseudorapidity, Transverse momentum

## Interfacial water: Atomic-scale imaging of solid-water interfaces

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### Abstract:

Solid-water interfaces have a prominent role in a variety of fields such as surface science, geochemistry, electrochemistry, energy storage or molecular and cell biology. Liquids near a solid surface form an interfacial layer where the molecular structure is different from that of the bulk. Yet the molecular-scale understanding of the interactions of liquid water with solid interfaces is unsatisfactory for the lack of high-spatial resolution methods. Here I will present an AFM-based method that provides atomic-scale resolution images of solid-liquid interfaces. Those images provide a new understanding on how water interacts with *real* hydrophobic and hydrophilic surfaces.

The presentation is divided in three sections. The first section is an introduction to the relevance of solid-liquid interfaces. The second section, presents the features and capabilities of 3D-AFM [1-3] to image with atomic resolution the three-dimensional interfacial structure of surfaces immersed in aqueous solutions. The third section reports the structure of interfacial water layers on different 2D materials from graphene to a few layer MoS<sub>2</sub>; from hexagonal boron nitride to a few layer WSe<sub>2</sub>. Those interfaces are characterized by the existence of a 2 nm thick region above the solid surface where the liquid density oscillates [4-6]. The distances between adjacent layers for graphene, few-layer MoS<sub>2</sub>, h-BN and pentacene are ~0.50 nm. This value is larger than the one predicted and measured for water density oscillations (~0.30 nm). The experiments demonstrate that on extended hydrophobic surfaces water molecules are expelled from the vicinity of the surface and replaced by several molecular-size hydrophobic layers.

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### Keywords:

interfacial water, solid-liquid interfaces, AFM, 2D materials

## Residual stresses and shear-induced overaging in boehmite gels

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### Abstract:

Colloidal gels respond like soft solids at rest, whereas they flow like liquids under external shear. Starting from a fluidized state under an applied shear rate  $\dot{\gamma}p$ , abrupt flow cessation triggers a liquid-to-solid transition during which the stress relaxes towards a so-called residual stress  $\sigma_{\text{res}}$  that tallies a macroscopic signature of previous shear history. Here, we report on the liquid-to-solid transition in gels of boehmite, an aluminum oxide widely used in industries to design catalyst supports, that shows a remarkable non-monotonic stress relaxation towards a residual stress  $\sigma_{\text{res}}(\dot{\gamma}p)$  characterized by a dual behavior relative to a critical value  $\dot{\gamma}c$  of the shear rate  $\dot{\gamma}p$ . Following shear at  $\dot{\gamma}p > \dot{\gamma}c$ , the gel obtained upon flow cessation is insensitive to shear history, and the residual stress is negligible. However, for  $\dot{\gamma}p < \dot{\gamma}c$ , the gel encodes some memory of the shear history, and  $\sigma_{\text{res}}$  increases for decreasing shear rate, directly contributing to reinforcing the gel viscoelastic properties. Moreover, we show that both  $\sigma_{\text{res}}$  and the gel viscoelastic properties increase logarithmically with the strain accumulated during the shear period preceding flow cessation. Such a shear-induced "overaging" phenomenon bears great potential for tuning the rheological properties of colloidal gels.

### Keywords:

colloidal gels, overaging, residual stress, memory

## Viscoelastic polymer flows in 3D porous media

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### Abstract:

Many energy, environmental, industrial, and microfluidic processes rely on the viscous flow of polymer solutions through porous media. In many cases, the macroscopic flow resistance abruptly increases above a threshold flow rate in a porous medium—but not in bulk solution. The reason why has been a puzzle for over half a century. Here, by directly visualizing the flow in a transparent three-dimensional (3D) porous medium, we demonstrate that this anomalous increase is due to the onset of an elastic instability in which the flow exhibits strong spatio-temporal fluctuations reminiscent of inertial turbulence, despite the vanishingly small Reynolds number. We find that the transition to unstable flow in each pore is continuous, arising due to the increased persistence of discrete bursts of instability above an onset flow rate; however, this onset value varies from pore to pore. Thus, unstable flow is spatially heterogeneous across the different pores of the medium, with unstable and laminar regions coexisting. Guided by these findings, we quantitatively establish that the energy dissipated by unstable pore-scale fluctuations generates the anomalous increase in flow resistance through the entire medium. Thus, by linking the onset of unstable flow at the pore scale to transport at the macroscale, our work yields generally-applicable guidelines for predicting and controlling polymer solution flows.

### Keywords:

viscoelasticity, rheology, flow instabilities, turbulence, disordered media

## Micro-viscometry of soft matter for clinical applications

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### Abstract:

The viscometry of minute amounts of liquid has been in high demand as a novel tool for biomedical diagnosis and engineering. While various microrheological techniques have shown the capability to deal with small volume of fluids, increasingly dominant interfacial effects of minute volume liquids complicate the measurement and analysis. Here, we present an atomic force microscope-based micro-viscometer that determines the viscosity of single sessile drops at the micro and sub-microliter scale. We circumvent the interfacial effects by measuring the negative-valued shear elasticity, originating from the retarded fluidic response inside the drop. For clinical applications, we implement the micro-viscometry to formulate the sperm sorting media, which enables the selection of high-quality sperm in conjunction with microfluidic techniques. Our results offer a quantitative methodology for viscosity measurements of extremely minute volumes of liquids, which could be generally applicable to viscometry of biomedical fluids.

\*I thank my co-workers J. K. Choi, J. H. Lee, W. Jhe, and D. Kim for carrying out these studies.

### Keywords:

atomic force microscopy, viscosity, soft matter, sperm sorting, male infertility

## Electrostatic potential of a uniformly charged triangle in barycentric coordinates

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### Abstract:

We compute the electrostatic potential of a uniformly charged triangle. Barycentric coordinates are employed to express the field point, the parametrization of the surface integral, and the gradient operator. The resultant analytic expression for the electrostatic potential is expressed in terms of the side lengths of the triangle, the altitude of the field point from the plane in which the triangle is placed, and the barycentric coordinates of the field point relative to the triangle. Our results are in good agreement with available numerical results. The asymptotic behavior of the analytic expression is investigated in special limits that satisfy known values. The resultant analytic expressions for the asymptotic regions are useful in improving the numerical convergence at boundaries. As an application, we provide a strategy to compute the electrostatic potential of a uniformly charged polygon. The electrostatic potential of a uniformly charged rectangle is considered as a simple example that agrees with a previous result. Appendices provide a complete set of integral tables that are necessary to evaluate the double integral over the barycentric coordinates, an explicit parametrization of the gradient operator in the barycentric coordinates, and useful coordinate-transformation rules between the barycentric and Cartesian coordinates.

### Keywords:

Electrostatics, Barycentric coordinate system, Polygon

## Interplay between Physics and Mathematics in Physics Education

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### Abstract:

The researches related to the interplay between physics and mathematics were reviewed, and the topic on the algebraic expressions in physics education, perspectives on the interplay between physics and mathematics, and students' and teachers' comprehension of mathematization were discussed. For this, the three perspectives of the interplay between physics and mathematics are discussed: the perspective of modeling, blending, and epistemological beliefs. The perspective of modeling for mathematization reveals the complexity of the physical-mathematical modeling in detail. The perspective of blending could be useful to analyze the dynamic process related to conceptual reasoning concerning the blending of two domains. The perspective of epistemological beliefs seems to be a crucial factor to predict students' performance on problem-solving. Thus, in the curriculum revision concerning the mathematization, teachers should consider the issue of students' epistemological beliefs critically. Students' understanding, difficulty, or view of the issue clearly shows that an explicit approach for the issue, especially their epistemological beliefs, is essential to improve their competency. Teacher preparation program should enhance their understanding of the issue, and encourage their change in classroom action. Considering the complexity of the mathematization and related educational issues, even though the development of an effective teacher preparation program could be an extremely challenging task, the next step would be to develop effective materials and programs for that.

### Keywords:

Mathematization, Interplay between physics and mathematics, Verbalization of physics knowledge

## 새물리 논문 결론부 서술의 특징 분석

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### Abstract:

학술 논문 작성 과정에서 결론부는 작성하기 어려운 부분으로 알려져 있다. 결론부에서는 사실에 근거한 결과 요약, 결과에 의미를 부여하는 의견이 함께 제시되기 때문에 객관성을 중시하는 연구 방법 및 결과 진술과는 다른 특징을 지닌다. 결론부 작성 과정에서 연구자에게 자율성을 부여하는 까닭에 오히려 더 작성하기가 난해하다는 견해도 있다. 이러한 이유들로 인해, 논문 작성법에 대한 전문 서적에서 결론부를 별도로 다루기도 한다. 또 논문 작성과 관련한 장르 분석 연구에서는 여러 형태의 결론부 모형을 제안하고 있다. 일반적으로 학문 분야에 따라 결론부의 구성 요소나 서술 방식이 다르다. 그런데 물리교육 연구에서는 자연과학과 사회과학의 특성이 복합적으로 발현되는 경향이 있기에, 결론부를 작성하는 연구자에게 부담이 가중될 수 있다. 이 연구에서는 새물리 게재 논문의 결론부를 분석하여 특징을 파악하고, 논문 작성을 위한 시사점을 도출하고자 한다. 연구 결과는 초보 연구자가 논문의 결론부를 작성할 때나 지도교수가 논문 작성을 안내할 때 활용될 수 있을 것이다.

### Keywords:

새물리, 논문 작성, 결론부, 장르분석

## Polymer based triboelectric nanogenerator and tactile sensor

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### Abstract:

Beyond the rigid or flexible frame-based electronics, the development of stretchable electronics for implementing wearable/attachable electronics or electronic/ionic skin, consisting of transistor, luminescence devices, smart sensors, and energy devices received great attention. It is required to be thin, light, stretchable, and transparent to be integrated with clothes/wears or attached on or implanted into curved human body. The triboelectric nanogenerators (TENG) convert mechanical energy into electrical energy is receiving great attention as a sustainable power source for portable/stretchable electronics because of its simple structure, many materials options, low cost/easy fabrication, and superior power output performance. In this presentation, we introduce polymer based stretchable, transparent, and high performance TENG that can harvest biomechanical energy and tactile sensing. We have fabricated ionic/nonionic polymer gel based dielectric layers and investigated its dielectric property, electrical conductivity, and triboelectric property. The fabricated polymer gel has improved its transparency and stretchability. Beside it exhibited an extremely improved dielectric constant and very strong triboelectric behavior that can contribute to enhanced TENG performance. In addition, we introduce a new type of tactile sensor based on charge displacement current that can sense position and pressure without electrode grid patterning.

### Keywords:

Triboelectric nanogenerator, dielectric, energy harvesting

# Sustainable energy generation based on triboelectric effect & dielectric polarization

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## Abstract:

As the energy crisis and global warming are emerging as major issues, the development of renewable and green energy based on alternative energy resources such as solar, wind, hydrogen or geothermal sources, has attracted considerable interest. The energy harvesting technologies based on these natural resources have been well established, and their use has gradually increased. Yet there are still many forms of energy sources in our living environment, which are not being utilized. Furthermore, owing to increasing energy demands, significant energy-related issues remain to be solved. Thus, we need to continue the efforts to develop innovative energy harvesting technology to overcome energy issues. Here, we introduce two strategies for a sustainable energy harvesting method based on triboelectric effect and dielectric polarization, and detailed topics are as follows,

- Triboelectric nanogenerator based on engineering design for long lifespan & high-output
- Triboelectric nanogenerator utilizing water as a triboelectric materials & self-ionization
- Triboelectric nanogenerator utilizing lubricant to control air breakdown
- Energy loss return gate via dielectric polarization
- Electrical stimulation for cell vitalization via body-mediated energy loss conversion system

## Acknowledgements

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## Keywords:

Energy harvesting, triboelectric effect, energy-loss, dielectric polarization

## Design of triboelectric effect-based system for its effective utilization

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### Abstract:

액체를 포함한 서로 다른 두 물질의 접촉 및 분리에서 비롯된 정전 신호 발생은 자가 발전 센서뿐만 아니라 다양한 유형의 에너지 수확장치 개발을 위한 새로운 메커니즘으로 각광받고 있다. 재료 및 화학적인 접근 기반의 기존 대부분 연구와 달리, 정전 신호 생성에서 기구학적 설계 기반의 접근법을 소개하고자 한다. 일반적으로 동력을 전달할 때 활용되는 다양한 전동요소를 정전 신호 생성 원리에 적용함으로써 출력 성능을 크게 높일 수 있으며, 이러한 출력 증대를 통해 정전 신호 생성 메커니즘을 보다 실용적으로 활용할 수 있다. 대표적인 예시로, 생체역학적 에너지 수확이 소개되며, 기구학적 설계 기반의 시스템 구성을 통해 신호 생성에 있어 유리한 효과를 분석하고자 한다. 더 나아가, 다양한 기계 요소들의 정상 작동 중 발생하는 정전 신호를 활용하여 작동 상태를 인지할 수 있는 자가 발전 센서로서의 정전 신호 발생 메커니즘의 역할에 대해 발표한다. 본 연구에서 소개하는 정전 신호 발생 메커니즘 및 기구학적 설계 기반의 시스템 제작의 융합을 통해 새로운 응용 분야를 개척해낼 수 있을 것으로 기대된다.

### Keywords:

정전소자, 기계요소, 시스템, 기구학적 설계, 자가 발전 센서

## Interfacial Engineering of Tribo-materials for enhancing TENGs

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### Abstract:

The triboelectric nanogenerator (TENG) is one renewable technology that utilizes environmental mechanical energies originating in nature, machines, vehicles, and humans. Its principal operation is based on contact-electrification and electrostatic induction. The contact electrification is related to the formation of surface charges on the tribo-materials, and the electrostatic induction is the polarization of tribo-materials and electrodes due to the electric field generated by the surface charges. Therefore, material engineering is an important technique to control triboelectric performance. The material engineering in a TENG can be divided into multiple categories: development of novel tribo-materials, formation of electron-trapping layer(s) in tribo-materials, surface modification, and interface engineering. Interface engineering, that utilizes interfacial effects, has been attracting attention due to its notable effectiveness and compatibility with surface engineering. Interfacial ferroelectric materials reinforce the polarization and provide an improved polarization performance by a polling process. Furthermore, a technique that forms interfacial polarization and improves dielectric constant by utilizing dielectric bilayer to achieve the enhanced triboelectric performance. Due to the difference in impedance and capacitance of dielectrics, the space charges are accumulated at the interface between dielectrics. The accumulated space charges occur the interfacial polarization with the electric field. Therefore, the polarization performance can be improved and corresponding triboelectric performance can be enhanced. In this work, to enhance the performance of TENGs, interfacial layer designs were utilized and their effect on triboelectric performance was investigated. We confirmed that the triboelectric performance varied with the interfacial layers. Furthermore, we found that the enhancing mechanism was related to the dipole direction, high polarization, and electron blocking beneath negative tribo-materials during operation. Finally, various applications such as illuminated LEDs and a capacitor charging were shown to demonstrate those effects.

### Keywords:

Interfacial engineering, Tribo-materials, Triboelectric nanogenerators (TENGs), Electron Blocking, Self-assembled Monolayer (SAM)

## Individual atoms as clocks and bits

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### **Abstract:**

Atoms absorb electromagnetic radiation at precise discrete frequencies. Knowing this, a recipe for making an atomic clock is simple to state: we first need an oscillator to produce the radiation and a device that fixes the radiation frequency for maximum atomic absorption. We then simply count cycles of the oscillator; the duration of a certain number of cycles defines a unit of time, e.g., the second. Today, the most accurate clocks count cycles of radiation corresponding to optical wavelengths, around a million billion per second. At this level, many interesting effects, including those due to Einstein's relativity, must be accounted for.

Atoms can also be used to store bits information. For example, we can label the atom's lowest energy state a "0" and a state of higher energy a "1." However, quantum systems such as atoms can also exist in "superposition" states, thereby storing both states of the bit simultaneously, a situation that makes no sense in our ordinary-day experience. Superposition leads to an exponential increase in memory and processing capacity. It would enable a quantum computer to simulate the action of other important quantum systems in cases where such a simulation would be intractable on a conventional computer.

Experiments in which laser-beam-manipulated "trapped" atomic ions are used to realize atomic clocks and the elements of a quantum computer will be described.

## 양자컴퓨팅 기법 소개

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### Abstract:

입자물리학에서 실험데이터를 효율적으로 분석하기 위해, 그리고 현상론의 복잡한 모델을 처리하게 위해 인공지능을 포함한 다양한 고급 컴퓨팅 기법들이 활용되고 있다. 최근에는 연구자들이 양자컴퓨터를 사용할 수 있게 되면서 이를 활용한 다양한 연구활동들이 진행되고 있다. 본 강연에서는 양자컴퓨터의 기본 이론 및 실제 구현에 대한 강의들을 제공하여, 젊은 연구자들이 최신 양자컴퓨팅 기법을 연구에 적용할 수 있는 발판을 마련해주려 한다.

### Keywords:

양자 컴퓨팅, 양자 얽힘, 양자 알고리즘

## 양자컴퓨팅 기법 소개 (Introduction to Quantum Computing)

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### Abstract:

2016년부터 IBM사는 대중에게 클라우드 기반 양자 컴퓨팅 서비스를 제공하고 있다. 이 강좌에서 우리는 IBM 양자 컴퓨터를 사용하여 EPR 쌍과 GHZ 상태 같은 간단한 형태의 양자 상태들을 만들어 본다. 이를 통해, IBM Quantum Composer와 IBM Quantum Lab에 대한 전반적인 이해를 제공한다.

### Keywords:

IBM quantum computer, circuit implementation

## 초전도 양자소자의 활용

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### Abstract:

중첩, 얽힘 등의 양자현상을 활용할 수 있는 유용한 양자소자에 대한 연구가 활발히 진행되고 있다. 그중 거시적 양자현상을 보이는 초전도체를 이용한 초전도 양자소자가 있다. 본 튜토리얼 강의에서는 초전도 기반 양자소자 중 대표적인 조셉슨 접합의 예를 중심으로 초전도기반 양자컴퓨터 및 양자센서 활용에 대해 논의하고자 한다.

### Keywords:

조셉슨 접합, 초전도 양자소자

## 한 물리학자의 학교과학 탐구: 초중등 물리교과를 중심으로

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### Abstract:

물리학에서 이론은 알려진 자연현상을 설명하거나 새로운 현상을 예측하게 하는 기능을 가질 뿐만 아니라 이들이 일어나는 원인이나 이유를 설명하는 기능을 가진다. 물리교육의 실험수업에서 발생하는 불일치 현상들은 실험 결과가 관련 이론으로 설명하지 못하는 경우에 발생한다. 물리교육의 현장에서는 많은 불일치 현상들이 발생한다는 보고들이 있다. 물리교육의 특성상 실험수업은 새로운 물리 지식을 찾는 것이 아니라 이미 알려져 있는 물리 지식을 교수하고 학습하기 위하여 이루어진다. 이러한 까닭으로 물리교육에서 다루어지는 사실, 개념, 원리나 법칙 등은 확고한 물리 이론을 근거로 설명될 수 있어야 한다. 그러나 실험수업에서 발생하는 불일치 현상들을 해결할 수 있는 이론적인 근거는 거의 찾아보기가 어렵다. 즉 불일치 현상들을 해결할 수 있는 이론적인 배경지식을 충분히 제공하지 못하고 있다. 특히 불일치 현상들은 현장 교사들의 노력이나 현장 여건의 개선 등을 통하여 해결될 수 없는 특성을 지니고 있어 관련 분야의 전문가들의 노력이 필요하다. 이 발표는 불일치 현상들의 해결과 추상적인 물리 개념 학습을 위하여 지난 10여년 동안 노력해온 발표자의 결과 중 일부를 공유하고자 하는 것이다.

# Analysis of Defects in Semiconductors with Deep Level Transient Spectroscopy

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## Abstract:

Deep level transient spectroscopy (DLTS) is very useful method to identify the defect states in the semiconductor materials. The defect states in semiconductor heterostructures and quantum structures such as quantum wells and dots are originated from lattice defects, impurities, and interface states, etc. These defect states can degrade the characteristics of semiconductor devices such as transistors, optical detectors, solar cells, light emitting diodes, and so on. In this talk, I will introduce DLTS method and its application to analysis of the electrical properties as well as defect states in the semiconductor epi-layers and quantum structures. In the solar cell structures, especially, it showed that the interface traps and lattice defects reduce an external quantum efficiency by retrapping and recombination of the separated carriers. To optimize the electrical properties of optoelectrical devices, the origins and energy levels of defect states should be analyzed.

## Keywords:

Defect states, Semiconductors, DLTS

## Excitons in semiconductors: Light-matter interactions

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### Abstract:

본 튜토리얼 세션을 통해 다양한 차원의 반도체에서 나타나는 엑시톤 상태의 기본적인 물리적 성질에 대해 알아보려고 한다. 또한 반도체 기반 공진기 소자에서 공간적으로 구속된 빛과 엑시톤의 상호작용에 의해 나타나는 준입자 상태의 물리적 특성에 대해 알아보고, 이를 활용하는 응용 기술에 대한 최근 연구동향에 대해서도 살펴보려고 한다.

### Keywords:

Exciton, Semiconductor, Light-Matter Interaction

## Molecular switches regulating structures and interactions of protein nanotubes

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### Abstract:

Cells are working by well-designed molecular machines for a variety of tasks needed for life: to transfer genetic blueprint, to define cell shape, and to transport nutrients. Microtubules are among major components of eukaryotic cytoskeletons, involved in cell division, maintaining cell shape and intracellular trafficking. Tubulins are protein building blocks that are naturally preprogrammed to assemble into hollow cylinders of MTs. **Recently** we reported the re-programming of tubulin shape control by charge switch creating new supramolecular architectures, eg. single or double layered tubulin tubules (*Small* 2020). These tubulin-based nano architectures have been utilized as a delivery platform for anticancer drugs (*Adv. Mat.* 2020). This seminar deals with the bio-physical and -engineering aspects of tubulin as a molecular machine of life. **Additionally**, tau protein as charge switch regulating structural transitions of microtubules will be described (*Biophys J* 2009, *PNAS* 2014, *Nat Comm* 2016).

### Keywords:

Microtubules, Tau, Bio-physics and -engineering

# 포스터발표논문

Poster session abstract

## Controlling Nucleation and Growth Parameters of AgCN Microwires on Two-Dimensional Crystals

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### Abstract:

Mixed dimensional van der Waals (vdW) heterostructures based on two-dimensional (2D) crystals have gathered intense research interest owing to emerging new physical and electrical properties. The precise control at the heterointerface in vdW heterostructure is the key to fully utilize coherent interaction between components. Here, we investigate in detail the growth and assembly mechanisms of one-dimensional (1D) chained molecules on various 2D crystals. AgCN microwires, as model 1D chain system, are assembled on the surface of 2D crystals with various lattice parameters, surface elements, and different surface treatment conditions. We find that the surface treatment of 2D substrates dramatically change the nucleation density, length and width of AgCN microwires. The growth behavior of 1D chains is modeled using Monte Carlo simulation and growth parameters including nucleation and growth rates are identified. The demonstrated control of 1D wire assembly on 2D will be useful for controlling the electrical and optical properties of 1D/2D van der Waals heterostructures.

### Keywords:

Growth Control, Two-Dimensional Materials, 1D/2D Heterostructure, AgCN

## TEM dark field analysis on domain boundary structure in twisted 2-D materials

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### Abstract:

In designing two-dimensional (2-D) van der Waals (vdW) heterostructures, one can manipulate the stacking angle between the two layers to engineer moire superlattices. More importantly, atomic reconfiguration occurs at the interface between the two layers, forming an array of commensurate domains and domain boundaries with emergent functionalities. Here, we note that the reconstructed domain structures and the corresponding functionalities are determined by the crystal symmetry of 2-D building block crystals and the twist angle between them. For instance, monolayer transition metal dichalcogenides (TMD) exhibits 3-fold rotation symmetry, and thus the twisted bilayer TMD with the stacking angle of  $120 \times n$  deg and  $120 \times n + 60$  deg make differences in terms of the resulting domain topology and the atomic configuration at the domain boundaries.

In this work, we employ transmission electron microscopy (TEM) dark field (DF) imaging technique to investigate the domain topology and atomic configuration at the domain boundaries. Due to the extremely thin nature of 2-D system, TEM DF analysis on twisted bilayer TMD can be understood assuming only a single event of electron scattering, so called kinematical diffraction theory. We investigate the atomic configuration at the domain boundaries by comparing the DF image intensity with the structure factor calculation results. With the quantitative analysis on the DF images, we could identify the lattice distortion vector associated with each domain boundaries. Our approach to investigate the DF images in a quantitative manner provides a new pathway to understand the atomic structures of reconstructed domain and domain boundaries in 2-D vdW heterostructures.

### Keywords:

TMD, 2D vdW heterostructures, dislocations, dark field TEM, kinematical theory

## All Solution-Processed van der Waals Thin-Film Electronics with High Performance and Low-Power Operation

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### Abstract:

Solution-processable van der Waals (*vdW*) materials, which have an atomic layered crystal structure, are promising building blocks for large-scale, high-performance electronics owing to high material quality and stability in addition to low-temperature processability. In particular, *vdW*-assembled thin films of transition metal dichalcogenides (TMDCs) in solution have recently shown great potential for using a high-mobility channel. However, utterly solution-processed *vdW* electronics have not yet been reported due to the lack of appropriate dielectric materials and fabrication processes. Here we report all solution-processed *vdW* thin-film transistors (TFTs), consisting of the TMDCs as a channel and the perovskite oxides as a high-*k* gate dielectric. The colloidal inks of each constituent layer were prepared by chemical or electrochemical exfoliation, followed by the sequential assembly into the semiconductor/dielectric heterostructure for constructing TFTs, all of which were performed at low temperatures under 250 °C. The fabricated MoS<sub>2</sub> TFTs with the Dion-Jacobson-phase perovskite dielectric exhibited excellent device characteristics, including ON/OFF ratio >10<sup>4</sup>. In addition, the use of high-*k* dielectric permits the operating voltage as low as ~3 V, enabling low power consumption. Furthermore, TFTs could be fabricated on flexible substrates, showing reliable device performances. Our demonstration on the low-temperature fabrication of high-performance TFTs opens a new route for cost-effective, scalable electronics capable of hetero-integration.

### Keywords:

van der Waals heterostructures, perovskite oxide nanosheets, molybdenum disulfide, low-temperature fabrication

## Effect of temperature on the EEA in WS<sub>2</sub> monolayer

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### Abstract:

TMD has been extensively studied by many researchers for their electronic structures and optical properties. Indirect to direct bandgap transition at monolayer limit and large exciton binding energy make their application to nanophotonic devices promising. However, their light emitting capability is limited by strong many-body interactions such as exciton-exciton annihilation (EEA) through the Auger recombination process and it is essential to pin down the fundamental properties of this process for enhancing the quantum yield.

In this work, the influence of temperature on the EEA of monolayer WS<sub>2</sub> on a gold substrate is studied. Power-dependent photoluminescence measurement is conducted from 300K to 3K to extract the Auger coefficient at each temperature. The interactions between excitons in WS<sub>2</sub> monolayer are effectively suppressed by the gold substrate that a WS<sub>2</sub> monolayer gives out pure excitonic PL emission even in the lowest temperature. Precise measurement of auger coefficient is realized in this condition.

We believe that our results provide more profound understanding of the Auger processes in TMD monolayers and give a control over the Auger processes and hence, enhancing the quantum yield of the material.

### Keywords:

Exciton-exciton annihilation, TMD

## Graphene encapsulated in high k-dielectric as charge trapping layer for MoS<sub>2</sub>-based memory devices

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### Abstract:

High- $\kappa$  dielectric material such as Al<sub>2</sub>O<sub>3</sub> has been used as both tunnelling and control oxides in non-volatile memory (NVM) device due to its capability to achieve low equivalent oxide thickness and lower leakage current compared to the conventional SiO<sub>2</sub>. On the other hand, two-dimensional (2D) materials such as Graphene and Molybdenum Disulfide (MoS<sub>2</sub>) have been promising candidates for new generation of electronic devices due to their high carrier mobility. In this work, we fabricated memory device using multiple discrete graphene strips encapsulated in Al<sub>2</sub>O<sub>3</sub> as charge trapping component and bottom CVD-grown MoS<sub>2</sub> act as channel. By tuning the applied electric field, charges can tunnel from channel through the thin dielectric layer and trapped in the Graphene floating gate, results in memory window of ~5 V. Moreover, our device exhibit the ability to store charge individually to discrete isolated graphene strips, results in potential multibit design.

### Keywords:

Memory, Graphene, MoS<sub>2</sub>, Charge trapping, Floating gate

## Remote surface charge-transfer doping in MoS<sub>2</sub> field-effect transistors

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### Abstract:

Two-dimensional (2D) transition metal dichalcogenide (TMDC) semiconductors such as molybdenum disulfide (MoS<sub>2</sub>) hold great promise for their outstanding electrical, optical, and mechanical performance. From a practical point of view, surface charge transfer doping (SCTD) is known to be an effective method to modulate the electrical properties of 2D semiconductors. However, although SCTD is a facile and non-destructive method, it could also introduce charged impurities that can hinder charge transport [1]. In this study, we overcome the shortcomings of SCTD through demonstrating a remote charge transfer doping by inserting a thin hexagonal boron nitride (h-BN) layer (< ~3 nm thickness) between MoS<sub>2</sub> channel and the n-type molecular dopants, benzyl viologen (BV). We characterized the electrical properties of MoS<sub>2</sub> field-effect transistors (FETs) with h-BN interlayer before and after doping (denoted as "remotely doped" device) with four-point probe measurements which can minimize the effect of the varying charge injection behaviors due to the BV doping. We identified a larger increase in the mobility of remotely doped MoS<sub>2</sub> FETs relative to its pristine (un-doped) state than that of the BV-doped MoS<sub>2</sub> FETs without h-BN interlayer, since remote SCTD can suppress charge impurity scattering because of the spatial separation by thin h-BN interlayer between BV and the MoS<sub>2</sub> channel. Our work suggests that the remote doping is a promising methodology for efficiently and reliably controlling the electrical properties of TMDCs.

### Keywords:

MoS<sub>2</sub>, Field-effect transistors, surface charge transfer doping, TMDCs

## STEM Image Analysis Based on Deep Learning: Identification of Vacancy of Defects and Polymorphs of MoS<sub>2</sub>

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### Abstract:

Identifying structural features in scanning transmission electron microscope (STEM) images of crystalline materials is important in studying structure-property correlations, but traditional methods for identification are often time-consuming and require expertise. Recent advances in deep learning for computer vision, in particular the use of convolutional neural networks (CNNs), holds promise for efficient high-throughput STEM image analysis. Here we investigate the generalizability of CNNs in identifying point defects and polymorphs in STEM images of transition metal dichalcogenides (TMDCs) in the presence of different levels of noise, aberrations, and carbon contamination. We focus on the application of ResUNet, a type of fully convolutional neural network (FCN), in identifying sulfur vacancies and different polymorphs of molybdenum disulfide (MoS<sub>2</sub>). The prediction of the FCN models toward extensive experimental STEM images was found to be comparable to that of careful hands-on analysis. Based on these results, we provide a guideline on best practices to train a deep learning model to identify structural features of interest in STEM images.

### Keywords:

Deep learning , TEM image analysis, Molybdenum disulfide, Defect, Polymorph

## Interlayer interactions in MoS<sub>2</sub> -ReS<sub>2</sub> heterostructures

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### Abstract:

Heterostructures stacked with two different monolayer transition metal dichalcogenides result in moiré superlattices due to the lattice mismatch or rotational misalignment [1]. Although there are many Raman studies on the heterostructure of transition metal dichalcogenide materials, there is a lack of Raman studies on the isotropic-anisotropic heterostructure. Therefore, we conducted a study on the heterostructures of MoS<sub>2</sub> which is an isotropic transition metal dichalcogenide material and ReS<sub>2</sub> which is an anisotropic transition metal dichalcogenide material.

MoS<sub>2</sub> and ReS<sub>2</sub> monolayers were fabricated using the mechanical exfoliation method, and heterostructures were fabricated using the dry-transfer method. MoS<sub>2</sub> has a honeycomb structure and it is consisting of stacks of S-Mo-S sandwiches held together by van der Waals interactions [2]. ReS<sub>2</sub> has an anisotropic structure, 1T', because Re has one more electron that makes a Re-chain [3]. The twist angle of the heterostructure was determined by using polarization-dependent second harmonic generation for MoS<sub>2</sub> and polarization-dependent Raman for ReS<sub>2</sub>. By observing interlayer interaction by low frequency Raman, it was confirmed that the two layers are interacting. It was found that the maximum intensity polarization of the mode 5 of ReS<sub>2</sub> varies depending on the twist angle of the heterostructure. Also, new peaks were discovered in the high frequency range of the Raman spectrum which are attributed to moiré phonons.

### References

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### Keywords:

Raman, 2D, MoS<sub>2</sub>, ReS<sub>2</sub>, phonon

## Optical Spectroscopy of 2H-MoS<sub>2</sub>/1T'-MoTe<sub>2</sub> Heterostructures

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### Abstract:

2H-MoS<sub>2</sub> is an isotropic two-dimensional (2D) material whose monolayer has a direct band gap of ~1.9 eV with a strong photoluminescence (PL) signal [1]. On the other hand, 1T'-MoTe<sub>2</sub> is an anisotropic 2D metal, exhibiting a temperature-driven structural phase transition to the Weyl semi-metallic T<sub>d</sub> phase at low temperatures. Although van der Waals (vdW) heterostructures are drawing great attention due to their fascinating optical and electronic properties, vdW heterostructures combining semiconducting 2H-MoS<sub>2</sub> and metallic 1T'-MoTe<sub>2</sub> have not been fully studied despite its vast opportunities to explore.

We prepared monolayer 2H-MoS<sub>2</sub> and bulk 1T'-MoTe<sub>2</sub> samples through the mechanical exfoliation method and stacked monolayer 2H-MoS<sub>2</sub> on top of bulk 1T'-MoTe<sub>2</sub> by using the dry transfer method. We conducted Raman and PL measurements on 2H-MoS<sub>2</sub>/1T'-MoTe<sub>2</sub> heterostructure samples both at room temperature and at low temperatures. For the heterostructure samples, we observed new Raman peaks in the ultra-low frequency region (<50 cm<sup>-1</sup>), and the PL signal was significantly different from that of the monolayer 2H-MoS<sub>2</sub>. The crystallographic axes of 2H-MoS<sub>2</sub> and 1T'-MoTe<sub>2</sub> were determined by using polarization-dependent second-harmonic generation (SHG) and Raman spectroscopy, respectively.

### References

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- [2] Yeryun Cheon, *et al.*, ACS Nano **15**, (2021) 2962-2970.

### Keywords:

2H-MoS<sub>2</sub>, 1T'-MoTe<sub>2</sub>, ultra-low frequency Raman spectroscopy, photoluminescence, van der Waals heterostructure

## Temperature-dependent piezoresponse force microscopy study of Moiré superlattices in twisted bilayer WSe<sub>2</sub>

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### Abstract:

Moiré superlattices in van der Waals heterostructures presents various physical properties such as superconductivity, magnetism, and topological edge states. Reconstruction of atoms within the individual layers occurs for small twist angles, yielding the periodic domain structures with different energy levels. Especially, ferroelectricity in the Moiré superlattices has recently attracted considerable attention due to its potential applications, including nonvolatile memories. Here, we present our recent efforts to study temperature-dependent piezoresponse of two-dimensional Moiré superlattices in twisted bilayer WSe<sub>2</sub>. By taking a line-by-line snapshot of their temperature varied response, we cautiously insist that visibility of ferroelectricity gradually goes down as the sample is heated. We discuss the origin of this piezoresponse change in terms of ferroelectric phase transition.

## Raman study of ReSe<sub>2</sub>/MoSe<sub>2</sub> heterostructures

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### Abstract:

Two-dimensional-material-based heterostructures produce novel phenomena due to distinctive interactions between the stacked layers. In the study of transition metal dichalcogenides (TMDs), there are several studies on isotropic/isotropic heterostructure. However, there is a lack of research on anisotropic/isotropic heterostructure.

ReSe<sub>2</sub>, one of the TMDs, is a semiconducting material which has a indirect (nearly direct) bandgap from monolayer to bulk [1]. ReSe<sub>2</sub> has an anisotropic crystal structure (1T', distorted tetragonal) unlike hexagonal MoSe<sub>2</sub> or WSe<sub>2</sub> because Re has one more electron, which makes a Re-chain [1]. MoSe<sub>2</sub> is an isotropic material with a hexagonal structure [2]. It has a direct bandgap only for the monolayer case [1-3].

We made ReSe<sub>2</sub>/MoSe<sub>2</sub> heterostructures by using mechanical exfoliation and dry-transfer. The directions of the Re-chain and the c-axis of ReSe<sub>2</sub> were determined by using polarized Raman spectroscopy [1, 4, 5]. The armchair direction of MoSe<sub>2</sub> is measured by the second harmonic generation [6]. We studied Raman modes in ReSe<sub>2</sub>/MoSe<sub>2</sub> heterostructure with different twisted angles. When the interlayer interaction between the constituent layers existed, we found that new low-frequency and high-frequency Raman modes appeared.

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### Keywords:

Hetero, ReSe<sub>2</sub>, MoSe<sub>2</sub>, Raman, TMDs

## Lithium ionic drift based memristor mimicking synaptic behavior with low power consumption

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### Abstract:

Neuromorphic devices imitating the human brain's data processing has been suggested as an advanced computing architecture to handle massive data processing. The main idea of the neuromorphic computing concept is involved with the parallel data processing of memory and processing units. However, neuronal integrated circuit based on typical silicon complementary metal oxide semiconductors (CMOS) is unsatisfied because of their low integration density. Thus, the satisfaction of scalable and high-performance neuromorphic devices requires a new concept serving synapse mimicking phenomena such as multi-level conductance and plasticity.

Therefore, we demonstrated lithium (Li) ion memristors mimicking the human brain with a low programming power consumption of 70 pJ per event. Since Li with low ionization energy and high ion mobility were utilized, the memristors were able to operate only with a voltage of 1 V and a time of 1 s. Furthermore, the resistive switching mechanism of the Li ion draft memristor was initially showed the ion migrations into PMMA insulating layer. The write once read many (WORM) properties of the memristor were studied for their I-V characteristics as a function of the dual sweeping voltage, and the conductance changes were also studied. Accordingly, we showed that the low power memristor exhibited the fundamentals of next generation neuromorphic systems, i.e., learning and memory. We help that these trials are of vital importance for further neuromorphic research.

### Keywords:

Neuromorphic, CMOS, memristors

## Effect of the ceria particle size on SiO<sub>2</sub> film polishing rate by adjusting synthesis molar ratio.

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### Abstract:

Recently, dynamic random-access memory (DRAM) has been scaled down to ~ 1 nm per year. Nano-unit cmp processes have become important to semiconductors that are getting smaller, and for this purpose, formation of small particles capable of reducing scratches during the cmp process has also become important. This study conducted synthesis to reduce the size of particles. Ceria particles were synthesized using Ce<sup>3+</sup>:H<sub>2</sub>O<sub>2</sub>:NH<sub>4</sub>OH. Synthesis was carried out according to the molar ratio of Ce<sup>3+</sup>, H<sub>2</sub>O<sub>2</sub>, and NH<sub>4</sub>OH materials. The size according to each molar ratio was measured and analyzed, and the polishing rate of sio<sub>2</sub> film was confirmed with these particles. Particle sizes of 100 nanometers or less could be observed, and a maximum polishing rate of 5600A/min was achieved.

### Keywords:

chemical mechanical polishing, ceria particle, synthesis, sio<sub>2</sub> film

## Measurement and theoretical approach to thermoelectrical properties in out-of-plane direction of MoS<sub>2</sub> films depend on layer numbers.

LEE Sang-Kwon \*<sup>1</sup>, CHOI Jae Won<sup>1</sup>, KANG Min-Seong<sup>1</sup>, KIM Gil-Seong<sup>1</sup>, PARK No Won<sup>1</sup>  
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### Abstract:

Our research presents the out-of-plane thermoelectric properties of mono to multilayer MoS<sub>2</sub> films, especially Seebeck coefficient and electrical conductivity. We used a chemical vapor deposition method to grow up the MoS<sub>2</sub> films and made Cu-sandwiched structure. This is the first study that measures the out-of-plane Seebeck coefficients of atomically thin mono- and bilayer MoS<sub>2</sub> at room temperature. In our experiments, out-of-plane Seebeck coefficients for MoS<sub>2</sub> films with one, two, and seven layers came out approximately 129.4, 143.3, and 152.2 mV/K. We presumed such difference occurred in the relation of MoS<sub>2</sub> layer numbers and the density of states of a system. In contrast to conventional thermoelectric materials, the electrical conductivities of these MoS<sub>2</sub> films have the same tendency as the Seebeck coefficients. Our results suggest that we can utilize thermoelectric devices with using high power factors of out-of-plane properties of MoS<sub>2</sub> thin films.

### Keywords:

MoS<sub>2</sub>, Monolayer, Seebeck effect, out of plane

## 화학기상증착법을 이용한 대면적 MoS<sub>2</sub> 박막의 합성 및 기초물성 연구

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### Abstract:

2004년 그래핀의 실험적인 발견 이후, 이론적으로 예측되었던 그래핀의 다양한 우수한 특성들이 실험적으로 규명되면서 이와 유사한 2차원 원자층 소재들(h-BN, BP, TMD) 또한 주목받아 활발한 연구가 이루어져 오고 있다. 그래핀과 마찬가지로 2차원 원자층 소재들 또한 스킵치테이프 방법으로 플레이크 형태로 임의의 크기와 모양 그리고 층 수로 준비된 샘플들이 주로 기초물성 연구에 많이 활용되고 있으며, 최근에는 화학 기상증착법을 활용한 합성 및 응용연구들이 활발하게 진행되고 있다. 화학기상증착법을 활용한 2차원 소재의 합성연구는 대면적으로 그리고 고품질로 원하는 층 수를 균일하게 소재를 합성하는 것을 목표로 발전해왔다. 합성하고자 하는 소재와 최종 목표에 따라 같은 기법을 사용하더라도 최적화된 레시피는 다르게 존재할 수 있기 때문에, 개별적인 다양한 연구 개발들에 대한 성공사례들이 보고되고 있다.

한편, TMD 물질의 경우, 기존에 보고된 화학기상증착법을 활용해 합성한 연구들을 보면 전구체 공급량의 조절이 쉽지 않아서 합성소재의 품질 조절에도 어려움이 존재하는 실험 설계로 수행된 연구가 상당히 많이 보고되고 있다.

이에 본 연구에서는 대면적으로 균일한 MoS<sub>2</sub>의 합성을 목표로 황 원소가 포함된 혼합가스와 금속산화물을 전구체로 사용하였으며, 황 혼합가스 공급량의 조절이 가능하도록 액세서리 장치를 고안하여 사용하였다. 고안된 장치와 방법을 통해 화학기상증착법을 활용하여 전구체 공급량에 따른 합성 양상을 탐색하고 최적화하는 연구를 수행하였다. 합성된 시료의 라만분광법에 의한 맵핑 분석을 통해 합성 조건에 따른 MoS<sub>2</sub> 박막의 두께와 품질을 확인하였다. 또한 SEM을 이용한 표면 분석을 진행하였으며, 전계효과 트랜지스터를 제작하여 기초적인 전기물성을 평가하였다. MoS<sub>2</sub> 박막의 합성 및 기초물성 연구결과와 관련하여 상세한 내용은 본 발표에서 보고할 예정이다.

### Keywords:

2D Materials, TMDC, CVD

## Tailoring the electronic properties of graphene via photoreduced silver nanoparticle decoration

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### Abstract:

Graphene has shown a great potential for electronic device applications due to its superb electrical and mechanical properties. To broaden the application range of graphene-based devices, it is necessary to control the electronic state of graphene properly. Here, we report the controllable p-type doping effect on single-layer graphene which is selectively coated with silver nanoparticles grown by the focused-laser-assisted photoreduction. The direct photoexcitation of graphene submerged in AgNO<sub>3</sub> solution leads to the synthesis of dispersed silver nanoparticles on the graphene surface. It has been shown that the morphology characteristics and coverage area of silver nanoparticles on graphene are adjustable by tuning the laser power and dwell time using scanning electron microscope analyses. Further, using the graphene-based field-effect-transistor devices, we have demonstrated the electronic state of graphene can be modified by laser irradiation conditions.

### Keywords:

graphene, silver nanoparticle, photoreduction, field-effect-transistor device

## Antisymmetrical Temperature Dependence of Longitudinal Spin Seebeck Effect Measurement in Pt/TMDC/YIG Multilayer Structure

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### Abstract:

It is well known that longitudinal spin Seebeck effect (LSSE) are generated in Pt/YIG structures. We observed an unintended in-plane Seebeck effect in Pt/WSe<sub>2</sub>/YIG Structure due to the antisymmetric lateral temperature distribution during LSSE measurement. By applying out-of plane temperature gradients in the Pt/WSe<sub>2</sub>/YIG structure, the modified in-plane Seebeck factor ( $\sim \Delta V_{a\parallel} / \Delta T_{\perp}$ ) was found to be  $\sim 1.0$ - $1.6 \mu\text{V}/\text{K}$  depending on the surface coverage of the WSe<sub>2</sub> Interlayer. Furthermore, the ratio of the effective in- and out-of-plane temperature differences ( $\Delta T_{a\parallel} / \Delta T_{\perp}$ ) was found to be a maximum of  $\sim 48.6\%$ , indicating a substantially high in-plane temperature contribution in LSSE measurements. Our findings indicate that the in-plane temperature contribution can be substantial in the LSSE measurement in a Pt/YIG structure using two-dimensional interlayers

### Keywords:

longitudinal spin seebeck effect, temperature distribution, two dimensional interlayer, transition metal dichalcogenide, in-plane voltage, Pt/YIG structure

## In situ imaging of chiral active site in high-Miller-index exposed nanoparticle

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### Abstract:

Chiral characteristics may be found almost everywhere, from microscopic biological components to cosmic scales. However, chirality in inorganic nanostructure is hardly found in nature. Despite their rarity, the fascinating features of chiral nanostructures inspire chemists to imprint chirality into nanostructures such as nanoparticles and nanoarrays. In the case of nanoparticles, chiral gold nanoparticles are primarily realized by the interaction of biological molecules for their potential applications in the fields of plasmonics, catalysis, and biotechnology. The chirality of the nanoparticles emerges from the interaction between biomolecule-assisted precursors and metal surfaces. Because of the handedness of biomolecule precursor, nanocrystal surfaces with the same Miller-index family interact differently for each geometry. The R/S chirality of crystal surface can explain enantioselective interaction at the chiral nanoparticle seeds. In the point of a biomolecule, same {hkl} Miller-families are divided into two sorts of indices with breaking mirror symmetry. However, measurement of chiral ligand interaction and identification of active sites in the nanoparticle has not been closely examined because of difficulties of 3D structural information. As a result, there is still a lack of scientific knowledge of the detailed mechanism of organic-inorganic interaction that results in chiral nanostructure geometry. In this poster, we will present *in-situ* imaging of High-Miller-index exposed gold nanoparticle, which is the seed of chiral gold nanoparticle with the dose of chiral ligand.

This research was supported by the National Research Foundation of Korea (NRF-2021R1A3B1077076).

### Keywords:

Coherent X-ray diffraction imaging, Chiral gold nanoparticle

## Opposite Raman Shift of Ring Stretching in Pyrrole Molecule Influenced by Ag Nanomaterials Attachment and Electron Addition

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### Abstract:

Surface-enhanced Raman spectroscopy (SERS) can detect some molecules in a non-destructive manner. Using SERS, we study the shifts in the Raman peaks of polypyrrole (PPy) with two different coordinated silver (Ag) structures, Ag nanoparticles (NPs) and Ag dendrite film. The SERS spectrum of PPy with Ag NPs shows a ring-stretching peak which is red-shifted compared to the ring-stretching peak in the Raman spectrum of PPy. In contrast, the spectrum of the PPy with the Ag dendrite film presents a blue-shifted ring stretching peak. The various coordinated Ag nanostructures result in opposite Raman shifts of the ring stretching peak; this phenomenon has been investigated and confirmed by density functional theory (DFT) calculations of the Raman shift of the pyrrole (Py) molecule with a Ag layer (SERS of PPy with Ag NPs) and that of a charge-transferred Py molecule (SERS of PPy with Ag dendrite films). This result demonstrates that DFT calculations can be an effective tool to scrutinize Raman shifts in SERS.

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology(2021R1A4A5031805).

### Keywords:

Surface-enhanced Raman spectroscopy, silver nanostructure, polypyrrole, density functional theory

## Gradual current modulation based on based on Au/Ni/Pb(Zr<sub>0.52</sub>Ti<sub>0.48</sub>)O<sub>3</sub>/Nb doped SrTiO<sub>3</sub> structure.

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### Abstract:

Emerging neuromorphic computing based on memristors has been presented as an artificial synapse for applications. To accomplish high recognition accuracy of a neural computing in memristor arrays, changes in weight values in the form of device conductance should be linear and uniform. Here we report a memristor with Au/Ni/Pb(Zr<sub>0.52</sub>Ti<sub>0.48</sub>)O<sub>3</sub>/Nb doped SrTiO<sub>3</sub>(0.5 wt%) metal/ferroelectric/semiconductor junction that shows enhanced behaviors with a gradual and stable device operation, as compared with a device without PbZr<sub>0.52</sub>Ti<sub>0.48</sub>O<sub>3</sub>, which enables highly recognition accuracy and the large-scale implementation of crossbar arrays. Precise controllability of ferroelectric domain by external voltage could gradually modulate interface barrier in the Nb doped SrTiO<sub>3</sub> semiconductor substrate. Our ferroelectric memristor with high linearity and low variation value may throw light on the way for ideal neural network.

### Keywords:

ferroelectric, neuromorphic device, gradual modulation

## Laser scribed carbon nanomaterials on flexible polyimide film and gas sensor application

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### Abstract:

A gas detection system that monitors harmful gases is a very important field to maintain the global environment and human health. In particular, since flexible devices applicable to various types of wearable applications are in the spotlight as future electronics, the development of materials and substrates for flexible gas sensing platforms is also on the rise. Carbon nanomaterials have been widely studied as a gas sensing material due to its excellent physicochemical properties as well as gas adsorption/desorption behavior and conductivity because of its high specific surface area. However, it is difficult to apply as a flexible device since it has the disadvantage of being inefficient in terms of cost and process time due to high-temperature heat treatment, and the prepared material becomes rigid after carbonization.

In this study, we fabricated laser-scribed carbon nanomaterials (LSC) for flexible gas sensor application using the laser-assisted CVD system with improved time- and cost-effectiveness, rather than the conventional high-temperature heat treatment method. Especially, polyimide (PI) film, a material with excellent heat resistance and flexibility, was used as a carbonization precursor and substrate, and it was possible to use it as a flexible sensor immediately after synthesis without a carbon nanomaterial separation process. The synthesized material has a stereoscopic 3D-structure, which is advantageous for sensing target gas, and has the response of electrical resistance changing to polarized molecules such as acetone, nitrogen dioxide, and ammonia.

### Keywords:

carbon nanomaterial, laser scribing, polyimide film, flexible device, gas sensor

## Metal-Polymer Composites for X-ray Radiation Shielding

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### Abstract:

X-ray is one of the most widely used techniques in the diagnostic medical, military, and non-destructive testing of semiconductors/food products, and so on. However, long exposure to X-rays causes detrimental damage to human beings. Lead, which is a heavy metal, is the only choice now for shielding against X-rays, but it is very heavy and toxic to be used. In this work, we developed non-lead shielding materials against X-rays by compositing polydimethylsiloxane (PDMS) and metal compounds. Several lanthanide series of elements, such as gadolinium and holmium, were tested for X-ray transmittance and processed for uniform dispersion into the PDMS matrix. The resultant metal-PDMS composites have demonstrated reasonable shielding properties against X-rays. Further enhanced performance is possible to improve the miscibility between PDMS and metal compounds.

### Keywords:

X-ray, Radiation Shielding, Metal Compound, PDMS

## Modulation of rectification induced by ion-gel gate in ferrocenyl-alkanethiolate molecular vertical junctions

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### Abstract:

In the field of molecular electronics, the ultimate goal to achieve is demonstrating electronic components like wires, diodes, memories, and transistors using single-molecule or bundle-molecules monolayers. Ferrocenyl-alkanethiolate molecule has been investigated as an appropriate candidate for realizing the molecular diode due to its rectifying feature caused by its redox nature and molecular orbital of ferrocene head group. However, controlling the molecular orbital energy level of molecular monolayers was considered difficult to demonstrate because of their structural limitations. Recently, vertical molecular transistors induced by ion-gel gating were developed with the contribution of a weak screening effect of the graphene monolayer.

Here, we've shown molecular rectifying junctions with a ferrocenyl-alkanethiolate molecule in the form of vertical structure of ion-gel/graphene/molecule/metal. The template-stripping (TS) method was used to make an ultra-flat low roughness gold bottom substrate to form a great quality of self-assembled monolayer of ferrocenyl-alkanethiolate molecules. The electric double layer formed at the interface between the graphene and ion-gel induced a strong electric field that affects the energy levels of the graphene electrode and the molecules. The modulation of the rectification ratio of the molecular junction was achieved from unity to  $\sim 7$  depending on the bias voltage and the gate voltage. The demonstrations of the ion-gel induced modulation of rectification ratio of the molecular junction showed a potential for designing novel functional elements for molecular electronics field.

### Keywords:

Molecular Electronics Devices, Molecular Electronics, Molecular Tunneling Junction, Ion-gel Gating

## Phase change random access memory를 위한 $\text{Ge}_2\text{Sb}_2\text{Te}_5$ 및 $[(\text{GeTe})_x/(\text{Sb}_2\text{Te}_3)_y]_n$ superlattice 증착조건 제안

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### Abstract:

빅데이터 시대와 뉴로모픽 연산을 위해서는 초고속, 고밀도, 저전력의 비휘발성메모리가 필요하다. 현재 비휘발성메모리로 사용되는 플래시메모리는 동작속도가 느리고 밀도를 줄이는 한계가 있어 차세대 메모리로는 부족한 부분이 많다. 그 대안인 여러 후보 물질 중  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ 는 Chalcogenide계 물질로 비정질상과 결정상이 존재하며 상 변화 시 전환이 빠르고 가역적으로 상변화가 가능하다. 또한 고속의 메모리 동작 특성과 나노 스케일로 제작이 가능해서 고밀도의 차세대 메모리로 각광 받고 있어  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ 는 연구가 활발히 진행되고 있다. 특히 에너지효율을 높이기 위한 연구도 진행되고 있으면 이에 해결방식으로 GeTe와  $\text{Sb}_2\text{Te}_3$ 을 순서대로 적층시키는 구조인  $[(\text{GeTe})_x/(\text{Sb}_2\text{Te}_3)_y]_n$  superlattice 구조가 제시되었다. 본 연구에서는 스퍼터를 이용하여 GeTe와  $\text{Sb}_2\text{Te}_3$  타겟을 반복적으로 한 층씩 적층하여  $[(\text{GeTe})_x/(\text{Sb}_2\text{Te}_3)_y]_n$  superlattice 구조를 증착하고 온도/저항 Van der Pauw 방식을 통해 진행하였다. 그 결과 30도에서 320도 온도 구간에서 상변화를 나타내는 저항의 급격한 변화를 확인하였다. 더하여 압력, 조성비, 증착전압과 같은 스퍼터링 파라미터 및 동시증착법 또는 superlattice와 같은 구조를 변화시켜  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ 의 상변화 특성을 비교 분석하였다. 그 결과 120도와 260온도에서 급격한 저항변화를 확인하였고 이를 X선 회절 분석결과 결정구조가 변화하였음을 확인하였다. 따라서 본 연구에서는 최적의 상변화 특성을 가지는  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ 의 스퍼터링 기반 조건을 제안한다.

### Keywords:

GST, Phase change memory, sputter

## Single-molecule measurements of mechanical interactions between the viral Spike glycoprotein and ACE2 receptor using optical tweezers

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### Abstract:

Single-molecule measurement of the mechanical interactions between viral glycoproteins and host cell receptors is essential to understand virus entry into host cells. In particular, the binding between the viral Spike glycoprotein and ACE2 receptor is a critical first step in SARS-CoV-2 infection. It constitutes a primary drug target in the current search for treatments of COVID-19. We have been using optical tweezers to investigate the mechanisms by which the S-glycoprotein binds to the ACE2 receptor. Here, we demonstrate how to detect the molecular interactions between the S-glycoprotein coated on the microbead and the ACE2 receptor expressed on the surface of living cells by utilizing the optical tweezers. We look forward to using this method in research to develop binding inhibitors that target the early stage of viral entry.

### Keywords:

Single-molecule measurement, S-glycoprotein, ACE2 receptor, SARS-CoV-2

## The intermediate structure study of metal substituted carbonic anhydrase II

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### Abstract:

Enzymes are catalysts for biological processes. Capturing and interpreting intermediate state of enzyme during its catalytic activity is crucial to understand its catalytic mechanism. Human carbonic anhydrase II (CA II) is a zinc metalloenzyme that catalyzes the reversible hydration/dehydration of  $\text{CO}_2/\text{HCO}_3^-$  and is considered as a good model protein for biophysics. Protein X-ray crystallography is most common way to achieve the protein structure. High pressure cryo-cooling, a technique originally developed for cryo-preservation of protein crystal sample, was used to obtain an intermediate state of CA II. Through a comparative study on the intermediate states of the zinc-bound native CA II and non-native metal-substituted CA IIs, we demonstrate that the characteristic metal ion coordination geometries (tetrahedral for  $\text{Zn}^{2+}$ , tetrahedral to octahedral conversion for  $\text{Co}^{2+}$ , octahedral for  $\text{Ni}^{2+}$ , and trigonal bipyramidal for  $\text{Cu}^{2+}$ ) directly modulate the catalytic efficacy. In addition, we reveal that the metal ions have long-range electrostatic effect on restructuring water network in the active site.

### Keywords:

Structural biology, Intermediate state, Enzyme mechanism

## Molecular mechanism underlying DNA damage repair by Neil3 glycosylase

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### **Abstract:**

Human genome is damaged by various factors such as ionizing radiation and toxic chemicals. If DNA damage is not properly repaired, it causes serious problems such as malignant diseases. Different repair pathways are chosen according to the types of DNA damage. For example, modified bases including 8-oxo guanine and abasic site, which induce mutations, are recovered by base excision repair (BER) pathway. BER pathway is initiated by DNA glycosylases, which recognize DNA base lesions. Among many DNA glycosylases, we studied Neil3, which can repair modified bases in G-quadruplexes as well as interstrand crosslink (ICL) during replication. We investigated how Neil3 resolves modified base in G-quadruplex, which is a novel DNA structure usually formed in human telomeric sequence using single-molecule FRET. We found that Neil3 changes the conformation of G-quadruplex while it recognizes an abasic site and finally cleaves the DNA backbone at the abasic site. In addition, we found that Neil3 resolves ICL in the fork structure of DNA.

### **Keywords:**

BER, DNA glycosylase, Neil3, ICL, G-quadruplex

## Roles of transcriptional pause in $\rho$ -dependent termination

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### Abstract:

The transcriptional pause is a critical step for transcription termination, but the mechanistic roles of the pausing time in  $\rho$ -dependent termination are not clearly understood yet. We recently found that  $\rho$ -dependent termination occurs via three independent routes (i. stand-by/decomposing, ii. catch-up/decomposing, and iii. catch-up/recycling), raising an important question of how they are distinctly utilized for the regulation of  $\rho$ -dependent termination. We find that the termination efficiency of only the stand-by/decomposing route has a positive correlation with the pausing time, an observation in direct contrast with the common belief that the stand-by termination route is faster than the catch-up termination routes, thus does not require a long pausing time. We also find that the slow response of the stand-by termination route is favorably utilized in regulation of  $\rho$ -dependent termination by *mgtA* and *ribB* riboswitches.

### Keywords:

Single-molecule FRET, Transcription Termination, pausing,  $\rho$ -dependent termination, Riboswitch

## Direct observation of target-search by CRISPR/Cas9

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### Abstract:

CRISPR/Cas9 (Cas9) is a sequence-specific DNA endonuclease that has been working as one of the most powerful genetic editing tools. Although the target search process of Cas9 affects editing efficiency and off-target effects, its mechanism is controversial compared to the elucidation of target recognition and cleavage mechanisms. Recent researches have revealed that Cas9 undergoes both three-dimensional (3-D) and one-dimensional (1-D) diffusion to identify its target among huge amounts of double-stranded DNAs. It, however, has not been investigated the searching process of Cas9 in real-time. Here, we directly observed the target search mechanism with single-molecule fluorescence assays, especially single-molecule tracking, to study Cas9 from *Streptococcus pyogenes* (SpCas9). By visualizing SpCas9 on the  $\lambda$  DNA-derived long DNA substrates, we could discern its movement. SpCas9 exhibited two modes of 1-D diffusion: sliding and intermittent DNA contacts (hopping). In addition, we found that the diffusion coefficient ( $D$ ) of SpCas9 was notably slower than the one of Cas12a derived from *Acidaminococcus* sp. (AsCas12a). Hence, based on diffusion, functional differences between SpCas9 and AsCas12a might be explained. Altogether, our results will provide a more detailed understanding of biological roles of Cas9 and should straighten out present issues in its applications.

### Keywords:

CRISPR/Cas9, Off-target effects, Single-molecule tracking, Target searching, Diffusion

## Enhancement of radiotherapeutic effect with radiation-guided nanoradiosensitizer in mouse brain tumor models

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### Abstract:

For radiation treatment combined with radio-sensitizer on intracranial tumors, a primary limiting factors is normal tissue toxicity. Targeted tumor treatment can potentially maximize tumor cure and minimize normal tissue toxicity. c-Jun N-terminal kinases (JNKs) regulates H2AX phosphorylation, which repairs DNA damage by radiation and its blocking can modulate radiosensitivity for tumor cells. HVGSSV peptide was found to bind specifically to the tax-interacting protein-1 (TIP-1) receptor expressed in irradiated tumor cells. The aim of this study is to establish a drug delivery system using the radiation-targeted peptide in a Lewis lung carcinoma (LLC)-bearing brain tumor mouse and to assess effect of JNK inhibitor-incorporated nanoparticle on brain tumor growth delay. The tumor cell lines used were murine LLC obtained from the American Type Culture Collection. The LLC-Fluc cell line was transfected with a Lentiviral vector containing the firefly luciferase (Fluc) Gene. The LGEse block copolymer was synthesized to fabricate SP600125-incorporated nanoparticles: SP600125 is radiation sensitizer. JIIN copolymer was conjugated to the radiation-targeted peptide to yield JIIN-HVGSSV polypeptide. Physicochemical and morphological properties were observed by transmission electron microscope (TEM) photo and particle size. Elevated expression of TIP-1 was found in irradiated mouse brain tumor. The experimental results indicated that TIP-1 is a molecular target that enables the selective binding of the HVGSSV peptide within irradiated xenograft tumors. Nanoparticles could enable sustained release of radio-sensitizer into the tumor. Radiation-guided JIIN delivery system can be effectively applied to synergistically inhibit the tumor growth by reducing DNA repair and enhancing apoptosis in radiation treatment of brain tumor.

### Keywords:

Radio-guided drug delivery, Nano particle radiosensitizer, JNK inhibitor, HVGSSV peptide, Mouse brain tumor model

## Study on Imatinib Binding to c-Src Tyrosine Kinase

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### Abstract:

c-Src tyrosine kinase plays a key role in cell differentiation and growth. Imatinib (Gleevec) is an effective inhibitor for suppressing the activity of Abl-tyrosine kinase. c-Src tyrosine kinase has a 47 percent similarity to Abl tyrosine kinase in the amino acid sequence. We investigate the binding of imatinib to c-Src tyrosine kinase by using MD simulation and molecular docking. In particular, we use a targeted MD simulation to generate several conformational structures in the process of the conformational change of c-Src tyrosine kinase from an inactive state to an active state. The results establish that most stable conformation of c-Src tyrosine kinase to imatinib, from among the various conformations, has the highest binding affinity.

## Transient dynamics of information transfer in a simple Markov model

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### **Abstract:**

Transfer entropy is an information-theoretic measure often used to infer causal relations in a complex system such as gene regulatory network. Using a simple Markov model inspired by gene regulatory network, I show that the causal relations measured by the transient entropy not only depends on the time-dependent probability distribution, but such a causal relationship can also be reversed with time. Therefore, the transfer entropy contains time-localized dynamic information not contained in the model parameters that is fixed for a given system. The result suggests that the interaction network inferred by the transfer entropy may change dynamically with time.

### **Keywords:**

Markov model, information theory, gene regulatory network

## The Brownian Motion of Conjugates of Magnetic Nanoparticles and Anti-CD3 Monoclonal Antibodies and the Drainage of Nanoparticles through Mice's Organs

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### Abstract:

An optimal Fc-directed conjugate of Foralumab (anti-CD3 monoclonal antibody, mAb) with the amine group-containing magnetic nanoparticles (MNPs) was prepared mAb-MNPs using the SiteClick antibody labeling kit, which provides instructions for an antibody control, buffer exchange, antibody carbohydrate domain modification, azide attachment, and azide-modified antibody purification and concentration procedures. The mAb-MNP conjugate was confirmed by observing transmission electron microscopy (TEM) images and energy dispersive spectroscopy (EDS) maps, including those of S elemental spectra and images. The average values of drift movement speed due to Brownian motion of MNPs and mAb-MNPs in PBS were measured as +3.16 pix/frame, 0.76 pix/frame on the x-axis and +6.70 pix/frame, +1.98 pix/frame on the y-axis, respectively. Particle size, concentration distribution, and intensity distribution were analyzed by nanoparticle tracking analyzer (NTA) for MNPs and mAb-MNPs with an actual size of 35 nm. The hydrodynamic diameter was found to be 180.0 nm and 258.8 nm on average for MNPs and mAb-MNPs, respectively. The 2× increase in drift velocity for mAb-MNPs could be attributed to Brownian motion in proportion to the higher value for the square of the radius of the conjugate according to Stokes' law. These results show that the conjugate of the anti-CD3 antibody, Foralumab, with MNPs has suitable fluidity in phosphate-buffered saline (PBS). In addition, in the use of MNPs conjugated with mAbs, a simple microneedle liquid patch can be attached to the skin to obtain injection efficiency, and an immunotherapeutic agent can be induced by attaching it to a target site. It is considered that the treatment effect can be maximized by reducing the burden on the patient and providing a sense of stability. The mAb-MNPs still migrate easily to sites of virus entry, making this conjugate useful for treating cytokine release syndrome (CRS) in COVID-19 cases. Also, we investigate the drainage and excretion criteria of nanoparticles through different organs(kidney, lung, liver, and spleen) according to their properties.

**Acknowledgments:** This research was funded by the Brain Pool program (2021H1D3A2A01099303) funded by the Ministry of Science and ICT and the Basic Science Research Program (2021R1I1A3054773) funded by the Ministry of Education through the National Research Foundation of Korea (NRF).

### Keywords:

anti-CD3 monoclonal antibody, magnetic nanoparticle, Brownian motion, Stokes' law, drainage

## Searching for Majorana bound state by Shapiro step measurement in $\text{FeTe}_{0.55}\text{Se}_{0.45}$ Josephson junction.

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### Abstract:

Topological superconductors have a Majorana bound state (MBS) at their boundaries or vortices on the surface. Such MBS follow non-Abelian exchange statistics, so they can be used as a fault-tolerant topological quantum computer.  $\text{FeTe}_{0.55}\text{Se}_{0.45}$  (FTS), an iron-based superconductor, is one of the candidates for topological superconductors. FTS is expected to have a topological surface state and zero-energy vortex bound state (ZVBS) under the external magnetic field. To prove the topological superconductivity of FTS, we fabricated full-van der Waals vertical Josephson junction through low-temperature micro-cleaving technique. We will discuss our investigation about the Shapiro steps upon irradiating microwave as a function of the strength of the external magnetic field.

### Keywords:

Iron-based superconductor, Shapiro steps, Topological superconductor, Majorana bound state

# Mechanism of Superconductivity in CrB<sub>2</sub> at High Pressure

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## Abstract:

After discovering the superconductivity with  $T_c=40$  K in MgB<sub>2</sub> about 20 years ago, many have tried to achieve higher  $T_c$  in AlB<sub>2</sub>-type compounds. However, these trials have failed, so far. Last year, Y. Qi and coworkers found superconductivity up to 32 K at 100 GPa in nonmagnetic MoB<sub>2</sub> that was isostructural to AlB<sub>2</sub> over 70 GPa [1]. Additionally, they observed superconductivity in the AlB<sub>2</sub>-type, yet antiferromagnetic CrB<sub>2</sub>, under high pressure. In CrB<sub>2</sub>, at 4 GPa the antiferromagnetism is suppressed, subsequently leading to a transition of AFM to superconductivity [1]. Finally, its  $T_c$  reaches 7 K at 110 GPa. These superconductors are different from the superconducting MgB<sub>2</sub>, but show several similarities to high  $T_c$  hydrates under mega bar [2].

In this presentation, we will address the electronic structure and the origin of the superconductivity of CrB<sub>2</sub> at the mega bar, using first principles approaches. Our calculations based on the Allen-Dyne equation well reproduce the experimentally observed  $T_c$  at 110 GPa, indicating an electron-phonon coupling mediated superconductivity. However, remarkably, in the lower pressure region, the theoretically calculated  $T_c$  is substantially different from the experimental observations. That will be discussed in the presentation. Furthermore, we will address similarities to the superconducting MoB<sub>2</sub> and high  $T_c$  hydrates.

## [Acknowledgements]

This research was supported by NRF of Korea Grants NRF-2019R1A2C1009588.

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- [2] Y. Quan, K.-W. Lee, and W. E. Pickett, Phys. Rev. B 104, 224504 (2021).

## Keywords:

first principles calculations, CrB<sub>2</sub>, high pressure superconductors

## Mirror symmetry breaking beyond critical doping in High $T_c$ cuprate superconductor

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### Abstract:

The phase diagram of cuprate High-temperature superconductors features an enigmatic strange metal region in which in-plane resistivity varies linearly with temperature. In this V-shaped region, there is general agreement that  $T^*$  or pseudogap temperature can be defined by deviation from linear resistivity below critical doping. However, there is no consensus on  $T_{up}$  or upturn temperature which is also defined by deviation from linear resistivity beyond critical doping. Here, we present Second harmonic optical anisotropy measurement on (Pb,Bi)2212 beyond critical doping. Taking our symmetry analysis from SHG, as well as resistivity and ARPES measurement, we found this mirror symmetry breaking occurs at  $T_{up}$ . This result may suggest  $T_{up}$  region beyond critical doping coincides with mirror symmetry breaking order.

### Keywords:

Second Harmonic Generation, High  $T_c$  cuprate superconductor, Mirror symmetry breaking

## Superconducting properties for HTS GdBCO CC with heat treatments

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### Abstract:

Ag/GdBCO/Buffer-layers/Stainless-Steel 구조를 가지는 GdBCO 박막선재(Coated Conductor: CC)들을 진공상태(V-series)와 산소분위기(O-series)의 열처리 조건에 따른 초전도 특성 변화를 분석하였다. V-series 및 O-series 시편들의 자기적 특성들을 조사하기 위해 Quantum Design 회사의 Physical Property Measurement System(PPMS)을 이용하였다. Zero-field-cooled(ZFC) 조건을 이용하여 자화도 (Magnetization:  $M$ )의 온도 의존성  $M(T)$  curve들을 얻고, 이를 통해 V-series 및 O-series 시편들의 열처리 조건에 따른 초전도 임계전이온도  $T_c$ 의 변화를 조사하였다. 또한, 자화도(Magnetization:  $M$ )의 자기장세기 의존성  $M(H)$  curve들을 얻고, Bean model를 이용하여 V-series 및 O-series 시편들의 열처리 조건에 따른 임계전류밀도  $J_c$ 의 변화를 조사하였다. 한편, V-series 및 O-series 시편들의 열처리 조건에 따른 비가역자기장(irreversibility magnetic field)  $H_{irr}$  선들의 변화 등을 조사하고, 온도에 증가에 따른  $H_{irr}$  선들의 감소에서 약한 감소(Weak-down)와 강한 감소(Strong-down)의 영역들을 확인할 수 있었다. 우리는 이러한 결과들과 다른 연관된 결과들을 논의할 것이다.

### Keywords:

GdBCO CC, 열처리, 자화도(Magnetization), 임계전류밀도, 비가역자기장(Irreversibility magnetic field)

## The vortex property of the $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_x$ with Torque Magnetometry

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### Abstract:

Thanks to the improvement of the fridge system, the low-temperature field is developed faster than before. Especially superconductivity become a large field in physics. Nowadays, the superconductivity material can sort by type 1, type 2. Most of the high-temperature superconductors belong to type 2. Type 2 superconductor has a relatively small coherence length than type 1. Several materials are even close to Fermi wavelength which means these can show the BCS-BEC cross-over phenomena. The coherence length of the type 2 superconductor is also shorter than the penetration depth of this material. This makes the vortex-pinning effect which appears at a mixed state of superconductor and a normal metal. Here we focus on the optimal doped  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_x$  (BSCCO) which is the high-temperature superconductor ( $\sim 90\text{K}$ ). We figure out the vortex effect of BSCCO and measure the magnetic moment under several hundred gauss fields. We find the vortex entry field according to temperature. This occurs the magnetic moment change which doesn't follow the Meissner effect. We use the torque magnetometry method to measure the magnetic moment. This is an interferometry-related method that has high sensitivity ( $10^{-7}$  emu).

### Keywords:

Superconductivity, Vortex, Type 2

## 스퍼터링을 이용한 고품질 Nb, NbN 초전도 박막의 전기적 특성 연구

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### Abstract:

Nb와 NbN은 초전도 물질로서 과거부터 활발하게 연구되어왔다. 또한 최근에는 탄소나노튜브(Carbon nanotube, CNT)에 박막으로 증착한뒤에 CNT 실을 만드는 방법등에 이용되어 다시 주목받고있다. 이러한 박막 증착에서 고품질의 Nb, NbN 박막을 만드는것이 중요한 역할을 하며, 스퍼터링, 전자 빔 증착, 열 증착등의 고품질 박막을 만드는 방법에대한 연구도 진행되고 있다. 본 연구에서는 스퍼터링을 이용한 고품질 Nb, NbN 초전도 박막의 제조와 전기적 특성에대해 연구하였다. 스퍼터링 시간, 기판온도 및 스퍼터링 파워등의 여러가지 조건을 이용하여 Nb, NbN 박막을 증착하였으며, 증착된 Nb, NbN 박막을 4 단자 I-V 측정을 통해 각 조건에 따른 전기적 특성을 확인하였고, 또한 초전도 전이의 유무 또한 확인 하였다. 본 연구에서는 스퍼터링을 이용한 박막 제작이 고품질의 초전도 박막을 제작하는데 좋은 방법임을 제시한다.

### Keywords:

thin film, superconductivity, Nb, NbN, sputter

# Josephson Junctions in Twisted NbSe<sub>2</sub> van der Waals Heterostructures

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## Abstract:

The dynamics of Josephson junctions (JJs) — the evolution of supercurrent in a region of weakened superconducting order — is a direct indicator of the underlying current-phase relation (CPR) in the superconducting junction. Although the fabrication of Josephson junctions often involve the nanofabrication and deposition of conventional superconductors, there has been a recent increase in the utilization of layered, cleavable superconductors such as NbSe<sub>2</sub> and BSCCO [1,2].

In this study, we fabricated bulk-like, multilayer, twisted NbSe<sub>2</sub> flakes using mechanical exfoliation and a PDMS assisted dry-transfer technique [3]. Magnetic interference and microwave response of these heterostructures are presented, consistent with the results of previous reports in literature [1,4].

An additional outlook on the application of these JJs, which most likely find themselves in the clean tunnel junction regime, for phase-sensitive measurements is presented.

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[4] Chen, Shixian, et al., *Physical Review B* 104.21 (2021)

## Keywords:

Josephson Junctions, NbSe<sub>2</sub>, Twistronics, vdW Heterostructures

## Epitaxial growth of van der Waals ferromagnetic metal MnTe<sub>2</sub>

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### Abstract:

Magnetic van der Waals(vdW) materials of which long-range magnetic order is stabilized by large magneto-anisotropy have drawn growing attention for their unique properties and potential applications to novel spintronic devices. In most of the known vdW magnets, the Curie temperature tends to decrease with reduced thickness due to thermal fluctuations and thus search for a 2D magnetic material with high  $T_C$  and robust magnetism even at two-dimensional limit is important for future applications.

Hexagonal MnTe<sub>2</sub> with 1T-transition metal dichalcogenide(TMDC) has been proposed to host 2D ferromagnetism with high  $T_C$  of 100 K in the monolayer limit. However, the 1T- phase is thermodynamically unfavored for Mn-Te binary system and has not been experimentally synthesized yet. In this work, 1T-MnTe<sub>2</sub> has been epitaxially grown by molecular beam epitaxy. Its ground state is confirmed to be a ferromagnetic metal with high  $T_C$  of 200K by angle-resolved photoemission spectroscopy(ARPES) and magnetotransport. Synthesis of a metastable material with 2D magnetism via epitaxy paves a new way to realize novel functional devices.

### Keywords:

Magnetism, Molecular beam epitaxy, Angle-resolved photoemission spectroscopy

## Magnetic exciton of multiferroic van der Waals material NiI<sub>2</sub>

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### Abstract:

A two-dimensional magnetic van der Waals material NiI<sub>2</sub> has two successive phase transitions at  $T_{N2}=78$  K into an antiferromagnetic phase and  $T_{N1}=59.5$  K into a proper-screw helimagnetic phase. It has been reported that NiI<sub>2</sub> forms six-directional multiferroic domains below  $T_{N1}=59.5$  K. Using infrared-visible spectroscopy, we measured the optical absorption of NiI<sub>2</sub> and found a sharp magnetic-exciton peak at 1.384 eV below 60 K where NiI<sub>2</sub> has is in the multiferroic phase. Further, the exciton peak has anisotropy with respect to the multiferroic domain directions, which we claim is due to the transition into the multiferroic states.

### Keywords:

van der Waals, multiferroicity, exciton, spectroscopy

## The physical properties of nanoparticle $AFe_2O_4$ ( $A = Fe, Co$ ) for biomedical applications

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### Abstract:

The crystallographic and magnetic properties of Fe oxides with potential applications as biomaterials have been studied.  $Fe_3O_4$  and  $CoFe_2O_4$  nanoparticles are prepared by high temperature thermal decomposition method. The samples are characterized by X-ray diffraction, vibrating sample magnetometer, and Mössbauer spectroscopy. It was confirmed that the lattice constants of  $Fe_3O_4$  and  $CoFe_2O_4$  were cubic spinel structures with  $Fd-3m$  space groups of  $a_0 = 8.3831 \text{ \AA}$  and  $a_0 = 8.3960 \text{ \AA}$ , respectively. The saturation magnetization value of  $Fe_3O_4$  was 71.47 emu/g, the coercive force was 10.25 Oe, the  $CoFe_2O_4$  saturation magnetization value was 65.78 emu/g, and the coercive force was 57.46 Oe. Exothermic experiments for hyperthermia were performed in an external magnetic field of 250 Oe and 109.8 kHz. The results show that at 800 s, saturation was achieved at 64.4 °C for  $Fe_3O_4$  and 77.5 °C for  $CoFe_2O_4$ . Mössbauer spectroscopy was performed to determine the phase of nanoparticles and to study electromagnetic interactions for their superparamagnetic and exothermic properties. In addition, LDH Assay was performed to measure the cytotoxicity of nanoparticles. When both  $Fe_3O_4$  and  $CoFe_2O_4$  nanoparticles were administered in an amount of 40 mg/ml, less than 20% of cells were apoptotic. Both samples were found to have good biocompatibility.

### Keywords:

$Fe_3O_4$ ,  $CoFe_2O_4$ , Mössbauer spectroscopy, superparamagnetic, biocompatibility

## The magnetic properties and biocompatibility study of nanoparticle $\text{MnFe}_2\text{O}_4$

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### Abstract:

The crystallographic and superparamagnetic properties of nanoparticle  $\text{MnFe}_2\text{O}_4$  for biomedical applications have been studied. The nanoparticles of  $\text{MnFe}_2\text{O}_4$  are prepared by high temperature thermal decomposition method. The structural and magnetic properties of the nanoparticles are investigated by X-ray diffraction, vibrating sample magnetometer, and Mössbauer spectroscopy. The crystal structure of the nanoparticles  $\text{MnFe}_2\text{O}_4$  was a single phase cubic spinel with a lattice constant  $a_0 = 8.3899 \text{ \AA}$ , and the average size was 8.75 nm. The saturation magnetization value of the  $\text{MnFe}_2\text{O}_4$  was 71.1 emu/g and the coactivity was 26.1 Oe. Mössbauer spectroscopy was performed to determine the phase of nanoparticles and to study electromagnetic interactions for their superparamagnetic properties. The exothermic experiment for hyperthermia was performed in an external magnetic field of 250 Oe and 109.8 kHz. The result shows that saturation was achieved at 66.3 °C for the  $\text{MnFe}_2\text{O}_4$  at 800 s. The cytotoxicity test was performed for biomedical applicability. LDH assay showed good biocompatibility. In addition, cell viability was improved in  $\text{MnFe}_2\text{O}_4$  coated with the biodegradable polymer poly(L-lactic acid) compared to  $\text{MnFe}_2\text{O}_4$ .

### Keywords:

$\text{MnFe}_2\text{O}_4$ , nanoparticle, Mössbauer spectroscopy, superparamagnetic, biocompatibility

## Temperature dependence Raman study of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ ( $x=0.0, 0.2, 0.3, 0.4, 0.5$ )

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### Abstract:

$\text{Ca}_2\text{RuO}_4$  is Perovskite crystal structure, and be issued with feature of Higgs mode and orbital selective Mott phase and others. With temperature dependence Raman spectroscopy, we have studied about phonon and electronic gap of  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ , element replaced from Ca to Sr about  $x=0.0, 0.2, 0.3, 0.4, 0.5$ . And we analyzed the result of Raman spectroscopy, and compared with the same sample result of angle-resolved photoemission spectroscopy.

### Keywords:

Raman spectroscopy, Angle-resolved photoemission spectroscopy,  $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ , phonon, electronic gap

## Temperature dependence of Raman spectrum from magnetic van der Waals $\text{Mn}_{0.5}\text{Fe}_{0.5}\text{PS}_3$ with a spin-glass state

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### Abstract:

Two-dimensional magnetism has played an important role in developing the modern understanding of magnetism.<sup>1</sup> With the arrival of magnetic van der Waals materials, experimental studies on 2D magnetism have made progress.<sup>2</sup> Spin glass is a unique magnetic state arising from competing magnetic interactions.<sup>3</sup> In this work, we studied the spin-glass phase of van der Waals  $\text{Mn}_{0.5}\text{Fe}_{0.5}\text{PS}_3$ , which is the first spin-glass van der Waals system. We measured the polarized Raman spectrum down to low temperatures and observed several features due to the spin-glass transition. First, we have studied with bulk  $\text{Mn}_{0.5}\text{Fe}_{0.5}\text{PS}_3$ , and then we did the same measurements with few-layer  $\text{Mn}_{0.5}\text{Fe}_{0.5}\text{PS}_3$ . In both cases of bulk and few-layer  $\text{Mn}_{0.5}\text{Fe}_{0.5}\text{PS}_3$ , the Raman spectra showed subtle changes, consistent with the nature of the spin-glass transition.

[1] Onsager, L. Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition. *Phys. Rev.* 1944, 65 (3–4), 117–149. <https://doi.org/10.1103/PhysRev.65.117>.

[2] Park, J.-G. Opportunities and Challenges of 2D Magnetic van Der Waals Materials: Magnetic Graphene? *J. Phys. Condens. Matter* 2016, 28 (30), 301001. <https://doi.org/10.1088/0953-8984/28/30/301001>.

[3] Mydosh, J. A. *Spin Glasses: An Experimental Introduction*; CRC Press: London, 1993.

### Keywords:

(Mn,Fe)PS<sub>3</sub>, spin glass, Polarized Raman Spectroscopy, Quasi-elastic scattering

## STUDY ON NEW KONDO LATTICE $Ce_3Fe_2Ge_{11}$

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### Abstract:

Expected  $Ce_3Fe_2Ge_{11}$  was grown for the first time by Indium self-flux method. The chemical composition has been identified through EDS (Energy Dispersive Spectroscopy) analysis. The system orders antiferromagnetically below  $\sim 5.2$ - $6.3$ K (TN), whose transition is observed as kink in magnetic susceptibility, electrical resistivity, hall effect and as a peak in specific heat capacity. The electrical resistivity with respect to the temperature follows logarithmic increase in decreasing temperature from 200K to 50K, suggesting strong local Kondo scattering contribution to the electron transport. At around 50K, the resistivity shows shoulder like feature with broad local maximum and increases drastically below  $\sim 20$ K with a hump at around TN. The overall feature resembles those of heavy fermion compound  $Ce_3Co_4Sn_{13}$ [1] and low density system  $CeNi_2-xAs_2$ [2]. Upon applied magnetic field, resistivity and specific heat gives strong anisotropic response between the magnetic field direction along and out of plane direction. Details of magnetic field dependence of the resistivity, specific heat and Hall coefficient will be presented and discussed.

### Reference

[1] E. L. Thomas et al., J. Solid State Chem. 179, 1642 (2006).

[2] Y. Luo et al., PNAS 112, 13520 (2015).

### Keywords:

Keywords:  $Ce_3Fe_2Ge_{11}$ , antiferromagnetic

## Synchrotron radiation spectroscopy study of a topological Kondo insulator candidate of CeNiSn

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### Abstract:

Non-symmorphic symmetry is important in determining topological states. For example, both experiments and calculations for a Dirac semimetal ZrSiS showed that the Dirac cone is protected by the non-symmorphic symmetry [1]. On the other hand, it was reported that the Kondo systems with non-symmorphic structures, such as CeNiSn and Ce<sub>3</sub>Bi<sub>4</sub>Pt<sub>3</sub>, might become topological insulators having the topological surface states [2]. In order to determine whether CeNiSn is a topological insulator, we have investigated the electronic structure of CeNiSn by employing angle-resolved photoemission spectroscopy (ARPES). We have measured the Fermi surfaces and band structures for three orthogonal crystallographic planes, and compared them with the corresponding band structures, obtained from the density functional theory calculations. In this presentation, we will discuss the role of the Ce 4f and Ni 3d states in determining the topological states in CeNiSn.

[1] L. M. Schoop et al., Nat. Comm. 7, 11696 (2016).

[2] Po-Yao Chang et al., Nature Physics, **13**, 794 (2017).

### Keywords:

Kondo insulator, CeNiSn, ARPES

## Tunable asymmetric spin wave excitation and propagation in a magnetic system with two rectangular blocks

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### Abstract:

Asymmetric spin wave excitation and propagation are key properties to develop spin-based electronics, such as magnetic memory, spin information and logic devices. To date, such nonreciprocal effects cannot be manipulated in a system because of the geometrical magnetic configuration, while large values of asymmetry ratio are achieved. In this study, we suggest a new magnetic system with two blocks, in which the asymmetric intensity ratio can be changed between 0.276 and 1.43 by adjusting the excitation frequency between 7.8 GHz and 9.4 GHz. Because the two blocks have different widths, they have their own spin wave excitation frequency ranges. Indeed, the spin wave intensities in the two blocks, detected by the Brillouin light scattering spectrum, were observed to be frequency-dependent, yielding tuneable asymmetry ratio. Thus, this study provides a new path to enhance the application of spin waves in spin-based electronics.

### Keywords:

spin wave, Brillouin Light Scattering measurement, dispersion relation, asymmetric propagation

## Dispersion characteristics of spin waves channeled in antiferromagnetic domain walls

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### Abstract:

Antiferromagnets are novel materials composed of sublattices of antiferromagnetically coupled spins that result in negligible magnetizations and have potentials for the application in spintronics owing to their unique features including ultrafast magnonic dynamics. For example, spin waves in uniformly ordered bipartite antiferromagnets have dispersion relations similar to solutions of the Klein-Gordon equation by considering the uniaxial anisotropy and their frequencies lie in the terahertz regime in common antiferromagnetic materials, while the forbidden frequency gap observed in those dispersion relations is estimated to be on the order of a few hundreds of gigahertz. Recently, channeling of spin waves in domain walls was proved to avoid such huge frequency gap in ferromagnetic materials and allow the low-frequency excitation of spin waves for the sake of less heat dissipation. Here, we show that the spin waves in antiferromagnetic domain walls have gap-less dispersion relations as well, according to the parameterization and formulations proposed by Hals *et al.* [Phys. Rev. Lett. **106**, 107206 (2011)].

### Keywords:

spin wave, domain wall, antiferromagnetic material

## Versatile MBE growth of tetrataenite L1<sub>0</sub>-FeNi film

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### Abstract:

Ordered hard magnetic L1<sub>0</sub>-FeNi, tetrataenite, has attracted attention as a good candidate for the rare-earth-free permanent magnet with comparable maximum magnetic energy product. In this work, high-quality FeNi films were fabricated using molecular beam epitaxy (MBE) on Al<sub>2</sub>O<sub>3</sub> (0001) substrate with different deposition routes i.e., co-deposition (CD), alternative monatomic layer deposition (AMLD), and 2 steps co-deposition (2SCD). XRD patterns indicated that the L1<sub>0</sub>-FeNi phase was successfully obtained using these three deposition routes from low to moderate substrate temperature. Surprisingly, the best substrate temperature for the CD route is 50 °C. By using 2SCD, it is possible to fabricate samples at higher substrate temperatures for better film crystallinity with the best substrate temperature of 200 °C. Whereas lower quality films were achieved using AMLD, attributed to the smaller diffusion of Fe and Ni in this growth route. More characterizations of the films using neutron reflectometer and vibrating sample magnetometer will be discussed. Our work provides a comprehensive picture of MBE growth of the L1<sub>0</sub>-FeNi film for the development of next-generation rare-earth-free hard magnetic materials.

### Keywords:

FeNi, MBE, 2 steps deposition, codeposition, magnetism, monatomic layer deposition

## Excitation-dependent emissive FeSe nanoparticles induced by chiral interlayer expansion and their multi-color bio-imaging

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### Abstract:

Layered transition metal chalcogenide nanostructures reveal unprecedented electronic and optical properties due to the unusual arrangement of interlayers and electronic interactions between them. Here, we report layered FeSe nanoparticles (NPs) coupled by *L*- or *D*-cysteine as a chiral stabilizer to show multi-colored excitation dependent emission (MEDE) for both single- and two-photon photoluminescence breaking conventional Kasha and Vavilov rules of luminescence, which is the first report in inorganic nanostructure system. Structural analysis shows the chiral stabilizer-induced interlayer spacing expansion in a FeSe NP. The MEDE in FeSe NPs is revealed to originate from the impurity coupled to the Mott insulator character of FeSe and chiral interlayer expansion through the first-principles electronic structure calculations and the classical molecular dynamics. Taking advantage of biocompatibility and multiphoton excitation in FeSe NPs, MEDE was utilized for bio-imaging of neuron cells and tissues altering excitation wavelength from visible to near-infrared range expanding the capabilities of multi-color bio-labeling.

### Keywords:

Excitation-dependent emission, Multiphoton excitation, Chiral nanoparticles, Mott insulator, Multi-color bio-imaging

## Rotating magnetocaloric effect (RMCE) in $RB_4$ (R=Gd-Tm) group

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### Abstract:

In order to overcome several problems of ordinary magnetocaloric effect (MCE) application, a new approach named 'rotating magnetocaloric effect (RMCE)' has been suggested and studied extensively in recent years. Since this effect can be realized by only rotating the direction of the magnetic materials in a constant magnetic field, there is neither mechanical losses caused by the moving of magnetic materials nor space restrictions for device integration. And as one might suspect, the most important two conditions for showing high RMCE efficiency are the high magnetic entropy change ( $\Delta S_M$ ) for a specific crystal direction and high magnetic anisotropy for the other direction one. According to these conditions, we concentrated on  $RB_4$  (R=Gd-Tm) group.  $RB_4$  (R=rare earth element) group is a representative geometrically frustrated system with an SSL (Shastry-Sutherland lattice) structures, indicating high magnetic entropy in  $RB_4$  system. It is also well known that  $RB_4$  group shows high magnetic anisotropy between two directions, i.e.  $H \parallel c$  and  $H \perp c$ . Furthermore, quadrupole ordering existing in  $RB_4$  (R=Dy, Ho) can also cause high value of rotating magnetic entropy change,  $\Delta S_R$ . We measured magnetization of  $RB_4$  (R=Gd-Tm) and calculated  $\Delta S_R$  using Maxwell's relations. As expected, high values of  $\Delta S_R$  were obtained for  $RB_4$  (R=Dy-Tm). Especially, the value of  $\Delta S_R$  for  $DyB_4$ , 18.9 J / kg K under 50 kOe at 11.5 K is comparable to the highest value of single crystal RMCE reported before. This work suggests  $DyB_4$  single crystal as an attractive candidate for RMCE material operating on  $H_2$  liquefaction temperature range. On the other hand, more specific discussion of abnormal  $\Delta S_R$  dependency of  $RB_4$  (R=Gd-Tm) will be described, too.

### Keywords:

$RB_4$ , RMCE, geometrical frustration, quadrupole ordering

## Role of Ti in magneto-crystalline anisotropy of Co/Pt thin film

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### Abstract:

Perpendicular magneto-crystalline anisotropy (MCA) is one important property for spintronics applications [1-3], which is advantageous for high thermal stability and low switching current [4]. Here, we present density functional study on the role of single Ti layer in magneto-crystalline anisotropy of Co/Pt thin film. In particular, the role of Ti, as insertion versus capping, is investigated with  $E_{MCA}$ . The insertion, Ti in between Co and Pt, shows  $E_{MCA} = 0.58$  meV/film. On the other hand, the capping, Ti placed on top of Co/Pt, exhibits  $E_{MCA} = 1.24$  meV/film, larger than Ti-insertion. From MCA analysis based on perturbation picture [5], the difference between insertion and capping is due to occupancy change of Pt  $|m|=1$  orbital.

[1] S. Wolf et al., Science **294**, 1488 (2001).

[2] I. Zutic et al., Rev. Mod. Phys. **76**, 323 (2004).

[3] A. Brataas et al., Nat. Mater. **11**, 372 (2012).

[4] Soon-Wook Jung et al., Appl. Phys. Lett. **92**, 202508 (2008).

[5] Ding-Sheng Wang et al., Phys. Rev. B **47**, 14932 (1993).

### Keywords:

density-functional theory, magneto-crystalline anisotropy

## Effect of valence fluctuation on the magnetic and thermoelectric properties of $\text{Eu}_8\text{CuNi}_{2.5}\text{Si}_{42.5}$ clathrate

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### Abstract:

Inorganic clathrates have been extensively investigated owing to their unique and intriguing atomic structure as well as their potential as superconducting and thermoelectric materials. The connection between the chemical ordering and the physical properties has however, remained elusive. Among the clathrate family, type-I clathrates are the most extensively considered due to their stable structures and variety of species. In the present study,  $\text{Eu}_8\text{CuNi}_{2.5}\text{Si}_{42.5}$  polycrystal crystal were synthesized using arc melting and then cold press. The guest and host atoms site occupancies were investigated with Rietveld refinement. The complete replacement of  $\text{Ba}^{2+}$  ions by  $\text{Eu}^{2+}$  ions was analyzed using the shift in PXRD and the Raman peaks. A homogenous morphology and presence of respective elements shown by the SEM- EDX mapping and XPS analysis. Magnetic studies perform for the  $\text{Eu}^{2+}$  clathrate sample shows an electron hopping between  $\text{Eu}^{2+}$  and  $\text{Eu}^{3+}$  ion and has the antiferromagnetic transition at 13 K. The clathrate sample is metamagnetic and has two field dependent antiferromagnetic phases at low magnetic field. The magnetic entropy calculated for the  $\text{Eu}_8\text{CuNi}_{2.5}\text{Si}_{42.5}$  compound comes to be 3.15 J/Kg-K.

### Keywords:

Clathrate, rare earth material, ferromagnetic, Type I structure, electron hopping

## Quantum-classical crossover in a molecular magnet embedded in S/F/S Josephson junction

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### Abstract:

Within the frameworks of the spin-coherent-state path integral method we consider quantum-classical escape-rate crossover of a superconductor-molecular magnet-superconductor(SMS) with the bias current and the external magnetic field. Employing the instanton technique and the nonlinear perturbation method near the top of the energy barrier, we obtain the phase boundary between the first- and the second-order crossovers. We demonstrate that the bias current plays a crucial role in determining the phase boundary and that the region for the first-order crossover is greatly suppressed by the supercurrent as well as the external magnetic field. These features are expected to be observable with existing experimental techniques.

### Keywords:

molecular magnet, quantum tunneling

## Study of the electronic structure of Kagome metal $AV_3Sb_5$ (A = K, Rb, Cs)

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### Abstract:

We have investigated the electronic structure of Kagome lattice materials of  $AV_3Sb_5$  (A = K, Rb, Cs) within the density functional theory (DFT). Kagome materials  $AV_3Sb_5$  show many intriguing physical properties such as charge density wave (CDW) transition around 80 ~ 100 K, superconductivity below 0.9 ~ 2.5 K, and  $Z_2$  topological surface states. We have studied these physical properties by computing their electronic band structures and phonon dispersions. From DFT calculations, we have found flat bands and Dirac cones possessing vanadium d orbital characters. Furthermore, we have confirmed that the CDW transition could be controlled by the dimensionality reduction. In future studies, we will investigate how the CDW transition is closely intertwined with the superconductivity. It would help us to understand unconventional and topological superconductivity exhibited in  $AV_3Sb_5$ .

### Keywords:

Density functional theory, Kagome lattice, Electronic structure calculation

## Electronic and magnetic structure of double perovskite BaLaCuOsO<sub>6</sub>: density functional theory

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### Abstract:

To understand the electronic and magnetic structure of BaLaCuOsO<sub>6</sub>, a newly synthesized antiferromagnetic 3d<sup>9</sup>-5d<sup>3</sup> double perovskite<sup>1</sup>, we carried out density functional theory calculation. Our numerical results reveal that the system shows C-type antiferromagnetic ordering and that its reduced magnetic moment observed in the experiment is due to the spin-orbit coupling as well as p-d hybridization. We also estimated exchange couplings which were found to be understood based on the superexchange mechanism. Although out-of-plane nearest-neighbor interaction is much suppressed, finite next-nearest-neighbor coupling enables the C-type ordering to be stabilized. Our results explain several experimental observations, providing a comprehensive understanding and insights into the electronic and magnetic structure of this 3d<sup>9</sup>-5d<sup>3</sup> double perovskite system.

[1] G. S. Thakur, H. L. Feng, W. Schnelle, C. Felser, and M. Jansen, Structure and Magnetism of New A- and B-Site Ordered Double Perovskites ALaCuOsO<sub>6</sub> (A = Ba and Sr), J. Solid State Chem. 293, 121784 (2021).

### Keywords:

double-perovskite, magnetism, density functional theory calculation

## A computational study of titanyl phthalocyanine on Ag(100) and on MgO/Ag(100)

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### Abstract:

Titanyl phthalocyanine (TiOPc), a non-magnetic molecule from the family of the metal-phthalocyanines (MPcs, C<sub>32</sub>H<sub>16</sub>N<sub>8</sub>M, M = Ti, V, Cu, *etc.*), is commonly used to dilute the isostructural magnetic compound VOPc to reduce the spin-spin interaction and enhance the coherence time of VOPc. [1]

In this work, we perform calculations based on density functional theory (DFT) to confirm that TiOPc adsorbed on the silver (100) surface remains non-magnetic (total spin  $S=0$ ), indicating that it can be used as a templating host for VOPc spin-qubits. [2] We study the effect of TiOPc-Ag hybridization by inserting a thin insulating buffer layer (MgO) between the TiOPc and the Ag(100) surface. Our findings show, in good agreement with experiments conducted in a low-temperature scanning tunneling microscope, that TiOPc retains its vacuum-like  $S=0$  electronic structure on both Ag and MgO/Ag substrates and is therefore suitable as a decoupling and a templating layer for isostructural spin-based qubits on a wide range of surfaces.

[1] Bonizzoni, C. *et al.* Coherent coupling between Vanadyl Phthalocyanine spin ensemble and microwave photons: Towards integration of molecular spin qubits into quantum circuits. *Scientific Reports*, 7(1), 1–8 (2017).

[2] Colonna, S. *et al.* Supramolecular and chiral effects at the titanyl phthalocyanine/Ag(100) hybrid interface. *J. Phys. Chem. C* 118, 5255–5267 (2014).

### Keywords:

#spinqubit #surface #metalphthalocyanine #titanylphthalocyanine #TiOPc, #VOPc, #vanadylphthalocyanine, #DFT, #DensityFunctionalTheory, #spin #qubit, #TiOPc/Ag #TiOPc/MgO/Ag #decouplinglayer, #scanningtunnelingmicroscope #STM

## Configuration of water molecules at the electrified electrochemical interfaces with graphene electrodes

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### Abstract:

A detailed understanding of the atomic and electronic structures of electrified electrochemical interfaces has critical implications for the development of advanced electrochemical devices. Graphene has been regarded as an ideal component for electrode materials in field of energy conversion and storage due to its unique electrical, thermal and mechanical properties. Despite the need for a better understanding of the device system in electrified situation with finite electrodes, first-principles characterizations based on the standard non-equilibrium Green's function (NEGF) approach have been so far mostly limited to the device system with semi-infinite electrodes due to the theoretical limitation of NEGF. In this presentation, taking the advantage of the multi-space constrained-search density functional theory (MS-DFT) formalism [1,2] that can handle the electrified finite electrodes, we firstly investigate the total enthalpy change of the water molecule on the electrified graphene electrode surface in fully first-principles scheme. Moreover, by carrying out molecular dynamics calculations based on MS-DFT, we will provide the configuration of condensed water at the electrified graphene-water interfaces and compare the interfacial water structures to that on metal electrodes. This study will show insight into the water configuration affected by electrified electrochemical interface

### Keywords:

Molecular Dynamics, Graphene, Electrified electrochemical interfaces

## Feasible experimental growth of novel aluminum nitride polytypes: A DFT perspective

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### Abstract:

We present the results of a first-principles study of the structural stability, electronic and optical properties of new polytypes of the aluminum nitride (AlN) (including those of the experimentally/theoretically known phases: wurtzite, zincblende, and rocksalt structures) to complement the picture of the pressure-dependent phase diagram of this industrially important compound. Along with the previously considered structures of AlN in other theoretical studies, we evaluated the dynamical stability of various novel phases, viz., SiC(4H), ZnS(15R), BeO, 5-5, TiAs, NiAs, MoC, Li<sub>2</sub>O<sub>2</sub>, and NiS, which were predicted recently in a study of high-pressure data-mining of more than 140,000 candidates of AlN structure, and claimed that they were either stable or near stable, based on the first-principles calculations. Based on the new AlN polytypes, all considered phase's physical properties are compared, and the common trends and differences are presented. According to the phonon band structures calculations, 9 phases of these new polytypes are free from the imaginary frequencies, indicating their adequate dynamical stability, which should be accessible to the experiment. Additionally, the calculated cohesive energies of the dynamically stable phases are comparable to that of the WZ-AlN and available literature. Furthermore, the electronic structures and optical results indicate that the polytypism of AlN is a practical tool for refining the physical and chemical properties. In other words, the exciting physical features of the new phases show them as promising candidates for new future electronic and optoelectronic applications for AlN.

### Keywords:

First-principles calculations, polytypism, structural stability, electronic structure, optical properties

## First-principles study of Janus 2D heterostructures for valleytronics applications

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### Abstract:

Since the discovery of graphene, many researchers have studied two-dimensional (2D) materials that exhibit various interesting physical and electrical properties. A lot of theoretical and experimental studies have been conducted on 2D van der Waals (vdW) heterostructures because they can be easily fabricated by mechanical exfoliation or delamination due to weak vdW interactions. Interestingly, 2D vdW heterostructures have shown superior properties to utilize 2D materials in nano- and electronic devices. In this study, we have investigated atomic and electronic structures of Janus 2D heterostructures using density functional theory calculations. Especially, we calculate band structures of Janus 2D heterostructures and focus on Rashba spin splitting and Zeeman-type spin splitting at the valleys by studying the effect of interaction between 2D materials in heterostructures. In addition, we investigate Berry curvatures of Janus 2D heterostructures depending on strain and out-of-plane external electric field. From the understanding of valley physics in Janus 2D heterostructures, we suggest the possibility of their applications in valleytronic and spintronic devices.

### Keywords:

Janus structure, Valleytronics, DFT

## Fast computation of lattice thermal conductivity using machine learning interatomic potentials

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### Abstract:

Lattice thermal conductivity is of central importance in materials engineering field. For instance, insulator for silicon-on-insulator devices needs high thermal conductivity to dissipate heat to the substrate, and thermoelectric materials are benefited from low thermal conductivity as it prevents unstoppable heat flow along the temperature gradient. A reliable approach for the theoretical evaluation of lattice thermal conductivity exploits ab initio calculations to determine both harmonic and anharmonic force constants to solve the Boltzmann transport equation (BTE). However, calculating the force constants demands atomic forces of thousands of supercells, which bottlenecks the ab initio approach.

Neural network potentials (NNPs) can accelerate the BTE approach by computing force constants, replacing costly ab initio calculations. NNPs trained by ab initio data set has an accuracy comparable to first principles at a fraction of computation time. In this study, we propose an approach combining NNP and BTE to calculate lattice thermal conductivity that satisfies two requirements for its general application: consistent choice data set and computational speed-up. In the former, we compare three different types of data set and the size of data set on the accuracy of transport properties. This work will widen the applicability of machine learning potentials by demonstrating a robust workflow to accurately calculate lattice thermal conductivities.

### Keywords:

machine learning potential, lattice thermal conductivity, phonon Boltzmann transport equation, accelerated computation

## Plasmonic catalysis in metallic nanoclusters: A time-dependent density functional theory study

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### Abstract:

Localized surface plasmons (LSP) can be generated at the surface of metallic nanoparticles under an external incident light. Provided that the light field is tuned to result in LSP resonance, a large amount of energy can be absorbed by the cloud of quasi-free electrons near the nanoparticle surface in the form of strongly enhanced local electric fields. The collective electronic density oscillations and intensity amplification of the incoming light field contribute to the generation of hot carriers at the surface. This mechanism can be employed to accelerate the chemical transformations on the plasmonic nanoparticles through hot electrons transfer to the nanoparticle-reactant interface. In here, based on real-time time-dependent density functional theory (TD-DFT), we investigate the optical and plasmonic properties of silver and aluminum nanoclusters through the analysis of the electronic charge density dynamics caused by an external perturbation. It is shown that the optical absorption spectra of the excited nanoclusters are significantly dominated by the LSP resonance frequency. To examine the plasmonic catalysis capability of these nanoclusters under an incident light, we study the chemical bond activation of methane and fluorine gas molecules, at the nanocluster-molecule interfaces.

### Keywords:

LSPR, TD-DFT, Plasmonic catalysis, Plasmonic nanoparticles, Bond activation

## topological classification of nodal-line semimetals with square-net structures.

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### Abstract:

In recent years, the topological semimetal phase with Dirac nodal line was observed in tetragonal  $P4/nmm$  space group materials with square-net substructure, such as  $AMnBi_2$  ( $A$ =alkali earth/rare earth metals) and  $ZrSiS$ -type materials. Also, the origin of the non-trivial topology was not clearly understood in previous studies.

In our work, we performed a first-principles electronic structure calculation and constructed effective tight-binding Hamiltonian including the distant-neighbor hopping between  $p$ -orbitals. Based on the developed out tight-binding model, we showed that the nontrivial topology comes from the interplay of electron-hole asymmetry and spin-orbit coupling. We show phase diagram as a function of electron/hole doping level and electron-hole asymmetry.

Moreover, we introduced three-dimensional energy dispersion and classified Fermi surface topologies of square-net material into six types. Our classification reproduces previously reported quantum oscillation results. Finally, we expect that our model of classification suggests a clue of magneto-resistance studies.

### Keywords:

nodal-line semimetal, Tight-binding model, First-principles calculation

## 열전도도 측정 장치 구축

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### Abstract:

열역학적계에 발생한 온도차는 열에너지의 흐름을 만들어내는 데, 고체계에서는 이러한 열에너지의 흐름은 전자와 포논을 비롯한 다양한 준입자들에 의해 이루어진다. 그리고 정해진 시간동안 가한 열에 따른 공간상의 온도분포를 측정함으로써 물질의 열전도도를 정하게 된다. 최근 열전도도 측정은 매그논이나 스피논과 같은 자기적 여기상태로 형성된 자기 준입자를 찾아내거나 그것의 동역학적 특성을 이해하는 데 많이 활용된다. 최근 발견된 준1차원  $S=1$  체인 시스템인  $\text{NiTe}_2\text{O}_5$ 에서는 상전이 온도 아래에서 질서변수가 이상 멱법칙을 보이며 온도에 따라 증가하고, 상전이 온도보다 높은 온도에서도 자기요동이 사라지지 않는 현상이 실험적으로 관찰된다. 우리는  $\text{NiTe}_2\text{O}_5$ 에서 보여지는 이처럼 특이한 자기 현상과 관련된 자기적 여기 상태를 온도 및 자기장 변화에 따른 열전도도로부터 이해하고자 한다. 이를 위해 우리는 Quantum Design사에서 제작한 열전도도 측정용 기구와 별도의 전자 기기들을 활용하여 열전도도 측정 장치를 구축하고자 하였다. 이번 발표에서는 이렇게 구축한 열전도도 측정 장치에 대해 발표하고 앞으로의 개선점에 대해 논하고자 한다.

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### Keywords:

열전도도, 열전도도 측정 장치

## Controlling metal-insulator transition of VO<sub>2</sub>(200)/R-Al<sub>2</sub>O<sub>3</sub>(012) thin film by interfacial strain

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### Abstract:

It is well known that vanadium dioxide (VO<sub>2</sub>) exhibits a metal-insulator transition (MIT) near room temperature,  $T = 68^{\circ}\text{C}$  and its transition temperature can be noticeably affected by the various substrates, often leading to the emergence of unexpected physical properties, e.g. intermediate structure phase, specific domain shape. Here, we focus on the effect of interfacial strain on MIT properties of VO<sub>2</sub> thin film prepared on R-Al<sub>2</sub>O<sub>3</sub>(012).

First, we monitored the temperature-dependent structure behavior of the VO<sub>2</sub> /R-Al<sub>2</sub>O<sub>3</sub>(012) in 3D reciprocal space from the measurement of theta rocking curve at the 9C beamline of the Pohang Accelerator Laboratory (PAL). To compare the electrical properties of the thin film to the structural change, 3D reciprocal space mapping and the resistance of thin films were measured simultaneously. We found that multi-domains with a specific angle started to appear in the thin film. Also, the signal for the Epi-layer grown along the substrate was observed at different  $q_x$  and  $q_y$  positions from the multi-domain.

Our results suggest the following: the behavior of multi-domain and epi-layer components at various temperatures. 1. The opposite behavior between the multi-domain and the epi-layer at the interface is present even after the structural phase change of the thin film, i.e. M1 to rutile. 2. The phase transition temperature decreases as the thickness of the thin film increases. 3. Regardless of the thin film thickness, the resistance of the thin film started to change only when the structural phase transition was completed. 4. When the angle between the multi-domain was changed, the electrical characteristics started to change. This can be direct evidence that, in addition to structural changes occurring within domains, structural correlations (domain boundary, twinning) between domains generated by multi-domain with different arrangements appear as an important mechanism for electrical properties (macroscopic).

Our work provides critical insight on how the interfacial properties affect the properties of MIT characteristics and the formation of the multi-domain.

### Keywords:

vanadium oxide, grain boundary, twinning, 3D RSM, Metal-insulator transition

# Fast Quantum State Tomography Implemented by Measurement Axis Adjustment

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## Abstract:

We developed a fast quantum state tomography method by choosing three independent measurement axes based on the initial statistical sampling of qubit state measurements. The measurement standard deviation (SD) is inversely proportional to the square roots of  $N$ , the number of readout, and proportional to the square roots of  $p(1-p)$  where  $p$  is a probability that state readout results in 0 (or 1). Accordingly, a straightforward way of reducing SD is to increase  $N$  which requires a large number of state-readout. An alternative way is to adjust measurement axes and, thus, modify the probability  $p$  of state readout. After the adjustment, we were able to obtain the equal error bound of SD with only  $2/3$  of  $N$  required previously. This method is independent of the 0/1 state resolution of the system. Therefore, the worse the system resolution, the more the required number of readout decrease.

## Keywords:

quantum state tomography, superconducting qubit, feedback measurement

## UV-Visible photoresponse enhancement at self-power and low bias mode by plasmonic nanoparticle treatment of Quasi Freestanding Graphene/vicinal SiC devices

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### Abstract:

Large area Metal-Graphene-Metal UV/Visible photodetector have been fabricated on quasifreestanding graphene (QFSG)/vicinal SiC (8° off-axis) wafer applicable for future low power consumption system. The migration of carriers in QFSG/vicinal SiC photodetectors under 365 nm (UV) and 405 nm (Visible) light irradiation by a built-in electric field (self-powered) and low bias (-10mV). The photocurrent gain and responsivity under UV/Visible light is significantly larger on QFSG/vicinal SiC due to the freestanding nature of topmost layer and absence of buffer layer, the main carrier scattering /trapping centers, unlike in epitaxial graphene (EG)/SiC(0001). Furthermore, photocurrent gain and responsivity are tuned by localized surface plasmon resonance (LSPR) phenomena using gold nanoparticles (AuNPs). In comparison to EG/SiC(0001), photocurrent is enhanced by 9-fold at self-power mode and nearly 120-fold at low bias mode in QFSG/vicinal SiC. Significant responsivity of QFSG/vicinal SiC after AuNPs treatment is  $\approx 1.65\text{mA/W}$  (at zero bias) and  $\approx 20\text{mA/W}$  (at -10mV) under illumination of 365nm light ( $P = 18\text{mW/cm}^{-2}$ ) and many-fold increase in responsivity with respect to that in EG/SiC(0001). The above results confirm that this QFSG/vicinal SiC combined with AuNPs possesses great potential in UV-Visible detection applications with minimum power consumption.

### Keywords:

Graphene/vicinal SiC, plasmonic nanoparticle, UV/Visible light, epitaxial graphene, localized surface plasmon resonance (LSPR)

## More than Morse: Observing an additional interaction between CO molecules with Lateral Force Microscopy

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### Abstract:

By functionalizing the tip with a single CO molecule, the spatial resolution of atomic force microscopy (AFM) can be drastically increased. The contrast produced by a CO tip can often be understood by considering Pauli repulsion and the tilting of the probe molecule. We have previously simulated this via a Morse potential and a torsional spring.

Here, we used Lateral Force Microscope, a variant of frequency modulation atomic force microscopy, to quantify the interaction between a CO tip and a CO on the Cu (111) surface. Interestingly, an additional feature appears in the measurement when we measured closer to the surface at the side of the surface CO. This new feature cannot be explained with our previous model. Following the results of other investigations, we include the electrostatic force in our simulations.

### Keywords:

Frequency modulation atomic force microscopy (FM AFM), Frequency modulation lateral force microscope (FM LFM), Scanning tunneling microscope (STM), Functionalized tip, lateral interaction in atomic scale

## Neutron skin thickness of $^{208}\text{Pb}$ using neutrino scattering in Quasiparticle Random Phase Approximation

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### Abstract:

$^{208}\text{Pb}(\nu_e, e)^{208}\text{Bi}$ 와  $^{208}\text{Pb}(\bar{\nu}_e, e)^{208}\text{Tl}$ 의 reaction cross section을 Quasiparticle Random phase Approximation 하에 계산하여  $^{208}\text{Pb}$ 의 neutron skin thickness를 이론적으로 얻어낼 수 있다. supernova에서 발생하는 neutrino를 관측하여 supernova 내부에서 발생하는 일을 관측할 수 있다. 또한 이번 J-PARC에서 만드는 neutrino beam을 이용하여 새로운 방법으로 관측을 할 수 있으며  $^{208}\text{Pb}$ 를 neutrino detector로 이용할 수 있다. 다른 모델로는 계산이 어려운 high energy state level를 QRPA 모델로 구조를 계산할 수 있다.

### Keywords:

structure

## Yukawa 퍼텐셜에 대한 슈뢰딩거 방정식의 두 가지 수치해석적 풀이

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### Abstract:

슈뢰딩거 방정식은 양자역학에서 입자의 상태를 표현하는 방정식으로 이를 풀면 입자의 고유 에너지와 고유 함수를 알 수 있다. 그러나 해가 알려진 몇 가지 퍼텐셜에 대한 경우를 제외하고는 해석적으로 푸는 것이 불가능하다고 알려져 있으며 따라서 슈뢰딩거 방정식의 수치해석적 풀이에 대한 연구가 진행되어 오고 있다.

본 연구에서는 두 가지의 수치해석적 방법으로 Yukawa 퍼텐셜에 대한 슈뢰딩거 방정식의 해를 구하고자 했다. Yukawa 퍼텐셜은 구면 대칭 퍼텐셜이므로 슈뢰딩거 방정식의 지름 방정식에 대해서만 우선적으로 고려하였다. 첫 번째 방법으로는 4차 Runge-Kutta 방법으로 방정식을 구현하고, 쏘아보기 법을 사용하여 고유해를 구하였다. 두 번째로는 Euler의 방법을 이용해 방정식을 구현한 후, 고유함수의 물리적인 경계조건과 수치해의 특성을 이용하여 고유해를 구하였다. 두 방법 모두 본 계산에 들어가기 전에 Coulomb 퍼텐셜에 대한 지름 방정식의 해석적인 해와 비교하여 방법의 유효성 및 타당성을 확보하였다. 이후 Yukawa 퍼텐셜에 대한 지름 방정식의 고유해를 계산하여 두 방법의 결과를 서로 비교 및 검증하였고, 선행 연구 결과들과 비교하여 Bohr 반지름의 500배에서 10배 사이의 screening length 대해 1s에서 3d 상태까지 1% 이내의 오차로 결과를 얻을 수 있었다.

### Keywords:

Yukawa potential, Schrodinger equation, Numerical method

## A Study on the Measurement of Half-life for $^{177}\text{Re}$ and $^{179}\text{Re}$ Isotopes by using 100-MeV Proton Accelerator

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### Abstract:

고에너지 양성자에 의한 핵반응은 다양한 분야에서 연구되고 있다. 특히 인공위성 및 국제우주정거장과 같은 우주 구조물에 대한 고에너지 양성자에 대한 영향 평가는 과거부터 지속적으로 연구되어 지고 있다. 또한 항성에서의 양성자에 의한 물질합성에 대한 연구 분야에서도 고에너지 양성자의 핵반응에 대한 연구는 항성의 구조 및 항성에서의 원소 합성과 매우 밀접한 관련을 가지고 있다. 뿐만 아니라 양성자를 이용한 핵 파쇄에 관한 연구에도 양성자 핵반응에 대한 중요한 연구들이 진행되고 있는 실정이다. 본 연구에서는 천연 텅스텐( $^{182}\text{W}$ :26.50%,  $^{184}\text{W}$ :30.64% 과  $^{186}\text{W}$ :28.43%)을 표적으로 한국원자력연구원 소속의 KOMAC에 있는 100MeV 양성자가속기를 이용하여  $^{177}\text{Re}$  및  $^{179}\text{Re}$  핵종을 생성하였다. 100MeV 에너지 양성자를 시료에 조사하여 고순도 Ge(HPGe)검출기를 이용하여 196.9 keV( $^{177}\text{Re}$ ) 및 289.97 keV( $^{179}\text{Re}$ ) 감마선 스펙트럼을 얻어 분석한 후 핵반응에 의해 생성 가능한 핵종 분석하여 각 핵종에 대한 반감기를 측정하였다. 본 연구를 통하여 얻어진 결과들은 과거 도출된 결과들과 비교 분석 하였다. 본 연구는 실제 고에너지 양성자가 물질 속에 입사함으로써 발생하는 물질변화의 양과 항성 속에서 만들어지는 물질들의 양을 동정하는데 매우 중요한 자료로 사용되어 질것으로 기대된다.

### Acknowledgement

This work was supported by the BB21+ Project in 2022.

### Keywords:

$^{177}\text{Re}$ ,  $^{179}\text{Re}$ , Proton Beam

## The Study of a Compositated Radiotherapy Method

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### Abstract:

In this study, a new radiotherapy method is proposed, which combine the proton therapy and Boron Neutron Capture Therapy (BNCT). In this method, firstly the BNCT is implemented, in which, with the radiation of thermal neutron, the He-4 ion and Li-7 ion are emitted to targeting destroy the local cell, and normally they stop at inside of the local cell due to their short ranges. As a result, the a large number of Li-7 are accumulated in the target cell. Then, the proton therapy is implemented. Based on the nuclear bombardment reaction:  $\text{Li-7}(p, \alpha)\alpha$ , beside of the dose from original proton beam, the addition dose of two emitting alpha particles (each with energy of about 8.6 MeV) can be induced in target cell. For evaluating the effects of this new compositated radiotherapy method, here, a Monte Carlo method is used. Through analysing the dose distribution of this method with comparison of BNCT and proton therapy, it can be concluded that under the same therapy effect, this method has advantage to reduce the radiation damage to normal tissue region.

### Keywords:

Radiotherapy Method, BNCT, Proton Therapy

## Momentum-Kick model에서 다중도 의존성 계산

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### Abstract:

Momentum-Kick model은 능선 구조(ridge structure)를 설명하는 모델이다. 능선 구조는 중이온 충돌에서 발생하는 입자들의 long-range(대략  $\Delta\eta > 2$ ) 부근의 분포 형태를 말한다. 지금까지 능선 구조는 쿼크-글루온 플라즈마(Quark-Gluon Plasma, QGP) 상태에 있는 유체의 집단 운동으로 만들어진다고 설명되었다. 충분한 에너지와 밀도를 가지는 중이온 충돌은 QGP를 만들 수 있지만, 양성자 간의 충돌과 같은 작은 계 (small system)에서는 QGP가 만들어지기 어렵기 때문에 QGP에 의한 능선 구조가 나타나지 않을 것으로 믿어왔다. 하지만 높은 다중도(multiplicity)의 양성자 충돌 실험 결과에서는 능선 구조가 관찰되는데, 이러한 현상을 설명하기 위해 운동학적 관점에서 접근한 모델이 Momentum-Kick Model이다. 이 모델은 입자 간 충돌에 의해 발생한 제트(jet)가 그 매질(medium)안의 쪽입자(parton)에 운동량을 전달하게 되고, 운동량을 전달받은 쪽입자들이 같은 방향으로 나열되어 집단 운동을 보임으로써 양성자의 충돌과 같은 작은 계에서도 능선 구조가 발생할 수 있다고 설명한다. 이 때 능선 구조가 나타나는 경향은 다중도에 따라 달라진다. 따라서 이 연구에서는 입자의 충돌을 역학적으로 계산한 뒤 모델에 다중도를 적용해 보았다. 제트와 쪽입자가 충돌하여 제트의 운동량이 전달되는 쪽입자들의 평균 갯수는 충격 변수(impact parameter)의 의존성을 가진다. 다중도 또한 충격 변수의 의존성을 가지기 때문에 충격 변수를 통하여 다중도를 모델에 적용하였다.

### Keywords:

Ridge, Momentum-Kick, Multiplicity

## Describe the Ridge structure in various high-multiplicity pp collision at $\sqrt{s_{NN}}=13\text{TeV}$ via Momentum-Kick model

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### Abstract:

Momentum-Kick 모델은 중이온 충돌에서 나타나는 실험결과의 near-side 부분에서 나타나는 능선 구조(Ridge structure)를 설명하는 모델이다. 이 모델은 상대론적 중이온 충돌기(Relativistic Heavy Ion Collider, RHIC)의 PHENIX(Pioneering High Energy Nuclear Interaction eXperiment)에서의 AuAu 200GeV 충돌과 거대 강입자 충돌기(Large Hadron Collider, LHC)에서의 PbPb 2.76TeV에서 near-side 영역의 실험결과를 성공적으로 기술할 수 있었다. 이 모델은 충돌 직후에 원뿔모양으로 나타나는 제트(Jet) 입자들이 주변의 medium 쪽입자들과 충돌을 일으키는 운동학적인 현상을 이용하여 능선 구조를 설명하는 모델이다. 중이온 충돌에서는 충분히 높은 밀도와 온도의 환경이 만들어지기 때문에 이러한 환경에서 생성되는 쿼크-글루온 플라즈마(QGP)현상을 전제로 하는 유체동역학을 이용하여 설명하는 것이 일반적이었다. 하지만, 양성자-양성자 충돌의 경우에는 QGP를 생성할 수 있는 충분한 밀도와 온도의 환경이 만들어지기 힘들기 때문에 능선 구조가 나타나지 않을 것이라 예상했었고, 일반적인 양성자-양성자 충돌에서는 능선 구조가 확인되지 않았다. 그러나, 고다중성의 경우로 한정할 경우에는 능선 구조가 관측되었으며, 다중성의 정도에 따라 입자들의 분포가 다른 것을 확인할 수 있었다. 그러므로, 우리는 능선 구조를 설명하기 위하여, 양성자-양성자 충돌에서도 똑같이 적용될 수 있는 Momentum-Kick 모델을 적용해 보고자 하였다. 양성자-양성자 충돌에서와 같은 작은 계의 경우에는 Jet 입자와 쪽입자들 사이의 운동학적인 현상이 더욱 드러날 것이기 때문에, Momentum-Kick 모델이 실험결과를 잘 설명할 수 있을 것이라 기대한다. 따라서 우리는 양성자-양성자 충돌의 다양한 고다중성 데이터에 Momentum-Kick 모델을 발전적으로 적용하여, LHC의 A Toroidal LHC ApparatuS(ATLAS), Compact Muon Solenoid(CMS) 실험 데이터에 나타난 능선 구조를 잘 설명할 수 있었다.

### Keywords:

Ridge, Heavy-ion, Momentum-Kick

## The measurement of the absolute light yield of crystal scintillators by utilizing silicon photodiodes

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### Abstract:

Silicon photodiodes have the advantage of high quantum efficiency in the range of visible wavelength, and it is matched well to the emission wavelength of the crystal scintillators. The crystal scintillator emits the light yield proportional to incident energy so that the accurate measurement of absolute light yield is important for gamma spectroscopy. We measure the absolute light yield of CsI(Tl), GAGG, BGO, LYSO, and NaI(Tl) by utilizing the silicon photodiode and avalanche photodiode. The electronic calibration constant and emission weighted quantum efficiency are used for the calculation. We report our test results and discuss the feasibility of utilizing silicon photodiodes in absolute light yield measurement.

### Keywords:

Silicon photodiode, Avalanche photodiode, Absolute light yield, Crystal scintillator

## Status of prototype Beam Drift Chamber(BDC) of the LAMPS Experiment

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### Abstract:

Beam Drift Chamber (BDC) is designed to reconstruct the beam trajectories for the Large Acceptance Multi-Purpose Spectrometer (LAMPS) which is made to study the dynamics between nucleons inside neutron-rich nuclei, with the rare isotope beam produced by the Rare Isotope Accelerator complex for ON-line experiments (RAON).

In order to understand the performance of the BDC, the prototype BDC have made and tested under the various conditions.

In this poster, improvements of the BDC design since last year and the present performance results will be shown.

And the prospect of the BDC with planned beam test also will be introduced.

### Keywords:

LAMPS, RAON, BDC, drift chamber, gaseous detector

## Measurement of Ac228 isomers by using Ra228 deposited CeBr3 scintillator

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### Abstract:

Recently, the COSINE-100 experiment observed new isomers in Ac228 at 6.28keV, 6.67keV and 20.19keV as a potential background for the dark matter search. In this study, we measured these isomers in Ac228 by using Ra228 deposited CeBr3 scintillator. CeBr3 crystal has fast decay time(~20ns) and high light output. We have studied selected events that are two pulse events and three pulse events. Ac228 is produced by beta decay of Ra228. Due to all beta decays from Ra228 to Ac228, gamma rays are always come out with beta particles. We prepared an encapsulated crystal with a radius of 4mm and a thickness of 5mm. And we adhered the crystal to the R12669 PMT (PhotoMultiplier Tube) surface using optical grease and measured the scintillation light emitted from the crystal. I will present a preliminary measurement of Ac228 isomer decay.

### Keywords:

CeBr3, Ac228, scintillator, nuclear decay

## Simulation for proton beam energy optimization for BNCT application

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### Abstract:

Li and Be are widely used as targets for neutron production in the accelerator-based BNCT. Neutrons produced from these reactions need a moderator to slow down their energy to the epithermal energy region. The generated neutron yield and energy from Li(p,n) or Be(p,n) varies depending on the energy of protons irradiated to the target. The higher the proton energy, the greater the neutron yield. But, a thicker moderator is required due to the increased neutron energy. In this study, Geant simulation was performed to investigate effective proton energy by considering this conflicting effect between proton energy and moderator thickness.

### Keywords:

moderator, epithermal neutron, Geant, BNCT

## Development and Application of positron lifetime spectroscopy

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### Abstract:

Recently the application of Positron Annihilation Lifetime Spectroscopy (PALS) is considered technologically important systems. The Positron Lifetime method involves a nondestructive probe to detect low levels of open-volume defects in a wide range of advanced material systems. This PALS allows examining structure of materials in sub-nanometer scale. This technique is based on the lifetime and intensity of ortho-positronium atoms in free volumes of given structures. It is mostly used for studies in material sciences, but it can also be used for in vivo imaging of the cell morphology. In KAERI, PALS was established and applied to study various defect studies. The free volume in polymer films such as polyethylene terephthalate, polyimide and nafion and the defect in structural metal alloys and semiconductor were analyzed by PALS. Also a slow positron beam transport system with <sup>22</sup>Na positron source is under developing for applying positrons on thin film studies. Even higher intense of positron production system is planned at ETRI with a high power laser system.

### Keywords:

Positron Annihilation, Lifetime, Defect, sub-nanometer scale

## Measuring and unfolding fast neutron spectrum using a stilbene scintillation detector

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### Abstract:

We propose an overall procedure for measuring and unfolding fast neutron energy spectrum using stilbene scintillation detector. Detector characterization was described, including information on energy calibration and detector resolution. Nonproportionality response of the detector was also observed. Digital charge comparison method was used for investigation of neutron-gamma pulse shape discrimination (PSD). A pair values of 600 ns pulse width and 24 ns delay time were found as the optimized condition for PSD. A unique technique was introduced to adjust stilbene proton response function (PRF) based on experimental pulse height spectrums. The PRF was corrected by 28% before being used in Geant4 Monte Carlo simulation to construct the detector response matrix. Spectrum unfolding was implemented using the Iterative Bayesian method. The unfolding performed well with simulation data and measured spectrums of Cf-252, AmBe and background neutron sources. Our approach is promising for fast neutron detection and spectroscopy.

### Keywords:

Fast neutron detection, Stilbene scintillator, Pulse shape discrimination, Monte-Carlo simulation, Iterative Bayesian spectrum unfolding

## Development of X-ray imaging system based on Raspberry Pi Camera

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### Abstract:

The field of X-ray imaging is continuously evolving with new applications in medical imaging and other fields. This report presents the preliminary results of the development of X-ray imaging system with a portable Raspberry Pi HQ Camera and thin luminescence film. The camera system was built from a Raspberry Pi 4/4GB and its official camera (RPi HQ Camera). The luminescence films were prepared by using polymer solution at different concentrations of CsI:Tl scintillator thin films or glasses. By using the combination of the Pi camera system and produced films, the system allows capturing high resolution of X-ray images. This system is promising and is now being developed for academic and medical imaging applications.

### Keywords:

RPi HQ Camera , luminescence , X-ray image

## 방사성동위원소 농도비를 이용한 RbCl 표적에의 양성자빔 입사 에너지 추정방법 연구

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### Abstract:

심장질환 진단 등에 이용되는 의료용 방사성 동위원소 Rb-82를 의료 현장에서 손쉽게 이용할 수 있도록 해주는 Sr-82/Rb-82 발생기 개발을 위해서는 모핵종인 Sr-82 생산이 필요하다. Sr-82는 천연연화루비듐 표적에 고에너지의 양성자빔을 조사할 때 일어나는 Rb-nat.(p,xn)Sr-82 핵반응에 의해 생성된다. 다양한 연구를 통해 Sr-82 생성에 적절하다고 할 수 있는 에너지 범위는 40~90 MeV로 알려져 있다. 국내에서 Sr-82 생산이 가능한 양성자가속기로는 한국원자력연구원 양성자과학연구단에서 운영 중인 100-MeV 선형 양성자가속기가 유일하며, 표적 조사 실험은 RI 생산용 표적 조사용 전용 빔라인에서 이루어지는데 이 때 표적에 입사되는 양성자빔의 에너지를 직접 측정하는 것에는 한계가 있다. 본 연구에서는 RbCl 표적에 조사된 양성자빔 에너지에 따라 생성되는 각각의 방사성동위원소의 생성량이 달라지고 이로 인해 표적 내에서의 방사성동위원소 비의 차이가 발생하는 점을 이용해 입사된 양성자빔의 에너지를 추정할 수 있는 가능성을 타진해 보고자 한다. 이를 위해 Sr-82 생산을 위한 실험결과와 계산결과를 비교하고 동위원소비의 차이에 대해 분석하고자 한다.

\* 본 연구는 과학기술정보통신부의 방사선기술개발사업 '고에너지 양성자가속기 이용 Sr-82 생산 및 발생기 기술 개발' 과제 (NRF-2017M2A2A2A05016601)의 일환으로 수행되었음.

### Keywords:

양성자가속기, 동위원소 농도비, Sr-82, Rb-82, 양성자빔 에너지

## Decomposing images of acoustic resonant modes into superposition of quasi-eigenmodes

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### Abstract:

When an incident acoustic wave is resonant with water-filled acoustic cavity formed in the center of an aluminum cylinder along its axis, acoustic quasi-eigenmodes are excited in the cavity. The spatial intensity distribution of the acoustic resonant modes can be imaged by using the schlieren method. We investigate the resonant modes of the acoustic cavity shaped following the Penrose unilluminable room, which has always a dark region wherever a light bulb is located inside the region. While most of the resonant modes are matched with quasi-eigenmodes computed with finite element simulation, some resonant modes are asymmetric, filling only a half region of the cavity, and not found in the simulation results, which we call a half-illuminated mode (HIM). In an open system, the near-degenerate quasi-eigenmodes have finite linewidths and biorthogonal each other. The HIM is the result of simultaneous excitation of the near-degenerate quasi-eigenmodes whose linewidths are overlapping. We have reproduced the resonant modes by optimizing the spatial overlap between the observed mode and the intensity distribution of linear superposition of the 20 quasi-eigenstates. We have also imaged the field distribution of the HIM in a stroboscopic way. The complex coefficients are computed by using biorthogonal relation and field distribution of the HIM.

### Keywords:

quasi-eigenmode, Penrose unilluminable room, schlieren method, open system, biorthogonal

## Polarization dependence of Degenerate Four Wave Mixing in DO3 doped polymer films

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### Abstract:

We study the polarization effect in degenerate four wave mixing in disperse orange 3 dye-doped PMMA thin film. Phase conjugate wave signals by Degenerate Four Wave Mixing were generated in two polarization configurations at 532 nm. The plane of polarization of the probe beam was arranged to be either parallel or perpendicular to that of pump beams. These two configurations result different responses to the increased temperature. The reorientation effect of the dye molecules was discussed in this process. The phase conjugate wave signal by polarization angle variation of the probe light was measured as a sine square function with respect to the polarization direction. The angular hole burning effect was discussed in disperse orange 3 dye-doped PMMA thin film.

### Keywords:

Degenerate four wave mixing, Phase conjugate wave, DO3, angular hole burning

## 자연 채광기용 프리즘 광학계의 설계 (Design of prism optics for Natural light illumination system)

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### Abstract:

최근 들어 녹색 에너지에 대한 많은 발전과 관심으로 그 응용 분야가 크게 증가하고 또한 에너지를 절약하고 건강한 조명을 만드는 수단으로 햇빛을 이용한 조명에 관심이 크게 대두 되고 있습니다. 자연광 조명 시스템에는 크게 세부분으로 구성되어 있는데, 빛을 모아주는 수집부, 빛을 전송하는 전송부 및 전송된 빛을 조명해주는 조명부로 구성되어 있습니다.

본 연구에서는 태양광 조명시스템을 이용하여 자연 채광능력과 공간효율성을 향상시키기 위한 방법으로 광학식 프리즘 형상의 돔 형태의 태양광 채광 시스템을 개발하고자 한다 .

이를 위해 돔내부에 최적 각도의 프리즘을 지닌 Fresnel Lens를 배치하여 기존 창문형 제품보다 집광효율 상승, 집광부 대비 광 이송부의 크기를 축소할 수 있으며 태양 궤적에 따른 최적의 설계 조건을 산출하고자 한다.

### Keywords:

Opticsl Design, Illumination system, prism optics

## 희토류 금속을 첨가한 Perovskite stannates $A\text{SnO}_3$ ( $A = \text{Ca}, \text{Sr}, \text{and Ba}$ )의 구조 및 광학 특성

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### Abstract:

$A\text{SnO}_3$ 에 희토류(Rare Earth, RE) 금속 이온( $\text{Dy}^{3+}$ ,  $\text{Er}^{3+}$ , and  $\text{Eu}^{3+}$ )을 첨가한 형광물질의 구조특성과 광 발광(Photoluminescence, PL) 특성을 연구하였다.  $A\text{SnO}_3 : X$  ( $A = \text{Ca}, \text{Sr}, \text{and Ba}$ ) ( $X$ =희토류 금속이온)시리즈 시료를 고상반응법으로 제작하였다. X-ray diffraction (XRD)와 Rietveld refinement 분석을 통해 첨가한 이온의 종류와 농도에 관계없이  $\text{CaSnO}_3$ 와  $\text{SrSnO}_3$ 는 Orthorhombic 구조를,  $\text{BaSnO}_3$ 는 Cubic 구조를 가짐을 확인하였고,  $\text{CaSnO}_3$ 가  $\text{SrSnO}_3$ 보다 구조 대칭성이 낮았다. 세 종류의 희토류 금속이온의 발광세기는  $\text{CaSnO}_3$ 에서 가장 강했고  $\text{BaSnO}_3$ 에서 가장 약하게 관측되었다. 이러한 결과를 통해 희토류 금속이온의 발광특성이  $A\text{SnO}_3$ 의 구조 대칭성과 밀접하게 연관된다는 것을 밝혀냈다. 이와 더불어, 광학 측정을 통해  $A\text{SnO}_3$ 의 전자 구조와 격자 동역학 연구를 진행하였다. Perovskite stannates를 시리즈의 비교연구를 통해 광전기 소재로서의 활용가능성을 살펴본다.

### Keywords:

Perovskite stannates, PL, XRD, RE

## Polymerase Chain Reaction 시스템의 Thermal cycling을 위한 레이저 파워 밀도 정량화

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### Abstract:

코로나19로 인해 많은 진단법 중에서도 높은 정확도를 가지는 Polymerase Chain Reaction(PCR) 진단에 대한 관심이 높아지고 있다. 히터를 이용하는 종전의 PCR thermal cycling은 검진에 소요되는 시간이 길며 온도 조절의 어려움이 있다. 이러한 문제점을 해결하기 위해 레이저를 이용한 PCR thermal cycling을 연구하였다. 레이저의 특성을 활용하여 PCR 샘플에 큰 에너지 밀도를 전달할 수 있기에 thermal cycling과정의 시간을 단축시킬 수 있다. 본 연구에서는 thermal cycling에 레이저를 적용할 때에 필요한 레이저의 에너지 밀도를 정량화하고자 한다. PCR 용액의 40~50% 이상이 정제수로 구성되기 때문에 본 연구에서는 정제수를 샘플로 사용하였다. 샘플인 정제수에 레이저를 조사하여 일어나는 온도 변화는 열 확산 방정식을 통해 나타낼 수 있으며, 이를 검증하기 위해 1450nm 파장의 레이저를 정제수에 조사하여 실시간으로 온도 변화를 측정하였다. 사용하는 레이저의 파장에 따라 필요한 에너지 밀도가 다르며, 레이저의 특성 및 작동 상태에 따라 효율적인 thermal cycling을 분석하고 정량화하였다.

### Keywords:

PCR(중합효소연쇄반응), laser power density(레이저 전력밀도), thermal cycling(열 순환)

## Photo-luminescent and Structural analysis on Dy<sup>3+</sup> doped alkaline-earth zirconates A<sub>1-x</sub>Dy<sub>x</sub>ZrO<sub>3</sub> (A=Ba, Sr, and Ca)

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### Abstract:

We investigated the photoluminescence (PL) and structural properties of AZrO<sub>3</sub> (AZO3), (A=Ba, Sr, Ca) doped with Dy<sup>3+</sup>. The AZO3 samples were synthesized by the solid-state reaction method. The Dy<sup>3+</sup> was doped at various ratios into AZO3 to investigate the effect of concentration of the Dy<sup>3+</sup> ions on the photo-luminescent emission. Rietveld refinement was performed on the X-ray diffraction patterns to obtain the crystal structural parameters. The emissions which are corresponding to <sup>4</sup>F<sub>9/2</sub> → <sup>6</sup>H<sub>15/2</sub> and <sup>4</sup>F<sub>9/2</sub> → <sup>6</sup>H<sub>13/2</sub> were observed from Dy<sup>3+</sup> doped AZO3 under UV excitation. The highest emission efficiency was achieved at 5 mol% and 3 mol% concentration of Dy<sup>3+</sup> ions in SrZrO<sub>3</sub> and CaZrO<sub>3</sub> respectively, while BaZrO<sub>3</sub> does not reveals enough emission. The change in asymmetry ratio between yellow and blue emissions from Dy<sup>3+</sup> ions in A-site varied host materials indicate that crystal field effects on Dy<sup>3+</sup> strongly related with surrounding environmental complexes of doped Dy<sup>3+</sup>.

### Keywords:

Photoluminescence, Dy<sup>3+</sup>, BaZrO<sub>3</sub>, SrZrO<sub>3</sub>, CaZrO<sub>3</sub>

# A Multimodal Imaging System for Digital Holographic Doppler Spectroscopy of Living Biological Tissues

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## Abstract:

A multimodal biodynamic imaging system is developed by introducing a beam splitter into the signal arm for simultaneous recording and reconstruction in tissue-dynamics spectroscopy(TDS). This is an integrated system of Fourier-domain digital holography(FDH), image-domain digital holography(IDH), and common-path digital holography(CDH). TDS is a fluctuation spectroscopy based on Doppler light scattering from intracellular dynamics that tracks subtle changes in intracellular motions in response to cancer therapeutics. TDS systems such as FDH and IDH used a Mach-Zehnder configuration that enabled low-coherence-gated optical sectioning. In the FDH configuration, the CCD camera is placed in the Fourier plane, whereas in the IDH configuration the CCD camera is placed in the image plane. In the CDH configuration, the object and reference waves share the same optical path from the sample interaction volume to the detector by using a grating and a spatial filter.

The performance of the multimodal system is verified by conducting various experiments using DLD-1 (human colon adenocarcinoma) spheroids as a target tissue sample. Power spectra and drug-response spectrograms obtained from two simultaneous recordings were compared for different configurations of the multimodal system. The experimental results show that the common-path configuration shows enhanced interferometric stability despite the very low resolution, whereas image-domain and Fourier-domain configurations show moderate sensitivity to Doppler frequency shifts caused by intracellular motions. FDH also shows moderate resolution with a good dynamic range, while IDH shows good resolution with a lower dynamic range than FDH. This work establishes the feasibility of the multimodal system for tissue-dynamics spectroscopy and indicates potential applications of the multimodal system to enable stable tissue-dynamics spectroscopy of living thick biological tissue for drug screening assays.

## Keywords:

digital holography, biological imaging, spectroscopy, interferometry.

## 측면 가공 커플러의 제작 조건에 따른 위상 이동 특성

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### Abstract:

이터븀이 도핑된 광섬유는 외부 펌프광의 광세기에 의존하여 굴절률 변화가 발생하는 비선형 효과를 통해 광섬유 간섭계에서 위상 이동을 유도할 수 있는 특징을 가지고 있다. 이러한 특징을 이용하여 위상 이동 간섭계를 구성하고 물리량의 변화를 측정하는데 활용하기도 한다. 이러한 특징을 광섬유 커플러에서 활용하고자 광섬유 측면을 가공하여 커플러로 제작한 측면 가공 광섬유 커플러를 제작하여 간섭계에 활용하여 위상 이동 특성을 측정하고자 하였다.

기존의 광섬유 커플러의 경우 수동소자로 광세기를 일정 비율로 분배하는 기능만을 가졌다. 하지만 이번에 제안한 광섬유 커플러는 측면 가공하는 조건에 따라서 광섬유에서 발생하는 위상 이동을 외부 펌프광의 인가조건에 따라서 가변할 수 있는 장점을 가진다. 특히 측면 가공 광섬유 커플러는 기계적인 이격을 발생시켜 커플러의 커플링 세기를 가변할 수 있어 가변 커플러로 사용할 수 있다. 이러한 장점에 위상 이동의 특성을 동시에 가질 수 있어 다기능 광섬유 커플러로 이용이 가능하다.

이러한 특징을 조사하기 위해서 광섬유 커플러의 측면 가공 조건인 측면 가공 깊이, 사용한 이터븀 광섬유의 길이 등을 변화시킴으로써 동일한 외부광이 인가되었을 때 위상 이동에서 어떤 변화가 있는지 측정하고자 하였다. 또한 가변 커플러의 광분배비에서의 파장별 차이에서의 영향도 동시에 살펴보고자 한다. 이러한 특징을 조사하여 위상 이동 제어가 가능하면서도 가변 커플러의 특징을 유지하는 최적의 가변 광섬유 커플러 제작에 활용하고자 한다.

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (grand no. NRF-2019R1A6A3A01095557 & no.NRF-2017R1A2B2009732)

### Keywords:

측면 가공 커플러, 위상 이동, 비선형 굴절률

## FDTD를 이용한 잘린 정팔면체 프레임 구조 나노 입자의 전자기장 분포 분석

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### Abstract:

FDTD를 이용한 잘린 정팔면체 프레임 구조 나노 입자의 전자기장 분포 분석

금속 나노 입자 표면에는 국부적으로 플라즈몬이 존재하여 도체 표면에서의 빛과 상호작용을 한다. 빛 에너지가 표면 플라즈몬으로 변환되면서 국소적인 전기장 증가 현상을 발생시킨다. 이러한 전자기장 증가 현상을 이용한 표면 증강 라만 산란 방법(SERS)은 미세한 라만 신호의 세기를 증폭시켜 소량의 분자를 검지하는 데 활용되어 왔다. 금속 나노입자는 표면 플라즈몬 여기가 용이해 국소 전자기장 증대 효율이 우수하여 이러한 SERS 방법에 광범위하게 활용되었으나, 일반적으로 전자기장 증대가 발생하는 지점인 핫스팟 위치를 제어하기 어렵고 전자기장 증대값 또한 한계가 있어 극미량의 분자 검지에는 한계가 있었던 것이 사실이다.

본 연구에서는 나노미터 크기의 내부가 비어 있는 잘린 정팔면체 (truncated octahedral nanoframe) 구조의 전자기장 분포를 유한차분 시간 영역법을 적용한 전산모사를 통해 연구하였다. 이 구조는 내부가 비어 있는 특성으로 인해 입자 내부에서도 핫스팟 형성이 가능하며, 규칙적 형상으로 인해 정렬이 용이하여 입자 사이에서 수 나노미터 이내의 나노갭 (nanogap) 형성을 통한 핫스팟 형성이 가능하는 등, SERS 방법을 위한 훌륭한 구조로 연구된 바 있다 [1]. 본 연구 결과, 전자기장 증대값은 최대 14 이상인 것으로 확인되었으며, 입자 사이의 갭에서 뿐만 아니라 구조체의 꼭지점 부분 등 다양한 위치에서 핫스팟 형성이 관측되었다. 따라서, 기존 구형 금속 나노입자 등 나노구조체에 비해 고감도 분자검지가 가능한 SERS 기판에 활용될 수 있을 것으로 기대한다.

### 참고문헌

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### Keywords:

Field Enhancement, Surface plasmon, Nanoparticle

## Electrical charge control of *h*-BN single photon sources

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### Abstract:

Color centers of hexagonal boron nitride (*h*-BN) have arisen as promising single photon sources due to their high brightness and narrow spectral linewidth at room-temperature. For the exploitation of *h*-BN quantum emitters for quantum communication applications, electrical manipulation of quantum emitters is highly desired. In this work, we show the electrical switching of photoluminescence from *h*-BN quantum emitters by controlling the charge transfer from the nearby charge reservoir. By applying a voltage to a pair of graphene electrodes sandwiching *h*-BN crystal, we could tune the Fermi level of *h*-BN defect by about several hundreds of meV. Within this tuning range, several localized quantum emitters could be electrically activated with an excellent on/off ratio and great repeatability. Among these quantum emitters, some of the emitters showed bidirectional voltage dependence which originates from the electrical control of the nearby charge trap sites. On the other hand, many other quantum emitters showed unidirectional voltage dependence which manifests the direct charge state manipulation of the *h*-BN defect centers. From the direct measurement of the charge transition level of these quantum emitters, we also found the crystallographic origin of the defect centers, which will provide useful information for the quantum control of *h*-BN quantum emitters for 2D material-based quantum information processing.

### Keywords:

Single photon sources, Hexagonal boron nitride, Charge transfer, Van der Waals heterostructures

## Study on thermal effect of end-pumped Tm:YLF crystal

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### Abstract:

Thermal effects are the main obstacle for achieving high power with good beam quality in solid-state lasers. To overcome the undesired thermal effects in laser crystals, thermal models were carried out using finite element analysis (FEA) for Tm:YLF laser crystal based on different dimensions, beam diameter, and heat load for predicting the focal thermal length and temperature and stress distribution in the crystal. FEA analysis gave an excellent quantitative prediction for heat and stress distribution and thermal lensing within laser crystals.

### Keywords:

Tm:YLF laser, FEA, thermal analysis

## GRIN Lens을 이용한 Relay Lens 설계에 관한 연구 (A Study on Relay Lens Design Using GRIN Lens)

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### Abstract:

최근 들어 코로나 19로 인하여 비접촉식 광학 방식의 의료용 계측장비 및 측정 장비가 크게 증가하고 있으며 각 분야에서 응용되고 있다.

본 논문에서는 고분해능이면서 간단한 구조적인 형태를 갖도록 Relay lens에 GRIN lens을 접목하여 새로운 형태의 의료용 광학계를 설계하고 분석하였다.

### Keywords:

Grin lens, Relay lens, Optical design

## The self-force on a single charged particle in the classical electrodynamics

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### Abstract:

고전전자기학에서 한 입자가 스스로에게 미치는 힘(self-force)을 계산하는 것은 이론물리학자들의 오랜 숙제였다. 이 힘을 제대로 계산하지 못하면, 원칙적으로는 어떠한 입자의 운동도 이론으로 기술할 수 없기 때문이다. 점전하에 대해서 이 힘을 처음으로 제대로 계산한 인물은 폴 디랙으로, 그의 계산에 따르면 self-force는 다음처럼 주어진다:  $\dot{p}_{\text{self}}^\mu = -(\alpha/R_c)\ddot{x}^\mu - (2/3)\dot{x}_\nu(\ddot{x}^\mu\dot{x}^\nu - \dot{x}^\mu\ddot{x}^\nu)$ , 여기서  $\alpha$ 는  $1/2$  혹은  $2/3$  이고  $R_c$ 는 입자의 반지름이다. 문제는 입자의 크기가 점일 것으로 가정했기 때문에 이 결과는 결국 무한대로 발산하게 된다. 디랙은 그래서  $p^\mu \propto \dot{x}^\mu$ 인 점을 이용하여 무한대로 발산하는 항을 무시했다. 그러나 이 발표에서는 입자의 크기가 점이 아니라 유한하다고 가정하고, 입자의 self-force를 다시 계산해본다. 흥미롭게도, 디랙의 결과와는 다르게, 다음을 얻을 수 있었다:

$\dot{p}_{\text{self}}^\mu = -(\alpha/R_c)(\ddot{x}^\mu + R_c\dddot{x}^\mu) - (2/3)\dot{x}_\nu(\ddot{x}^\mu\dot{x}^\nu - \dot{x}^\mu\ddot{x}^\nu)$ . 하나의 항이 추가되었으며, 이 때문에 입자의 운동량은 이제  $p^\mu \propto \dot{x}^\mu + R_c\ddot{x}^\mu$ 를 만족해야된다. 이러한 새로운 결과로 인해서 어떤 새로운 현상이 나타날 수 있는지를 발표 마지막에 논의해볼 것이다.

### Keywords:

Electrodynamics, Radiation reaction, Self-force

## Dark photon search using $B \rightarrow K l l$ decay at Belle.

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### Abstract:

We are going to present recent update on dark photon search using  $B \rightarrow K^{(*)} l^+ l^- l^+ l^-$  decay at Belle.

During b to s transition we can consider something like dark higgs can be produced, the dark higgs can be decay to two dark photons, and dark photon decays two leptons. We only studied electron and muon case. For the case of tau and dark photon decay to two pion, we didn't studied due to huge backgrounds.

This presentation includes signal extraction, background study, control sample study, and estimated upper limit of branching fraction using MC.

We used 772M  $B\bar{B}$  pairs which corresponds to  $711 \text{ fb}^{-1}$  integrated luminosity for control sample study.

And also used 10 streams of  $B\bar{B}$ ,

6 streams of qq, 50 streams of rareB and 20 stream of ulnu to evaluate this result. Each stream is corresponds to  $711 \text{ fb}^{-1}$  full Upsilon(4S) Belle Montecarlo samples.

### Keywords:

Belle, Dark photon

## Search for ALP through $B \rightarrow K a'$ ( $a' \rightarrow \gamma\gamma$ ) decay with Belle experiment

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### Abstract:

In this research, we are looking for one of the BSM particle, spin-less pseudoscalar Axion Like Particle(ALP), which expected to partialy decay into a gamma pair. This research is aiming calculating upper limit of branching fraction of  $B \rightarrow K a'$  ( $a' \rightarrow \gamma\gamma$ ) decay mode to find the evidence of existence of ALP.

We use MC data from Belle experiment, the asymeric e+e- collider experiment held in KEK, Japan which collect 710 fb<sup>-1</sup> of Y(4S) data.

### Keywords:

Belle Experiment, B Meson, ALP

## Search for $B \rightarrow X_s \nu \bar{\nu}$ decay in Belle II experiment

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### Abstract:

$b \rightarrow s \nu \bar{\nu}$  decay is theoretically clean and related to the right-handed current. Because there is no right-handed current in the standard model, this decay is interesting. By measuring the upper limit of the branching ratio of  $b \rightarrow s \nu \bar{\nu}$  decay, limits on the right-handed component of the Wilson coefficient can be obtained. In this presentation, we present  $B \rightarrow X_s \nu \bar{\nu}$  analysis in Belle II experiment. We used sum of exclusive method.  $B \rightarrow K^{(*)} \nu \bar{\nu}$  MC sample is produced by the form factors. Non resonant  $B \rightarrow X_s \nu \bar{\nu}$  sample is produced by the Fermi motion model. Powerful tools like full event interpretation(FEI) and FastBDT are used in the analysis.

### Keywords:

EWP, B physics, Belle II

# Data Acquisition Software Development for Belle II Detector Operation.

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## Abstract:

Belle II experiment is a high-energy physics experiment at the SuperKEKB electro-positron collider. With high-luminosity, we can make high precision measurement of rare decays and CP-violation in hadrons and leptons to probe new physics beyond standard model.

In this presentation, we present DAQ software development to make stable detector operation, including slowcontrol, monitoring system, software validation and so on.

## Keywords:

Belle II, DAQ

## Upcoming Beyond the Standard Model Searches in Belle II

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### Abstract:

In this session, 3 decay mode searches in Belle II experiment will be introduced.

$ee \rightarrow \mu\mu\mu\nu_D\nu_D$  is the mode for searching the dark sector through U(1) kinetic mixing. Muons come from the dark photon will be searched.

In  $D^0 \rightarrow V\gamma$ , CP violation is expected to be seen. Because of its low branching ratio, this decay mode is hard to be detected, but we expect Belle II has enough luminosity for the research.

Final part is the mode for the lepton flavour violation.

### Keywords:

Belle2

## Search for $B^0 \rightarrow l \tau$ decays at Belle experiment

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### Abstract:

We study the leptonic decay  $B^0 \rightarrow \ell^\pm \tau^\mp$  with  $\tau$  leptonic decay channels,  $\tau$  to 3 leptons. We used MC simulated data from Belle detector at KEKB e+e- collider, producing  $\Upsilon(4S)$  particle that decays to two B mesons. In this study, one B meson is regarded as signal B (decays to  $l \tau$ ) while the other B meson is fully reconstructed by semileptonic full event interpretation (FEI).

After skimming and basic quality control with momentum and angular variable cut, the precise quality control is done with the machine learning, by using the Toolkit for Multivariate Data Analysis with ROOT. We used the multi-layer perceptron (MLP) with 3 variables, to optimize the signal purity and background suppression.

The variable  $p_l^*$ (the primary lepton momentum on CM frame) is selected to extract signal events. The distribution of signal and background  $p_l^*$  is used to build the probability density function of signal and background. The combined PDF is used to fit background MC to estimate the signal yield. The corresponding MC upper limits are calculated. The control sample study also will be done to validate the analysis process.

### Keywords:

Belle, KEKB, B meson, Missing Particles, Machine Learning

## 전자-양전자 충돌실험에서 생성된 이중 암흑광자가 뮤온 쌍으로 붕괴하는 모드에 관한 연구

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### Abstract:

전자-양전자 충돌실험에서 생성된 이중 암흑광자가 각각 뮤온 쌍으로 붕괴하는 모드[1]를 초고성능컴퓨팅을 활용하여 연구하였다. 신호사건은  $e+e \rightarrow A'A'$ ,  $A' \rightarrow \mu+\mu^-$  이다. MadGraph5을 이용하여 simplified model[2]로부터 신호사건을 생산하였다. 신호사건생산에 많은 양의 계산이 필요하므로 선행 연구[3]를 바탕으로 KISTI 슈퍼컴퓨터5호기를 최적화하여 신호사건을 생산하였다. 신호사건과 관련된 질량중심에너지, 암흑광자질량, 결합상수에 대한 의존도를 알기 위하여 산란단면적을 스캔하였다. 이로부터 전자-양전자 충돌실험에너지(Belle II, FCC, CEPC, ILC 등)에서 산란단면적이 최대가 되는 암흑광자질량을 도출하였고 이것을 재구성(reconstruction)에 적용하였다. 전자-양전자 충돌실험에서 이중 암흑광자 채널을 재구성하기 위해서 독립형 틀(stand-alone frame)을 기반으로 Delphes 검출기 시뮬레이션[4]을 수행하였다. 이로부터 검출기 효율(detector efficiency)을 도출함으로써 각 실험에서 예상되는 신호사건의 수를 제시하였다. 향후 미래 전자-양전자 충돌실험에서 이중 암흑광자가 뮤온쌍으로 붕괴하는 모드를 탐색하는데 도움이 될 것이다.

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### Keywords:

암흑물질, 암흑광자, 전자-양전자 충돌실험, MadGraph5

# The pileup jet identification algorithm performance of CMS Run2 data

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## Abstract:

With increasing luminosity in LHC, a jet coming from additional collision (pileup) increase the complexity of the reconstruction.

A machine learning based algorithm has been used in CMS to mitigate the jet from pileup.

We study the efficiencies of the algorithm using the tag-and-probe method with Drell-Yan events categorizing the region by the jet momentum balance.

The data used for the measurement is collected by CMS experiment in Run2 at  $\sqrt{s}=13$  TeV.

## Keywords:

CMS

# Kinematic Significance of Mass Presence in Powheg Top Pair Decay

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## Abstract:

With increasing number of data planned from the future run of LHC, there are much more opportunities to measure various parameters. One of the possibilities is measuring  $V_{cb}$  component of CKM matrix using semi-leptonic decay of top pair production process. To check the plausibility of this study, a good Monte Carlo simulation is essential. While there are various samples of background generated through Powheg, the signal sample of semi-leptonic top pair decaying to c quark and b quark pair is not yet generated in Powheg due to simplification of CKM matrix to only including Cabibbo angle. Therefore, the generation of semi-leptonic top pair production decay into c quark and b quark pair is presented, using Powheg and Madspin. The difficulty rises when considering the particle mass involved in the process. Powheg, through its complex mechanism, generates massive particles after decay, while Madspin assumes zero mass as it was given in the collision. The kinematic difference from this mass difference is studied.

## Keywords:

$V_{cb}$ , Powheg, CKM Matrix

## Study of interference effect in heavy $W'$ boson search using Monte-Carlo simulation

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### Abstract:

Understanding the effect of interference is crucial as it could modify existing main observable and this change reflects the new particles mass and also the coupling strength to standard model fermions. For  $W'$  to electron and neutrino search, we investigated the interference effect on the transverse mass distribution to determine upper limits for the mass of  $W'$ . The left-handed  $W'$  boson interfering with the  $W$  boson in the same final state is simulated at the leading order in proton-proton collisions at  $\sqrt{s}=13$  TeV. We show that there are qualitative effects on the behavior of the new physics  $W'$  signal at the intermediate region, where the background and signal are mixed, and also the tail region, where the background is free. Therefore, the Interference effects become a robust strategy for searching new heavy resonance even not accessible at the LHC.

### Keywords:

BSM,  $W'$ , Interference, LHC

# A Study on ME0 Background Estimation Using FLUKA Simulation in CMS Experiment

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## Abstract:

ME0, a R&D project of the next-generation muon detector, is ongoing as a part of phase II upgrade of the CMS(Compact Muon Solenoid) experiment. ME0 adds 6 data points at the high-eta region of CMS, where a strong magnetic field is applied, so that it is considered to improve the resolution of muon momentum greatly. However, ME0 is expected to be affected by very severe background effects, because it is placed in the region very close to IP(Interaction-Point). I estimated background levels in the major background channels, using FLUKA, a specialized simulation tool for the experimental particle physics. Also, I compared various ME0 environmental models and derived the most effective environment model for the background shielding. Studies on simulation in photon, electron and positron, charged hadron and neutron background channels are presented in this presentation.

## Keywords:

CMS, Simulation, Background, GEM, ME0

## Pulse Shape Discrimination for the JSNS<sup>2</sup> experiment

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### Abstract:

The JSNS<sup>2</sup> (J-PARC sterile neutrino search in J-PARC sputtering neutron source) experiment explores neutrino oscillation at a short baseline of 24m with the neutrinos produced by the 3GeV 1MW proton beam on the mercury target in the J-PARC's MLF. Neutrinos are detected through the Inverse Beta Decay (IBD) in the gadolinium (Gd)-loaded Liquid Scintillator (LS) in the JSNS2 detector. Discrimination performance of IBD signals from the Fast neutrons (FN) backgrounds is one of the very important issues in the JSNS2 which can be achieved by analyzing the pulse shapes of the photomultiplier tubes. In JSNS<sup>2</sup>, we developed Pulse Shape Discrimination (PSD) algorithms based on Likelihood and Deep Learning. In this poster, we summarize PSD algorithms in the JSNS2 and their performance with the data taken in 2021-2022 physics runs.

### Keywords:

JSNS2, PSD, Likelihood, CNN, DNN

# Study of WZGamma production and anomalous quartic gauge couplings in fully leptonic final state at High-Luminosity LHC using Machine Learning Method

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## Abstract:

The High-Luminosity LHC will be operated at the center-of-mass energy of 14 TeV with the largest integrated luminosity ever,  $3000 \text{ fb}^{-1}$ . It is expected to observe rare processes in the Standard Model. The triple vector boson production that has a high sensitivity to variations in the quartic gauge couplings is a fundamental test of the behavior of the electroweak sector of the SM. We report the prospect for the observation of the fully leptonic WZ process and the expected exclusion limit on the anomalous quartic gauge couplings in the HL-LHC environment. The machine learning algorithm is adopted to efficiently classify signals and backgrounds.

## Keywords:

HL-LHC, Triple Vector Boson Production, Machine Learning, aQGC

## Cosmic Muon Identification at JSNS<sup>2</sup>

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### Abstract:

The JSNS<sup>2</sup> experiment aims to search for the existence of sterile neutrino oscillations with  $\Delta m^2$  near  $1\text{eV}^2$  at J-PARC MLF. A 1MW beam of 3 GeV protons incident on a spallation neutron target produces an intense neutrino beam from muon decay at rest. The experiment will search for muon antineutrino to electron antineutrino oscillations which can be detected by the inverse beta decay interaction followed by gammas from neutron capture on Gd. Cosmic-muon induced Michel electrons and neutrons make a contribution to accidental backgrounds against the sterile neutrino search. In order to their effective reduction, we have developed the identification method for the stopping muons and the through-going muons using a veto information. The selected Michel electrons are useful for detector calibration including determination of an absolute energy scale.

### Keywords:

JSNS<sup>2</sup>, Sterile neutrino, Michel electron

## Detection efficiency study for KDAR neutrino in JSNS2 experiment

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### Abstract:

JSNS2 (J-PARC Sterile Neutrino Search at J-PARC Spallation Neutron Source) experiment will search the unique ability to precisely measure monoenergetic 236 MeV neutrinos from charged kaon decay-at-rest (KDAR). KDAR neutrino gives the Optimized data for studying the neutrino-nucleus interaction, energy reconstruction, and cross sections in the hundreds of MeV energy region. A 1 MW proton energy (3 GeV) is sufficient to produce kaons efficiently at J-PARC Materials and Life Science Experimental Facility and, also in consideration of the facility's beam intensity, it represents the best facility in the world to accomplish this physics. In this presentation, detection efficiency of KDAR neutrino and systematic uncertainty study through the Monte Carlo will be reported.

### Keywords:

JSNS2, kaon decay-at-rest, J-PARC MLF, detection efficiency

# Jet Assignment in Dileptonic Top Pair Events using Machine Learning

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## Abstract:

Since the discovery of the top quark, many measurements of its properties such as the mass, cross-sections, and decay width have been performed. When top quarks are produced in proton collisions, additional jets can be produced together and many standard model signatures feature the same decay products. To measure the properties of the top quark it is very important to be able to reduce the background while identifying all the decay products. In this study, we propose assigning the decay products of top quarks by using a machine learning method based on self-attention, which can extract information about the relationships between the decay products.

## Keywords:

Machine Learning

## JSNS<sup>2</sup> trigger for a sterile neutrino search

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### Abstract:

The JSNS<sup>2</sup> experiment aims to search for sterile neutrinos with  $\Delta m^2$  near  $1\text{eV}^2$ . A 3 GeV J-PARC proton beam incident on a mercury target produces an intense neutrino beam from muon decay at rest which oscillates to anti-electron neutrinos. The JSNS2 detector is located at 24 m baseline from the target. The detector has a fiducial volume of 17 tons filled with GdLS, that efficiently can detect anti-electron neutrinos via the inverse beta decay reaction followed by a gamma signal from the captured neutron on Gd. The trigger to take the sterile neutrino events is set up. In this presentation, the trigger scheme for sterile neutrino at the JSNS<sup>2</sup> experiment will be described.

### Keywords:

sterile neutrino, JSNS2, Trigger

# Energy Calibration Study of an Electromagnetic Calorimeter Trigger System in the Belle II Experiment

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## Abstract:

The Electromagnetic Calorimeter Trigger system (ECLTRG) is one of the crucial components in the online trigger system in the Belle II experiment. The ECLTRG is composed of 576 Trigger Cells (TC), and one TC is a bundle of about 16 CsI(Tl) Crystals. The detected energy and timing of an event and also the number of clusters, etc, are used to generate various physics and Bhabha triggers.

In order to obtain the accurate total energy in TC, the Energy correction is performed by comparing energies recorded in ECL and ECLTRG, respectively. Then new attenuation coefficients are obtained and updated by reflecting this calibration.

We report the process of calibration in the ECLTRG and how to find and how to fix problematic TCs.

## Keywords:

Energy Calibration, Electromagnetic calorimeter, Trigger system, Belle II, Attenuator Coefficient

## A test of trapping and cooling of electrons with the antiproton trap for the GBAR experiment

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### Abstract:

The GBAR experiment is to measure the gravitational acceleration of antihydrogen atoms in a terrestrial gravitational field. A penning-malmberg trap is built for antiproton trapping for GBAR. For the accumulation and cooling of antiprotons, an electron cooling method is used. The electrons are injected into a harmonic potential well at the center of the trap with homogeneous magnetic fields, and a faraday cup is used to measure the released electrons from the trap. Number of trapped electrons is estimated by analyzing an electric signal from the faraday cup. The cooling of trapped electrons is confirmed by the change of energy distribution of the released electrons.

### Keywords:

GBAR,, Antiproton, penning-malmberg trap, electron

## Development of dynamic web interface for the CMS RPC detector efficiency monitoring

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### Abstract:

In the CMS RPC group, static-web pages have been used to summarize detailed results of detector performance studies for each run. This static-web based solution has a limitation in extracting useful information to be used by different analyzers since plots are stored in a static images, not a machine-readable format. We developed a dynamic web interface based on the JavaScript and HTML5 to solve the problems. The d3.js technology allows functionality to do a simple analysis with binding data and graphical elements on a graphical interface. On our web interface, results of the CMS RPC performance studies such as the efficiencies are shown on the various projections of RPC chamber's geometry along with the efficiency distribution on 1-D histogram. The plots are updated dynamically with the selection criteria by few mouse-clicks.

### Keywords:

CMS, RPC, Monitoring

# Search for Charged Lepton Flavour Violation in top quark interaction with muon and tau in pp collisions at $\sqrt{s} = 13$ TeV

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## Abstract:

Recently, studies of charged lepton flavour violation (CLFV) are performed by ATLAS and CMS experiments. Collision data used for this analysis are collected by the CMS experiment at the LHC during Run II period and the corresponding integrated luminosity is  $138 \text{ fb}^{-1}$  at center-of-mass energy of 13 TeV. This analysis is focused on top quark production ( $q \rightarrow t\mu\tau$ ) and decay ( $t \rightarrow q\mu\tau$ ) in the CLFV process. Effective field theory is adopted for model independent approach. The results are interpreted in terms of scalar, vector, tensor-like CLFV four-fermion effective interaction. There is no excess found in our analysis. Therefore, the expected limits of signal strength are set at 95% confidence levels, and branching fractions for top CLFV interactions are calculated.

## Keywords:

CMS, Top, CLFV, BSM

## Unusual optical phonon behaviors in strained monolayer WS<sub>2</sub>

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### Abstract:

화학 증기 증착 방법으로 성장된 단일 층 WS<sub>2</sub>의 표면 굴곡에 따른 광학 포논 변화를 연구하기 위해 편광 라만 산란 실험을 수행하였다. 원자힘현미경 이미지를 통해 울퉁불퉁한 표면 또는 주름이 한 방향으로 정렬되어 있는 표면을 지니는 단일 층 WS<sub>2</sub>가 성장되었음을 확인하였다. 이들 WS<sub>2</sub> 샘플 각각에 대한 편광 라만 산란 스펙트럼으로부터 E'과 A<sub>1</sub>' 포논 모드를 확인할 수 있었다. 흥미롭게도, 울퉁불퉁한 표면의 WS<sub>2</sub>로부터의 편광 라만 산란 실험 결과, E' 포논의 세기는 이론적으로 예측되는 편광 선택 규칙을 벗어나는 결과를 보였다. 주름진 표면을 지니는 WS<sub>2</sub>에서는 E' 포논 반응이 눈에 띄게 변화되었다. 특히, 주름 형성에 의한 단축 인장 변형에 의해 E' 포논 모드가 편광 의존도가 서로 다른 두 개의 포논으로 분리되었음을 알 수 있었으며, 이를 통해 성장된 단일 층 WS<sub>2</sub>의 변형이 어느 정도 일어났는지 계산할 수 있었다. [이 연구는 2019년도 정부(과학기술정보통신부)의 재원으로 한국연구재단의 지원을 받아 수행되었음 (No. 2019R1A2C1003366)]

### Keywords:

WS<sub>2</sub>, 변형, 라만 분광학, 광학 포논

## 반투명하고 유연한 그래핀/WS<sub>2</sub> 수직 이종접합 자가발전 광검출소자

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### Abstract:

높은 광투과도와 전기전도도를 가진 그래핀과 광특성이 뛰어난 2차원 전이금속 칼코게나이드 물질을 조합한 2차원 물질 기반 이종접합 구조는 우수한 광전 특성을 바탕으로 광전소자 분야 응용을 위한 많은 연구가 진행되고 있다. 본 연구에서는 2차원 물질인 WS<sub>2</sub>와 bis(trifluoromethanesulfonyl)-amide (TFSA)가 도핑된 그래핀을 순서대로 유리 기판뿐만 아니라 휘어지는 poly(ethylene terephthalate) 기판 위에도 전사시켜 TFSA-그래핀/WS<sub>2</sub> 수직 이종접합 광검출소자를 제작하였다. 이 광검출소자는 자외선에서 가시광선에 걸쳐 광반응을 나타내었는데, 가시광 영역에서 평균 투과도가 40 %에 이를 정도로 반투명하였으며, 특히 0 V에서 광반응도가 델타함수처럼 커지는 자가발전 특성을 보였다. 광검출소자의 성능 지수인 광반응도, 양자효율, 및 광검출능은 400 nm 파장에서 각각 0.14 AW<sup>-1</sup>, 40 %, 및 2.5x10<sup>9</sup> cm Hz<sup>1/2</sup>W<sup>-1</sup>로 이전 연구결과들과 비교했을 때 비슷하거나 크게 나타났다. 또한, 곡률 반경이 4 mm일 때 3000회 반복 굽힘 테스트 후에도 초기 광반응도 성능이 88% 이상 유지되는 우수한 휘어짐 특성을 보였다. 본 발표에서는 위의 실험 결과들을 토대로 그래핀/WS<sub>2</sub> 이종접합구조 광검출소자의 특성과 물리적인 메커니즘에 대해서 논의하고자 한다.

### Keywords:

2차원 물질, 도핑된 그래핀, 수직 이종접합, 유연 광검출 소자, 반투명

## GaN 표면 위에 MOCVD로 성장된 2차원 이황화 몰리브덴의 성장특성 연구

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### Abstract:

이황화몰리브덴(MoS<sub>2</sub>)는 전이금속 디칼코게나이드(TMDCs) 중 하나로, 단일층 또는 수 층으로 얇아졌을 때 발생하는 새로운 광학적, 전기적 특성으로 인해 지난 십수년간 다양한 분야에서 연구되고 있다. 특히 최근에는, MoS<sub>2</sub>를 포함한 TMDC 단일층 물질을 대면적에서 균일하게 성장하기 위한 방법으로 유기금속 화학증착법(MOCVD)을 활용한 성장기법이 개발되었다. 한편, 대표적인 III-V족 화합물 반도체 중 하나인 GaN는 그 결정면 중 하나인 c-면과 TMDC 물질들의 격자구조의 형태와 격자상수가 1% 이하의 차이로 굉장히 유사한것이 확인되었다. 따라서, GaN의 c-면을 성장면으로 하는 TMDCs, 그 중에서도 가장 격자상수가 일치하는 물질 중 하나인 MoS<sub>2</sub>의 성장은 기존에 많이 시도된 amorphous SiO<sub>2</sub> 기판 위에 성장한 것보다 더 나은 성장 품질 및 광전기적 특성을 보일 수 있을 것으로 기대할 수 있다. 본 연구에서는, 같은 MOCVD 장비 안에서 SiO<sub>2</sub> 기판과 GaN 기판에서 각각 성장된 MoS<sub>2</sub> 물질의 구조적, 광학적 특성을 관찰하고, 특히 GaN의 표면 상태에 따른 MoS<sub>2</sub>의 성장 형태를 비교하였다. 이를 통해 GaN를 고품질의 2차원 TMDCs 성장을 위한 플랫폼으로서의 가능성을 확인하고자 했다.

### Keywords:

MoS<sub>2</sub>, GaN, MOCVD, 격자상수

# Monolithic Interface Contact Engineering to Boost Optoelectronic Performances of 2D Semiconductor Photovoltaic Heterojunctions

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## Abstract:

In optoelectronic devices based on two-dimensional (2D) semiconductor heterojunctions, the charge transport across the interface is a critical factor to determine the device performance. Even though much effort has been recently made to improve the generation and dissociation of excitons in 2D semiconductors, effective strategies that can enhance charge extraction at the contact interface have rarely been explored. Here, we report an unexplored approach to boost the optoelectronic device performances of 2D heterojunctions via the phase-transition-induced modulation of the interface band alignment. In the proposed device, the atomically thin  $\text{WO}_x$  layer, which is monolithically formed by layer-by-layer oxidation of  $\text{WSe}_2$ , is used as a hole transport layer. When the  $\text{WO}_x$  interlayer was introduced at the semiconductor/electrode interface, the power conversion efficiency of the  $\text{WSe}_2$ - $\text{MoS}_2$   $p$ - $n$  junction devices increased by about an order of magnitudes, from 0.7 to 5.0%, maintaining the response time. The enhanced characteristics can be understood by the formation of the low Schottky barrier and favorable interface band alignment resulting from the monolithic phase transition, as confirmed by band alignment analyses and supported by first-principle calculations. In addition, by fabricating a more optimized  $\text{WO}_x$ - $\text{WSe}_2$ -Ti-Au device capable of improved light absorption and efficient electron transport, the performance was further improved to  $\sim 0.8$  V with  $V_{OC}$  close to the bandgap and  $\sim 7$  % for PCE. Our work suggests a new route to achieve band engineering in the heterostructures toward realizing high-performance 2D optoelectronics.

## Keywords:

2D materials, Interface Engineering, optoelectronics

## Faraday Geometry의 외부 자기장에서 InAlAs/Al<sub>40</sub>Ga<sub>60</sub>As 단일 양자점의 자기 광학적 특성 분석

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### Abstract:

외부 자기장이 가해졌을 때 전자들이 가지는 스핀 상태가 Zeeman splitting의 현상을 보이는 것은 널리 알려져 있다. 이러한 Zeeman splitting은 특히 discrete 한 에너지 상태를 가지는 반도체 양자점에서 더욱 명확하며, 이는 양자점이 가진 에너지 구조를 분석하는데 도움이 된다. 또한 외부 자기장은 양자점 내부에 구속된 엑시톤에 추가적인 구속 효과를 주고, 이는 양자점의 발광 특성의 변화로 나타난다. 이러한 추가적인 구속 효과는 해당 양자점의 구조에 의한 구속 에너지에 반비례한다. 따라서 이러한 외부 자기장에 의한 diamagnetic shift를 관측함으로써 반도체 양자점의 구조적 특징을 분석할 수 있다. 본 연구에서는 Faraday Geometry의 외부 자기장을 걸어주며 저온에서 magneto-photoluminescence 실험을 진행하였다. 특히 InAlAs/Al<sub>40</sub>Ga<sub>60</sub>As 단일 양자점 시료에서 Zeeman splitting과 diamagnetic shift를 관측하였고, 이후 편광에 따른 photoluminescence 실험을 통해 분리된 두 신호의 편광 특성을 분석하였다.

### Keywords:

Zeeman splitting, Diamagnetic shift, Semiconductor quantum dots, Faraday geometry

## Evaluating the time constant of p-n GaAs junctions with estimating the quantum efficiency of the junctions by photo-reflectance spectroscopy

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### Abstract:

In this work, the characteristic time constant of p<sup>+</sup>-n and p<sup>+</sup>-i-n GaAs junctions was investigated by photo-reflectance spectroscopy. Using the exponential behavior of the photo-reflectance signal, a limitation is introduced for the chopping frequency of photo-reflectance from the time constant point of view. Finally, an explicit formulation is derived for the characteristic time constant of the junction. This proposed semi-empirical formulation relates the characteristic time constant to photo-voltage, excitation wavelength and intensity, permittivity, depletion width, and the most important, the quantum efficiency of the junction. Employing this formula and estimating the related parameters from the photo-reflectance spectrum, one can estimate the quantum efficiency of the junction. The formula examined for two structures: a p<sup>+</sup>-n GaAs junction and a p<sup>+</sup>-i-n GaAs solar cell for different excitation intensity, and the quantum efficiency of the junctions estimated by the method. The proposed method can be used as a contactless method to compare the quantum efficiencies of the junctions.

### Keywords:

Time constant, Quantum efficiency, Photoreflectance, Phase diagram, Chopping frequency

## Ab initio study of metal-induced gap states at the metal-insulator interfaces

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### Abstract:

Interfaces between superconducting metals and thin oxide layers play a crucial role in a Josephson tunnel junction used in quantum information processing circuits. Josephson junctions are comprised of two superconducting electrodes divided by a thin insulator. In this case, extra electronic states can be formed at the bandgap region of oxide layers. These states are often referred to as metal-induced gap states (MIGSs). We present an *ab initio* study of atomic and electronic properties of interfacial heterojunctions built by sandwiching aluminum oxide ( $\text{Al}_2\text{O}_3$ ) layers between aluminum (Al) and gold (Au) electrodes. For *ab initio* calculations, we use the Vienna *ab initio* simulation package (VASP). The generalized gradient approximation (GGA) in the form of the PBE-type parameterization is employed. The ionic pseudopotentials are described via the projector augmented wave, and the cutoff energy for the plane-wave basis is set to 400 eV. We consider various atomic configurations between metal electrodes and insulating layers occurring in Al/ $\text{Al}_2\text{O}_3$ /Al and Au/ $\text{Al}_2\text{O}_3$ /Al heterostructures. Our calculations reveal that MIGSs are formed at the bandgap region of  $\text{Al}_2\text{O}_3$  layers with different interface configurations. In addition, we focus on the effects of MIGSs on the potential barriers at the interfaces present in the heterostructures.

### Keywords:

*ab initio* study, Josephson junctions, MIGSs, oxide layers, superconductivity

## Cross-linked Polyvinylpyrrolidone-induced Interface Trap Suppressed carrier transport with Electron Doping

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### Abstract:

The stability and reproducibility of van der Waals materials have been regarded as most important issues for the commercial applications. Instability of the materials leads spontaneous morphological and chemical transformation in air, and moreover it limits the doping process which is one of most important components for semiconducting electronics and optoelectronic industry. Here, we suggest the practical methods for n-doping of the tungsten diselenides ( $WSe_2$ ) mediating the Se-vacancies by simply coating the polyvinylpyrrolidone (PVP). The lone paired electrons of oxygen in polymer bonds with the chalcogenide vacancy site and donates the electrons; as a result, simultaneous effects of stabilized structure with interface trap suppression and carrier type conversion by electron doping is realized. The carrier type of  $WSe_2$  is converted from p-type to n-type with threshold voltage varying from 30 to -30 V. Further the vacancy-induced interface traps density is nearly 500 times reduced with stabilized activation energy. The study not only provides practical doping and passivation method for ultrathin materials but comprehensive understating and insights about chemical reaction and electronic transports inside materials.

### Keywords:

$WSe_2$ , PVP, interface trap, passivation

## Reducing Fermi level pinning effect at MoS<sub>2</sub>-Mo<sub>2</sub>C interfaces by using Mo<sub>2</sub>C as an electrode through dry transfer

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### Abstract:

Schottky Barrier Height (SBH) in the metal/semiconductor interface is a potential barrier by the work function difference. We can predict the height if we know the work function of each metal and semiconductor. However, it is difficult to obtain the expected barrier height from the work function difference due to Fermi level pinning effect, which could be reduced by minimizing defects in the interface of semiconductor.<sup>[1]</sup> Research on Two-Dimensional (2D) semiconductors has been studied. MoS<sub>2</sub>, the most representative 2D semiconductor showed the pinning effect for various metals at interface.<sup>[2]</sup> Here, Molybdenum Carbide (Mo<sub>2</sub>C) crystals are grown by Chemical Vapor Deposition (CVD) process.<sup>[3]</sup> Mo<sub>2</sub>C reveals 2D metallic behavior and has a work function of 4.8eV by Ultraviolet Photoelectron Spectroscopy (UPS) spectrum. We fabricated MoS<sub>2</sub>-Mo<sub>2</sub>C heterostructure device through dry transfer of Mo<sub>2</sub>C onto MoS<sub>2</sub>. Dry transfer can be expected that defects that might occur in existing processes such as evaporating would be reduced. We obtained the linear dependence electrical properties of MoS<sub>2</sub>/Mo<sub>2</sub>C device. Schottky barrier height was calculated from current measurement by temperature, and it noticed that Fermi level pinning effect is minimized because barrier height value (~0.5eV) is similar with the difference between the work function of Mo<sub>2</sub>C and the conduction band of MoS<sub>2</sub>.<sup>[4]</sup>

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### Keywords:

Schottky barrier height, Fermi level pinning effect, 2D semiconductor, Mo<sub>2</sub>C, Dry transfer

# Unveiling Hidden Surface Channel in Two-dimensional Multilayers

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## Abstract:

Thus far, numerous 2D van der Waals (vdW) materials have been reported with interesting optoelectronic properties mainly originating from their atomically thin nature. Among them, a black phosphorus (BP) multilayer is known to be extremely sensitive to ambient conditions, whereas a rhenium disulfide (ReS<sub>2</sub>) is relatively very stable comparing to BP. This contrasting feature makes them ideal platform to study the effects of surface adsorbates and surface oxidation on top of 2D materials. Here, we unveil a hidden surface channel in p-type black phosphorus and n-type rhenium disulfide multilayers originating from undesired ambient adsorbates and surface oxidation which not only accumulate holes on the surface of materials but also deteriorate their carrier mobility. The observed disappearance of a second peak in the transconductance curve under ambient conditions strongly implies the absence of the top-surface channel inside the 2D multilayers, which is a feasible indicator for the cleanliness of the top surface. Moreover, the almost invariability in the drain bias polarity-dependent turn-on voltage for the bottom channel under ambient conditions indicates the exclusive contribution of surface adsorbates to the formation of the top channel in 2D multilayers. Our study will provide a deep insight into the distinct carrier transport in 2D multilayer based optoelectronic devices and diverse sensor applications.

## Keywords:

2D van der Waals (vdW) materials, Black Phosphorus, Rhenium Disulfide, Carrier transport, Hidden surface channel

# Gate-induced photocurrent hysteresis in multilayer WSe<sub>2</sub> field effect transistor

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## Abstract:

Two-dimensional transition metal dichalcogenide(2D-TMDs) have been attracting enormous attention as promising materials for their interesting electrical, optical, and mechanical properties. Following the possibility of fabricating new optoelectronic devices, photodetector application, and thin-film transistors, a number of research have been carried out to understand the fundamental exciton physics and carrier relaxation mechanism in the 2D-TMDs. As a one of the powerful techniques to characterize the light-matter interaction, photocurrent spectroscopy provides a method to analyze the non-radiative excitonic states that need to be deeply understood for optimizing light-emitting devices based on 2D-TMDs. However, the electrical hysteresis of the transfer curve and surface sensitive properties of the 2D-TMDs hinder precise and consistent photocurrent measurements. Therefore, it is necessary to investigate the factors influence on the inconsistent photocurrent spectrum.

In this study, we fabricated a multilayer WSe<sub>2</sub> back-gated field effect transistor. We measure wavelength-dependent photocurrent with a conventional photocurrent experimental setup using lock-in amplifier. In the photocurrent spectrum, A-exciton transitions is clearly observed. The negative gate bias leads to A-exciton spectral broadening implying the scattering of excitons with the gate bias induced injection (doping) of free charge carriers. However, the time-dependent variation in the photocurrent spectrum obstructs systematic characterization. The further study needs to be performed to clarify and solve this inconsistency, for instance, by fabricating hysteresis-free WSe<sub>2</sub> FET device.

## Keywords:

Photocurrent spectroscopy, WSe<sub>2</sub> field effect transistor, Photocurrent hysteresis, TMDCs

## 징케이션 조건에 따른 알루미늄 기판 위 니켈-붕소 무전해 도금에 관한 연구

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### Abstract:

현재 IC의 기능이 높아짐에 따라 IC회로는 복잡해져가고 있고, 반도체 칩이 소형화, 고집적화, 고성능화됨에 따라 패키징 기술의 발전이 요구되고 있다. 일반적으로, IC bonding 패드 물질로 알루미늄(Al)이 가장 많이 사용되고 있고, solder bump를 이 Al 패드위에 올릴 때, 하부금속층 형성을 위해 니켈 도금박막을 형성하고 있다. 산화되지 않은 Al은 무전해 니켈도금에 대해 반응을 일으켜 박막형성이 가능하지만, 산화가 잘되는 Al 특성상 표면에 형성된 산화층이 니켈의 도금형성을 방해하게 된다. 따라서, Al 표면을 활성화시키고 접착력을 향상시키기 위해 주로 징케이션(zincation) 법을 활용하고 있다.

본 연구에서는 Al base 기판의 기판위에 회로를 구성함에 있어, 고온 무전해 도금에서 발생할 수 있는 기판의 손상이나 기판과 형성 금속간의 응력의 영향 제거, 공정비용절감 등을 위해 저온에서 니켈-붕소(Ni-B) 무전해 도금욕을 이용하여, 징케이션 조건에 따른 성장된 Ni-B의 특성을 분석하였다. 징케이션 표면 처리된 Al 또는 Ni-B 무전해 도금된 Al 표면의 특성 분석은 광학현미경(Optical Microscope), FE-SEM(Field Emission Scanning Electron Microscope) 등을 사용하여 표면의 결함 및 미세구조를 측정하고 XAS(X-ray Absorption Spectroscopy)를 이용하여 결정구조의 변화를 조사하였다.

### Keywords:

Ni-B 무전해 도금, XAS(X-ray Absorption Spectroscopy)

## Photosensitive Field-Effect Transistors Using n-type NDI-C6 and p-type Rubrene Organic Semiconductors

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### Abstract:

루브렌(rubrene)은 p형 유기 반도체로 전계 효과 트랜지스터, 광검출기, 광메모리에 연구되고 있다. 본 연구에서는 n형 유기 반도체 중 하나인 나프탈렌 디이미드(naphthalene diimide, NDI-C6)를 이용하여 n형 전계 효과 트랜지스터(n-channel field-effect transistor, FET)를 제작하였고, rubrene FET와 특성을 비교하였다. NDI-C6에 385 nm LED 광원에 의한 광전류는 -3.85 nA로 측정되었다. 레이저 공초점 현미경(laser confocal microscope, LCM)을 이용해 NDI-C6와 rubrene의 광발광(photoluminescence, PL) 및 흡수 스펙트럼을 측정하여 나노광학 특성을 비교, 분석하였다. NDI-C6와 rubrene LCM PL 피크는 각각 524 nm, 555nm에서 관찰되었다. NDI-C6와 rubrene의 하이브리드 나노구조체를 제작하여 나노광학 특성을 측정 및 분석하고, 이종접합 (heterojunction) FET를 제작해 전하전달과 광전자 특성을 측정하였다. 제작한 NDI-C6/rubrene 시스템에서 입력전압 변화에 따른 전기발광(electroluminescence) 특성 결과를 논의한다.

### Keywords:

organic semiconductor, field-effect transistor, organic n-channel transistor

## **Fabrication of the quantum dot-stacked microscale wires by using a micropipette-combined QTF-AFM and optical setup**

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### **Abstract:**

Recently, research on microscale patterning in a specific spot has been extensively studied on various field. Among these advanced technologies, e-beam lithography, which uses electrons to print, and dip-pen lithography, which uses a pipette like a pen, are widely used [1]. However, the above two methods have fatal drawbacks. First, in the case of the e-beam, a fairly high voltage is required to proceed with the experiment, and in the case of the dip-pen, there is a risk of tip damage, so it is impossible to print a large number of copies [2]. Therefore, in this experiment, we are going to introduce a method that can print a large number of prints without needing a high voltage and without worrying about damage to the tip. Simply by bringing the tip of the pipette very close to the surface of the sample, a very small water column is created between them, and the water column served as a passageway between the two. Therefore, the quantum dot solution in the pipette comes out through this passage, forming a microscale wire [3]. After forming a microscale wire made of quantum dots on the surface of the sample in this way, in this experiment, PL measurement will be performed to confirm that the component of the generated wire is made up of quantum dots [4].

### **Keywords:**

Micropipette, QTF-AFM, quantum dot, PL

## MoS<sub>2</sub>/WS<sub>2</sub>의 이종접합구조에서 비틀림각도에 따른 발광특성 연구

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### Abstract:

2차원 전이금속 디칼코게나이드(Transition metal dichalcogenides, TMDs) 단층들로 구성되는 2차원 이종 접합구조들은 빛과의 강한 상호작용, 층간전하의 빠른이동, 그리고 밸리(valley)에 의존하는 광학 선택성 등 다양하고 독특한 특성들이 나타나며 이로 인하여 새로운 물리적인 현상이 기대될 뿐만 아니라, 전자 및 광전자 소자로서 응용가능성도 큰 관심을 받고 있다. 두 단층을 접촉하여 이종접합구조를 제작하면 격자의 차이나 회전에 의한 불일치(misalignment)로 인하여 주기적인 새로운 전위가 추가되는 모아레 초격자도 형성될 수 있으며, 이로 인한 새로운 길이/에너지 스케일은 양자현상을 제어하는 강력한 수단이 될 수도 있다. 특히 MoS<sub>2</sub>와 WS<sub>2</sub> 단층간의 격자 매개변수 차는 ~0.16%로 거의 무시할 수 있는 격자 불일치를 가지며, 이들은 이미 잘 알려진 것처럼 type 2 형태의 띠틈격 (bandgap) 정렬이 일어난다. Type 2기반의 이종접합구조는 층간에서 효과적인 전하의 이동 및 분리가 일어나고 상대적으로 수명(lifetime)이 긴 층간 엑시톤이 형성된다. 엑시톤, 모아레 엑시톤, 층간 엑시톤들과의 혼성화(hybridization)는 인접한 단층사이의 비틀림 각도에 강하게 의존할 것으로 예상된다. 본 연구에서는 화학기상증착법 및 전사기법을 이용하여 다양한 비틀림 각도를 가지는 MoS<sub>2</sub>/WS<sub>2</sub>이종접합구조를 제작하였으며, 이런 이종접합구조는 Raman, photoluminescence (PL), differential-reflection(DR) 등의 분광기법과 2차 고조차 발생 측정기법(Second Harmonic Generation)을 이용하여 이종접합구조에서 비틀림 각도에 따른 광학적 특성을 연구하였다. 특히 이종접합구조의 비틀림 각도들 중에서 특정한 범위의 각도에서 각각의 단층들과 비교하여 이종 접합에 의한 PL 최고점(peak)과 세기의 변화 및 의존성을 관찰하였다. 우리는 이러한 새로운 발광현상들에 대하여 각각 단층의 엑시톤과 층간 엑시톤에 의하여 혼성화된 (hybridized) 엑시톤의 형성과 관련이 있다고 판단하였으며, 이런 실험적인 결과들은 이론적 예측들을 바탕으로 그 원리를 설명하고자 하였다.

### Keywords:

2차원, 전이금속 디칼코게나이드, 이종접합구조, 엑시톤, 층간 상호작용

## A study on Te and MoS<sub>2</sub> for CMOS inverter fabrication

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### Abstract:

The semiconductor industry tended to scale down in channel length according to Moore's law. However, as the channel length of the transistor was scaled down to the nanometer range, a Short Channel Effect (SCE) happened. As a solution to this, a transistor using a Trans Metal Di-Chalcogenide(TMDC) has been proposed. TMDC is a type of two-dimensional material that has a band gap and its type is determined by the defect of the material. Unfortunately, Carrier mobility of TMDC is hundreds, which is lower than silicon based devices. However, recent studies found that 2D Te is a material with carrier mobility of hundreds, even though it is a p-type material. In this study, CMOS inverter is fabricated on heavily p-doped silicon wafer, with MoS<sub>2</sub>, representative n-type TMDC, and 2D Te. Threshold voltages and carrier mobilities are calculated with the transfer curves and output curves of P, N- MOSFET measured by probe station and KEITHLY's 4200 instrument at vacuum and room temperature. Based on the data, the voltage transfer curve of the CMOS inverter with 2D materials is modeled. Through this study, it is expected that 2D Te can be used to fabricate low-power logic elements.

### Keywords:

MOSFET, 2D Materials, MoS<sub>2</sub>, Tellurene, CMOS Inverter

## CVD 단일공정에 의한 2차원 $WS_xSe_{1-x}$ 박막의 증착 및 Se 양의 조절을 통한 띠간격 에너지 조절

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### Abstract:

2차원 야누스(Janus) dichalcogenide 물질은 여러 새로운 양자 현상의 발현으로 매우 높은 관심을 받고 있다. 본 연구에서는 선행연구로 확인된 제작방법인 공정 전/후 처리가 없는 단일 CVD 공정에 기반하여, chalcogen 원소 S와 Se의 조성비를 달리하여 띠간격 에너지의 조절이 가능한  $WS_xSe_{1-x}$ 를 제작하였다. 먼저 두 단계로 이루어진 온도조절을 통하여 S와 Se를 순차적으로 활성화시켜  $WS_xSe_{1-x}$ 를 성장하였다.  $WS_2$ 에서 열처리 과정 중 W-S결합구조에서 결합이 붕괴된 뒤 S원소가 Se원소로 치환되는 성장 메커니즘을 바탕으로 Se 파우더를 10, 20, 30, 40 mg으로 바꿔가면서 x 값을 변화시켜 제작한  $WS_xSe_{1-x}$ 의 광루미네선스(Photoluminescence) peak가 각각 1.9, 1.85, 1.81, 1.65eV로 변화하는 것을 확인하였는데 이는  $WS_xSe_{1-x}$ 의 띠간격 에너지가 x 값에 매우 민감하게 의존한다는 사실을 나타낸다. 이를 포함하여, 제작된  $WS_xSe_{1-x}$ 의 광학적 및 구조적 특성을 라만 산란 및 광루미네선스로 분석한 결과를 바탕으로 그 물리적 성장 메커니즘에 대해서 논의한다.

### Keywords:

2차원 물질, 띠간격 에너지, 단일 CVD 공정,  $WS_xSe_{1-x}$ , 광루미네선스

## Raman mapping study of hBN-encapsulated monolayer WS<sub>2</sub>

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### Abstract:

수직으로 쌓여 있는 이차원 헤테로구조는 얇고 유연한 전자소자와 광전자소자 응용을 위한 차세대 물질로서 주목받고 있다. 하지만, 헤테로구조를 제작하는 과정에서 형성된 층과 층 사이의 기포는 전기 및 광 특성의 공간적인 변화를 일으키는 원인이 된다. 이 연구에서는 hBN/WS<sub>2</sub>/hBN 헤테로구조에 대한 공간 분해된 라만 산란 연구를 통해서 기포에 의한 단일 층 WS<sub>2</sub>의 물리 특성 변화에 대해서 보고한다. WS<sub>2</sub>에서 대표적으로 관측되는 E' 포논과 A<sub>1</sub>' 포논에 대한 넓은 영역에 걸친 라만 이미지를 분석한 결과, 기포가 형성되어 있는 계면의 위치와 기포에 의한 WS<sub>2</sub>의 전자 밀도 변화에 대한 정량적인 정보를 얻을 수 있었다. 기포가 전자 밀도에 영향을 끼치는 것과는 대조적으로 기포뿐만 아니라 hBN에 의한 WS<sub>2</sub> 층의 변형 효과는 미미한 것으로 나타났다. 이러한 결과는 E' 포논과 A<sub>1</sub>' 포논 사이의 상관관계 분석을 통해서 더욱 두드러지게 나타났다. [이 성과는 2019년도 정부(과학기술정보통신부)의 재원으로 한국연구재단의 지원을 받아 수행된 연구임 (No. 2019R1A2C1003366)]

### Keywords:

Raman spectroscopy, WS<sub>2</sub>, hBN, Bubble

## Enhanced Photoluminescence and Photoresponsivity of Photodetector using Perovskite MAPbI<sub>3</sub> Hybridized with Au-Nanoparticles

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### Abstract:

유기-무기금속 할로겐 화합물 페로브스카이트(organic-inorganic metal halide perovskites)는 고효율 태양 전지, 광 검출기, 발광다이오드, 센서 등에 응용되고 있으며, 메틸암모늄 요오드화납(methylammonium lead iodide, MAPbI<sub>3</sub>)이 대표적 물질이다. 본 연구에서는 고용해 용액법과 화학증착법을 결합하여 MAPbI<sub>3</sub> 결정성 박막을 제작하였고, 나노광학 및 광 검출기(photodetector) 특성을 연구하였다.  $\pi$ -공액 고분자전해질인 poly(9,9-bis(4'-sulfonatobutyl)fluorene-alt-1,4-phenylene) potassium (FPS-K)를 MAPbI<sub>3</sub> 박막 표면에 보호막(passivation layer)으로 스핀 코팅했고, 기능이 있는 금 나노 입자 (Au-NP)를 하이브리드하여 표면 플라즈몬 공명 (surface plasmon resonance coupling; SPR) 조건에서 에너지 전달 효과를 연구하였다. MAPbI<sub>3</sub> 박막에 FPS-K와 Au-NP 처리 후에 SPR 에너지 전달을 통해서 PL 효율의 증가와 시간분해 (time-resolved) PL 스펙트럼을 통해서 엑시톤 수명의 변화를 관찰하였다. AuNP/FPS-K/MAPbI<sub>3</sub> 하이브리드 광 검출기의 광전류와 광반응도 값의 증가를 입사된 광원의 파장 또는 세기의 함수로 측정, 분석하였다. AuNP/FPS-K/MAPbI<sub>3</sub> 광 검출기의 반응성이 가장 우수한 파장은 735 nm였으며, 빛 인가에 의해서 전류 값이 약 100배 증가하였고, 금 나노 입자와 고분자 전해질을 하이브리드 하기 전과 후의 전류 값의 차이도 약 70 배 정도로 관찰되었다.

### Keywords:

surface plasmon, perovskite, methylammonium lead halide, gold nanoparticle, photodetector

## Role of Quantum Capacitance in Double-Gate Negative Capacitance Field-Effect Transistors

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### Abstract:

The subthreshold swing (SS) of metal oxide field-effect transistors (MOSFETs) is limited to 60 mV/dec by the Boltzmann limit. To overcome the Boltzmann limit, negative capacitance field-effect transistors (NCFETs) using the negative capacitance behavior of ferroelectrics have been investigated actively. While significantly affecting inversion layer charge density in nanoscale devices, quantum capacitance is an obstacle to achieving hysteresis-free subthermionic SS of NCFETs [1]. We will report a computational study of the role of quantum capacitance primarily in double-gate (DG) NCFETs, where the density of states (DOS) and quantum capacitance can be readily controlled by modulating the degree of quantum confinement. The EDA Tool was supported by the IC Design Education Center.

[1] W. Cao and K. Banerjee, Nat. Commun. 11, 196 (2020).

### Keywords:

NCFET, quantum capacitance, double gate

## Optical and electrical properties of Sn-doped $\beta$ -Ga<sub>2</sub>O<sub>3</sub> thin films

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### Abstract:

Optical and electrical properties of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and Sn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> thin films grown on Si substrates via radio frequency magnetron sputtering deposition are investigated. Thermal annealing at 900°C for two hours was performed after the deposition of films at 500°C to improve crystalline quality. X-ray diffraction (XRD) and X-ray photoemission spectroscopy measurements were used to determine the structural and compositional properties of the films. XRD results showed that the amorphous phase was observed in all the as-grown thin films, and they became crystalline after the post-treatment process. The electrical properties of the annealed films were evaluated via a four-point probe method and Hall effect measurement. The  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> films showed n-type conductivity with electron mobility of 163 cm<sup>2</sup>V<sup>-1</sup> s<sup>-1</sup> and carrier concentration of 1.32x10<sup>17</sup> cm<sup>-3</sup>. Using spectroscopic ellipsometry, the thickness of thin films and the optical constants between 0.7 and 6.0 eV were determined. We estimated the optical gap energy of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and Sn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> layer using Tauc method. The optical gap energy was 4.902 eV for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> films. With increasing Sn content, the lattice constants increased, and the optical gap energy decreased. Optical structures owing to defects were found below optical gap energy in the dielectric function spectra, which were determined using point-by-point curve fitting. Using cathodoluminescence (CL) spectroscopy, multiple peaks were found in the range from 1.5 to 2.9 eV. The CL peaks correspond to transitions between valence (conduction band) and defect-induced gap states.

### Keywords:

Ga<sub>2</sub>O<sub>3</sub>, Sn doping, spectroscopic ellipsometry, cathodoluminescence, defect level

## Structural and optical properties of perovskite film in terms of precursor solution preparation method

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### Abstract:

Perovskite solar cells are known as commercially useful solar technologies because they have high power conversion efficiency with low manufacturing costs, and research on them has been actively conducted recently. However, in the solution process-based perovskite film, problems with reproducibility and stability due to the difference in the molar ratio between the stoichiometrically calculated precursor material and the resulting product have been reported. Therefore, in this research, a perovskite film was manufactured using a precursor mixture, a mechanical grind, and a single crystal precursor manufacturing method in terms of the precursor solution preparation method. Optical characteristics were analyzed using photoluminescence (PL) and time-resolved PL spectroscopy, and structural analysis was performed with X-ray diffraction and scanning electron microscopy. Compared to other preparation methods, the single crystal-based perovskite film exhibited the strongest PL intensity and long lifetime, and the sample using the mechanical grind method showed asymmetric PL characteristics with shoulder peak due to unintended composition fluctuation. These results will contribute to the production of reproducible perovskite solar cell devices.

### Keywords:

perovskite, precursor, stoichiometry, photoluminescence

## Photoluminescence와 photoreflectance를 이용한 InAlGaAs/GaAs Quantum Dot 광학적 특성분석

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### Abstract:

본 연구는 MBE를 이용하여 성장한 InAlGaAs/GaAs Quantum dot의 In 조성 변화에 따른 광학적 특성을 광 발광 과 광 분광법을 통하여 조사하였다. InAlGaAs QD 샘플은 반 절연성 GaAs(100) 기판위에 성성장 하였다. 300nm의 버퍼층위에 InAsGaAs QD를  $Al_{0.71}In_{0.29}As$ 과  $Ga_{0.83}In_{0.17}As$  그리고 InAs submonolayer 를 주기적으로 성장하는 디지털 합금방식으로 성장 후 300nm 배리어 성장을 하였다. In 조성이 42%, 52%, 62%의 변화에 따라 PL 발광중심은 1.35, 1.32, 1.32 로 감소함을 보이다 62%에서는 동일함을 보였다 이는 In 조성의 증가로 인한 QD의 균질성과 구조적 변화에 의한 영향이다. PR결과 GaAs 버퍼층의 신호와 QD에 의한 신호가 동시에 확인되었다. In 조성의 증가에 따라 QD 영역의 신호의 변화 경향 역시 PL의 경향과 유사함을 확인하였다.

### Keywords:

photoreflectance, photoluminescence

## 뉴로모픽 컴퓨팅을 위한 전기화학적 금속화 셀 기반의 나노-스케일 아날로그 인공 시냅스 소자

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### Abstract:

4차 산업혁명 시대가 도래함에 따라 인공지능 기술이 비약적으로 발달하고, 현재 가장 널리 사용되는 폰노이만 컴퓨팅의 한계를 뛰어넘기 위해 뉴로모픽 컴퓨팅에 대한 연구가 활발히 진행되고 있다. 인공지능의 학습 및 추론의 능력을 가속화 시키기 위한 새로운 컴퓨팅 패러다임에는 인공 시냅스 소자의 연구 및 개발이 필수적이다. 일반적으로, chalcogenide 물질 (예: GeSe, GeS<sub>2</sub>, GeTe, ZnTe 등) 내에서 Ag 또는 Cu의 mobility가 매우 빨라 낮은 전압(low voltage, <1 V)에서 저항 변화 (resistive switching)가 가능하다고 알려져 있다. 본 연구에서는 chalcogenide 물질인 GeS<sub>2</sub>를 switching layer로 사용하고, switching layer내의 Ag filament의 formation과 rupture dynamics를 이용한 인공 시냅스 소자를 개발하였다. 나노-스케일 (618 × 618 nm<sup>2</sup>)의 TiN bottom electrode에 10nm 두께의 GeS<sub>2</sub> (switching layer), 10nm 두께의 Ag (source layer), 그리고 20nm 두께의 Pt (contact electrode)를 순서대로 sputtering 공정을 이용하여 deposition을 진행하였으며, 이를 통해 단일 인공 시냅스 소자를 제작하였다. 또한, voltage pulse의 amplitude가 증가함에 따라 Long-term potentiation (LTP)과 Long-term depression (LTD) 특성에서 conductance의 변화량이 증가하는 것을 확인하였다. 그리고, 인공 시냅스 소자의 LTP/LTD 특성을 생물학적 시냅스의 비선형적인(non-linear) dynamics를 표현한 수식을 이용해 fitting을 진행하였고, 디바이스의 특성을 이용한 하드웨어 기반 딥-뉴럴 네트워크 (DNN) 시뮬레이션을 통해 92.92 %의 우수한 분류 정확도를 나타내는 것을 확인하였다.

### Keywords:

Electrochemical metallization cell, Neuromorphic computing, Synaptic device

## Temperature Dependency of Optical Characteristics in PbI<sub>2</sub>/Alq<sub>3</sub> Hybrid Structure: Observation of Fabry-Perrot Resonance

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### Abstract:

아이오딘화 납(PbI<sub>2</sub>)은 자연적으로 이차원 판상 구조의 결정을 형성하는 반도체 물질로, 저온에서 위스퍼링 갤러리 모드(whispering gallery mode, WGM)가 관찰되는 흥미로운 물질이다. Alq<sub>3</sub> (tris(8-hydroxyquinolino)aluminium)은 1986년 유기 발광 다이오드(OLED)의 발광층으로 처음 사용된 유기 반도체 물질이다. 본 연구에서는 재결정(recrystallization)을 통해 수백 nm 두께의 육각판 PbI<sub>2</sub>를 제작하였고, 그 위에 Alq<sub>3</sub>를 유기 분자빔 에피택시(organic molecular beam epitaxy, OMBE) 방법으로 증착해 하이브리드 구조체를 제작하였다. PbI<sub>2</sub>/Alq<sub>3</sub> 하이브리드 구조체에서 PbI<sub>2</sub>의 두께에 따르는 photoluminescence (PL) 스펙트럼에서 패브리-페로 간섭[Fabry-Perrot (F-P) interference]에 의한 공명현상을 관찰하였다. 또한 PbI<sub>2</sub>와 Alq<sub>3</sub>의 온도에 따른 PL 스펙트럼의 변화를 관찰하였고, 간섭현상에 의해 증폭되는 파장 대역이 변화하는 것을 확인하였다. 공명현상이 F-P 간섭에 의한 것임을 확인하기 위해 수직 입사에 의한 F-P 공명이 일어나기 위한 조건식  $2D = (m - 1/2) \times \lambda/n(\lambda)$ 를 이용해 공명이 발생한 파장을 비교하여 분석하였다. 극저온 3 K에서 PbI<sub>2</sub>/Alq<sub>3</sub> 하이브리드 구조체의 PbI<sub>2</sub>의 레이저 신호를 490 nm에서 관찰하였고 F-P 공명 신호의 최대값이 608nm에서 나타나 주황색의 빛이 PbI<sub>2</sub>/Alq<sub>3</sub> 가장자리에서 발광하는 것을 관찰하였다. 200 K까지 온도를 높이면 PbI<sub>2</sub>의 레이저 신호는 사라지고 Alq<sub>3</sub>의 고유의 스펙트럼의 형태가 드러나면서 F-P 공명 신호가 청색편이(blue-shift) 하는 것을 관찰하였다. 레이저 세기와 온도에 따른 PL 스펙트럼의 변화를 통해 PbI<sub>2</sub>/Alq<sub>3</sub> 하이브리드 시스템에서 전하, 에너지 전달 현상에 대해 논의한다.

### Keywords:

PbI<sub>2</sub>, Alq<sub>3</sub>, Fabry-Perrot resonance

## Characteristics of amorphous Ga<sub>2</sub>O<sub>3</sub> thin film growth on Ti substrates at low temperatures using MOCVD

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### Abstract:

Ga<sub>2</sub>O<sub>3</sub> has a wide energy bandgap of 4.7~4.9 eV and high break voltage of 8.0 MV/cm and a much higher Baliga's figure of merit of 3571 than GaN and SiC, so it is expected to be used in next-generation ultra-high voltage power semiconductors.[1] Currently, devices can be fabricated by homoepitaxy of Ga<sub>2</sub>O<sub>3</sub> crystals, but there are limitations to device performance improvement due to high defect density and low thermal conductivity existing in the substrate. Accordingly, many studies are being conducted to overcome the above-mentioned disadvantages and to fabricate a high-performance device by using a heterojunction thin film using various types of substrates. However, among various substrates, there have been few research results on metal substrates. Using metal substrates not only be able to solve the problem of thermal conductivity but also to provide various types of device applications. Therefore, research on the growth of Ga<sub>2</sub>O<sub>3</sub> heterojunction thin films using metal substrates is very important.

In a previous study, the growth of heterojunction Ga<sub>2</sub>O<sub>3</sub> on a Ti substrate at high temperature using MOCVD resulted in a rough surface. In this study, the heterojunction Ga<sub>2</sub>O<sub>3</sub> thin film growth was performed on Ti substrates at low temperatures using MOCVD to improve the surface flatness, and the characteristics of the crystal phase change were also observed through high temperature heat treatment. TMGa (trimethylgallium) and H<sub>2</sub>O were used as atomic gallium and oxygen sources. High purity nitrogen(5N) gas was used as carrier gas with flow rates of 400 sccm and 7sccm through the H<sub>2</sub>O and TMGa bubbled system, respectively. The growth temperature was varied from 350°C to 500°C with an increment of 50°C, and the characteristics of Ga<sub>2</sub>O<sub>3</sub> Schottky barrier diodes (SBD) depending on the growth temperatures were evaluated. Structural and electrical properties of the thin films were evaluated using I-V measurement and field emission-scanning electron microscope(FE-SEM). As a Schottky electrode, Ni/Au was deposited on the Ga<sub>2</sub>O<sub>3</sub> thin films, and electrical characteristics of the vertical Schottky diode of Ga<sub>2</sub>O<sub>3</sub>/Ti structures were evaluated. The surface morphology strongly depends on the growth temperature. The flatness of the thin films improved when the growth temperature was higher than 450°C. After heat treatment, the I-V measurement result showed that decreased forward biased current and increased leakage current might be due to the change of crystal phase, grain boundary and density of oxygen vacancy.

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### Keywords:

Ga<sub>2</sub>O<sub>3</sub>, MOCVD, Thin film, Power semiconductor

## Growth of Ga<sub>2</sub>O<sub>3</sub> thin films on Si substrates and transformation of crystal phase by thermal treatment

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### Abstract:

본 연구에서는 다양한 형태의 고기능의 소자를 제작하기 위해서는 homo-epitaxy 이외에도 hetero-epitaxy 성장이 매우 유용한 기술이 될 수 있으므로 Si 반도체의 높은 기술의 완성도와 Ga<sub>2</sub>O<sub>3</sub> 박막의 우수한 물질적 특성을 활용할 수 있는 hetero-epitaxy 성장을 시도하였다. 유기 금속 화학 증착법(metal organic chemical vapor deposition, MOCVD) 방법을 이용해 온도에 따라 어떤 특성들을 가지는지 확인하기 위해서 Si 기판 위에 undoped Ga<sub>2</sub>O<sub>3</sub> 박막을 각각 500 °C, 550 °C, 600 °C, 650 °C, 700 °C의 성장온도에서 30분간 성장하여 900 °C의 온도에서 10분간 열처리하였다. X-선 회절 분석(X-ray diffraction, XRD) 결과로 500 °C, 550 °C에서 성장한 경우에는 비정질(amorphous)특성을 보였으며 900 °C 열처리한 후에는 다결정(polycrystal)로 성질이 변화하는 것을 확인하였다, 표면 형상 분석 결과 500 °C, 550 °C에서 성장하여 900 °C 열처리하였을 경우 매끈하고 평탄한 박막이 관찰되며 600 °C 이상에서 성장한 박막의 표면이 500 °C, 550 °C의 비교적 저온에서 성장한 박막의 표면보다 큰 거칠기를 가지고 다결정화(polycrystal) 되는 것을 확인하였다. 따라서 vertical SBD(Schottky barrier diode)를 제작하기 위해서는 매끈하고 평평한 박막이 필수적이므로 550 °C에서 성장한 박막을 이용해 device를 제작하였다. I-V 측정 결과 900 °C 열처리 전 후 표면산화, 결정상의 변화의 원인으로 전기전도도의 차이를 확인하였다. 또한 vertical SBD(Schottky barrier diode)으로 제작된 photodetector의 활용가능성을 확인하기 위해 I-V curve를 통해 암/광전류 측정한 결과 암전류보다 266nm UV 파장 영역에서 훨씬 뛰어난 광전류 특성을 보이는 것을 확인하였다.

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### Keywords:

MOCVD, Ga<sub>2</sub>O<sub>3</sub>, Schottky barrier diode, photodetector, hetero-epitaxy

# Implementation of Capacitor-less Integrate-and-Fire Neuron with Oxygenated Amorphous Carbon based Memristor

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## Abstract:

4차 산업혁명과 더불어 인공지능 기술의 필요성이 대두되면서 막대한 양의 정보 저장 및 처리를 위한 컴퓨팅 기술의 출현이 요구되고 있다. 하지만 현재의 컴퓨팅 구조인 폰 노이만(von-Neumann) 구조에서 인공지능의 학습 및 추론을 구현하면 데이터 병목 현상(von-Neumann bottleneck)으로 인해 시스템 전체 성능이 감소하고 높은 전력 소모를 발생시키기 때문에 인간의 뇌 구조를 모방한 Spiking-Neural-Network(SNN) 연구가 전 세계적으로 활발히 진행되고 있다. SNN의 신호 생성 및 정보 처리를 위해서는 대규모 인공 뉴런들이 요구되는데, integrate 기능을 모방하기 위해 Capacitor가 주로 사용된다. 하지만 Capacitor는 면적이 최소  $100 \mu\text{m}^2$  이상을 차지하기 때문에 high neuronal density를 달성할 수 없다. 따라서 인공 뉴런의 높은 밀도를 달성하기 위해 Capacitor가 없는 인공 뉴런 구현이 필수적인데, 본 연구에서는 인공 뉴런의 integrate 기능을 oxygenated amorphous carbon 소자를 이용하여 모방하였으며, sense amplifier 및 SR-latch 회로를 이용해 인공 뉴런의 fire 기능 및 reset 기능을 구현하였다. Integrate 기능을 모방한 인공 뉴런 소자의 resistive switching layer는 25 nm 두께의  $\alpha\text{-CO}_x$  을 DC magnetron sputtering system을 이용하여 증착 하였으며, 하부 전극인 20 nm 두께의 Al 및 상부 전극인 20nm 두께의 Pt 역시 DC magnetron sputtering system을 통해 증착 하였다. 제작된 oxygenated amorphous carbon 기반 인공 뉴런 소자는 가해지는 전압의 크기에 따라 integrate 변화량이 증가하는 것을 확인하였으며, 주변회로(Current-mirror-type sense amplifier 및 SR-latch)를 discrete C-MOSFETs으로 설계하고 하드웨어적으로 연결하여 생물학적 뉴런의 integrate-and-fire 기능을 성공적으로 모방하였다. 또한, 설계된 oxygenated amorphous carbon 기반 인공 뉴런의 Spiking Deep Neural Networks(SDNN) 적용을 테스트 하기 위해 특성을 추출하여 SDNN 시뮬레이션을 진행한 결과, 손 글씨 이미지 데이터셋(MNIST)에 대한 높은 분류 정확도(~93%)를 달성하였다.

## Keywords:

ReRAM, Neuron, Memristor, capacitor-less

# Triboelectrification in ferromagnetic NiO-Ni-MgO nanocomposite: Synthesis, device fabrication, and energy harvesting performance

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## Abstract:

Triboelectric nanogenerator (TENG) has recently received wide attention for abundant mechanical energy harvesting due to low-cost, high-energy conversion efficiency, and vast structural diversities [1,2]. Typically, the research area on TENGs, dominated by metals and polymers, often requires obscured synthesis routes. Hence, the alternative method of using the composites directly, as a triboelectric layer synthesized via a cost-effective fabrication route, can essentially extend the application [3]. Therefore, we present a systematic investigation on synthesizing a ferromagnetic NiO-Ni-MgO nanocomposite via a cost-effective mechanochemical synthesis process and its utilization as a positive triboelectric layer in the fabricated TENG device to harvest biomechanical energy in real-life applications. The structural and microstructural analyzes reveal the formation of a three-phase face-centered-cubic structured composites. The magnetic study exhibits a robust ferromagnetic behavior. The coexisting ferromagnetic Ni and antiferromagnetic NiO phases determine the overall properties. The nanocomposite, acting as a positive triboelectric layer, helps convert the accessible waste mechanical energy into suitable electrical energy. The TENG device with an area of 2cm<sup>2</sup> delivers the voltage of 35 V, current of 130 nA, and power density of 0.72  $\mu\text{W}/\text{cm}^2$  at  $10^8 \Omega$  load resistance. Further, the TENG device was employed to harvest the biomechanical energy during palm pressing (output voltage:15 V, current: 88 nA) and foot pressing (output voltage: 21 V, current: 109 nA). These results elucidate the promising utilization of the nanocomposite as a positive triboelectric layer, suitable for several energy harvesting device applications.

**References:** [1] S. Li et al., *Energy & Environmental Science* 13 (2020) 896-907; [2] S. Yong et al., *Advanced Energy Materials* 11 (2021) 2101194; [3] M. Sahu et al., *Mater. Lett.* 301 (2021) 130290.

## Keywords:

Nanocomposite, Ferromagnetism, Exchange bias, Triboelectric

## Study on the Array of the Transparent Photodetectors

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### Abstract:

본 연구는 3차원 이미지 획득을 위한 그래핀 기반의 투명 센서 연구로, 평면 기판과 곡면 기판 특성을 분석하였다. 본 발표는 이 중 센서 특성에 초점을 맞춰 소자를 제작 및 분석하였다. 사용된 구조는 ITO-Si-ITO, ITO-Si-Graphene 투명 센서로, 2x2, 5x5로 구성 되었으며 약 75퍼센트의 투과도를 보이며, 다양한 광량의 불연속적 R, G, B 광원과 I-V 측정을 통하여 광응답특성과 양자효율 특성을 분석하였다.

현재 제작된 센서는 낮은 투명도와 양자효율을 보이지만, 본 연구실의 다수인자 광 측정 구조를 사용하여 개선할 예정이며, 곡면 기판이 아닌 유연 기판을 사용한 소자의 안정성 등을 측정할 예정이다.

이외의 본 연구의 투명 특성과 유연한 특성을 이용하면 거울이나 유리등에도 이용이 가능하고 곡면인 피부와 같이 다양한 형태로 이용할 수 있기 때문에 실생활에 밀접하게 사용될 수 있을 것으로 보인다.

### Keywords:

Graphene, 3D Sensor, Transparent Sensor, Curved Sensor

## Observation of Biexcitons in Perovskite Single Crystals with High Photoluminescence Quantum Yield

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### Abstract:

Halide perovskites (HP's) have emerged as novel materials for light-emitting applications owing to superior optical properties and cost-effective solution-based preparation methods. Nevertheless, their optical properties and fundamental exciton physics are quite elusive. It is believed that biexcitons created from combining two excitons are stable only in low-dimensional environment where exciton-exciton binding is strongly enhanced by quantum and dielectric confinements. In this presentation, comparing the photoluminescence (PL) spectra between cleaved internal pristine surface and ordinary external surface for  $\text{CH}_3\text{NH}_3\text{PbBr}_3$ , we demonstrated that they indeed do exist in pristine quality of three-dimensional (3D) HP single crystals for the first time. The existence of biexcitons is clearly evidenced at low temperature with a binding energy of  $\sim 3.9 \pm 0.3$  meV according to i) exciton-biexciton population dynamics, ii) biexcitonic spectral feature of inverted Boltzmann shape, iii) resonant two-photon excitation of biexciton, iv) optical selection rule under resonant circularly polarized two-photon excitation. By using fine scale of PL excitation spectroscopy, we identified polariton effect and unique exciton fine structures: longitudinal (L) and transverse (T) excitons that energy splitting is obtained 3.7 meV. In contrast, the PL spectrum for ordinary external surface dominates P-band emission arising from inelastic exciton-exciton scattering and biexciton peak is entirely vanished. This implies that defects play an important role in many-body exciton-exciton interactions. Finally, we claimed the PL efficiency of the biexcitons in 3D HP single crystals is higher than that of the biexcitons in low-dimensional HP because the biexciton Auger process in 3D single crystals is quite negligible. The discovery of the high-efficient 3D biexcitons improved fundamental understanding of their exciton and biexciton physics, and light-emitting applications.

### Keywords:

Perovskite single crystals, Biexciton, Exciton fine structure, Resonant two-photon excitation, Exciton physics

## Improvement of SnO<sub>2</sub> electron transport layer prepared using calcium chloride additive for perovskite solar cells application

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### Abstract:

Perovskite solar cells (PSCs) have recently proven rapid power conversion efficiency of more than 25%. A SnO<sub>2</sub> thin film as an electron transport layer (ETL) has similar physical properties to TiO<sub>2</sub>, but charge extraction is more efficient for perovskite, so many studies have been conducted recently. In addition, the SnO<sub>2</sub> ETL is prepared using a simple and efficient methods to obtain high-performance PSC. Here, we have investigated the electron transport properties of SnO<sub>2</sub> thin film with different amount of calcium chloride additive for improvement of perovskite solar cells. As a result, calcium chloride-added SnO<sub>2</sub> thin film can significantly improve the performance of the device compared to pure tin oxide. When using 1.5 mg/ml calcium chloride-added SnO<sub>2</sub>, the power conversion efficiency of PSCs improved significantly from 18.8% to 19.5% on average and from 19.1% to 20.6% on champion devices.

### Keywords:

perovskite

## 준직접 에너지밴드갭 Si의 광특성

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### Abstract:

육각 형태의 Si 결정의 광특성을 조사하였다. 실리콘(Si)은 현재 주요 산업 분야에서 매우 중요한 재료로 사용되고 있다. Si은 외부 조건인 압력과 온도에 의해 다양한 상(phase) 구조를 갖는 동소체(allotrope)이다. 동소체는 같은 종류의 원소이지만 원자수가 다르거나 원자의 배열 상태, 원자간 결합 구조가 달라 특성이 달라지는 물질을 말한다. 예를 들면, 산소(O<sub>2</sub>)와 오존(O<sub>3</sub>)는 산소 원소의 동소체이고, 다이아몬드와 흑연은 탄소 원소의 동소체이다. Si의 동소체 중 육각 형태의(hexagonal) Si은 간접 천이의 정육면체(cubic) Si과 비교하여 0.6 eV에서 1.69 eV의 준직접 밴드갭을 가지고 있어 미래의 다양한 분야에서의 응용이 기대되는 재료이다. 본 연구에서 육각 형태의 Si 결정 발광소자의 제작방법은 열방출되는 Al heat sink를 이용하여 Al 기반의 PCB 기판 위에 Si 결정을 실버 페이스트로 전극을 형성하여 I-V와 광특성을 측정하였다. 발광특성은 740 nm의 주 피크가 측정되었으며, I-V 특성에서 소자의 저항은 1 Ω<sup>Ω</sup>, 턴온 전압은 8 V로 측정되었다. 일정한 턴온 전압을 가지며 발광하는 형태의 금속 반도체 소자로 판단된다. 그 결과 1.66 eV - 1.75 eV의 주 피크가 관측되었으며 이는 육각형 Si (2H) 구조의 준직접 밴드갭에서 비롯된 것으로 판단된다. 이 결과로부터 준직접 밴드갭을 가지는 Si 결정의 광학적 특성은 새로운 Si 관련 광전자 소자의 적용에 기여할 것으로 기대된다.

### Keywords:

준직접에너지밴드갭 Si, 육각형태 Si, Si 동소체, 광특성, Si 발광소자

## 슈퍼커패시터 응용을 위한 코발트 인화물의 합성 및 특성

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### Abstract:

재생 불가능한 에너지 자원의 급속한 고갈과 점차적으로 감소하는 화석 연료로 인해 연구자들은 효과적인 에너지 저장 목적을 위해 재생 가능하고 자연 친화적인 대안을 찾고 있다. 여러 에너지 저장소자 중 슈퍼커패시터는 비용 효율성, 급속 충전 능력, 긴 사이클 수명 등의 많은 장점으로 주목받고 있다. 수십 년 동안 슈퍼커패시터는 기존 커패시터와 이차전지사이의 격차를 해소하면서 개발 중이다. 탄소기반 재료, 전이금속 산화물/수산화물, 전이금속 칼코게나이드, 전도성 고분자 및 전이금속 인화물/인산염으로 구성된 여러 전극 재료가 지난 몇 년 동안 개발되고 있다. 특히, 황화물/셀레늄화물과 같은 전이금속 칼코게나이드는 높은 산화환원 활성 부위, 높은 이론 용량 및 성능 향상으로 인해 많은 관심을 받고 있다. 본 발표에서는 2단계 방법으로 코발트 셀레네이트-코발트 인화물 복합물질의 합성을 나타낸다. 초기에 코발트 셀레네이트는 손쉬운 단일 단계 수열합성법을 통해 빠르게 합성되었다. 풍부한 산화환원 활성과 형태학적 이점을 통해 더 높은 면적 용량을 나타냈다. 그리고 다음 단계에서 인산화 공정을 수행하여 코발트 셀레네이트-코발트 인화물을 형성했다. 생성된 전극물질은 개선된 areal capacity를 제공했다. 또한, 코발트 셀레네이트-코발트 인화물과 활성탄 전극을 사용하여 하이브리드 슈퍼커패시터 셀을 제작해 특성을 평가하였다.

### Keywords:

슈퍼커패시터, 코발트 인화물, 전기화학특성

## Study of ultrafast amorphization and re-crystallization on phase-change materials

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### Abstract:

Phase-change memory utilizing sufficient phase-change speed between amorphous and crystal phase-change materials (PCMs) in sub-nanosecond time scale<sup>1–4</sup> is becoming universal electronic memory<sup>5,6</sup>. For faster processing memory module in computers, development of new PCMs whose phase-change speed is more rapid than conventional PCMs are in demand.<sup>7–9</sup> There have been reported<sup>2,4,10</sup> that the high-speed switching can be achieved by the phase transition from the transient non-thermal state to amorphous state, where the transient non-thermal state is generated by femtosecond optical excitation. The previous studies provide overall information related to the time range, however, a crucial information on amorphization process is not yet available.

Here, we report ultrafast reversible atomic re-arrangement on phase-change (amorphization and recrystallization) in Ag, In, Sb, Te based phase-change materials by employing time-resolved X-ray diffraction (trXRD) in a wide range of reciprocal space. Laser triggered picosecond to sub-nanosecond scale amorphization and re-crystallization of phase-change materials are traced by powder diffraction. This study will shed light on devising the materials for next-generation memory, such as phase-change random access memory (PRAM).

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### Keywords:

Phase change materials

## Temperature-dependent photoluminescence in Green InGaN/GaN light-emitting diodes with the Si-doped graded short-period superlattice (GSL).

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### Abstract:

Temperature-dependent photoluminescence is used to investigate the carrier transport and localized states of the Green InGaN/GaN light-emitting Diode (LEDs) with regarded silicon doping short-period InGaN/GaN GSL superlattice. Selecting the PL spectra taken over the temperature range 25-300K and fixed power ( $P=700\mu\text{W}$ ). The emission mechanism is generally because of the spatial indium fluctuation leading to indium-rich regions acting like the quantum dots. The emission from the InGaN region due to the exciton-localized at potential minima is called the excitation localization effect. The QW emission peak shows the well-known S-shaped (decrease-increase-decrease) temperature dependence. The potential fluctuations in the energy band structure are known as the band tail states. These states would capture the excitons and carriers and make the localized carrier and bound excitons. Due to the confinement of the electrons and holes at the same site, the potential fluctuations provide the efficient luminescence centers strongly. The strong value of the localization means the tail's deeper extension into the forbidden band and the strong luminance are generated. The linewidth variation as a function of the temperature represents a W-shaped (decrease-increase-decrease-slowly increase-increase). Because of large potential fluctuation and deeper tails in the high In component structures (green LED), the excitons can capture easier by the defect states. The donor-bound excitons are the dominant emission source at low temperatures, and free exciton will be improved in the emission mechanism. The knee point in the integrated PL intensity curve under light irradiation was observed. When the excitation energy is higher than the barrier bandgap, both the barrier and the well are excited. This anomalous phenomenon can be interpreted because of the carrier transport along with the quantum barrier and carrier transport between different localized states. The observed anomalous optical phenomenon is related to the carrier transport behavior known as carrier mobility.

### Keywords:

InGaN/GaN MQW, photoluminescence, Green InGaN/GaN light-emitting diodes, localization effect

## Investigating of InAs/GaSb single quantum well band structure using eight-band k.p model discretized with finite difference method

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### Abstract:

Theoretically, we investigated the first transition energies of unstrained InAs/GaSb single quantum wells (SQW) for different well widths based on band structure simulation. In this work, Kane's 8-band k.p model, which includes Luttinger parameters, is used to calculate the energy levels, while all second-order terms correspond to the contributions to remote bands. We have used MATLAB software to code the finite difference approximation method (FDM) to solve the k.p Hamiltonian. The discretization procedure is based on the backwards-forward difference form of the FDM. It is assumed that the structure has grown in the direction [001]. The discretizing of the differential equations leads to the reduction to the eigenvalue problem to be solved for discretized transition energies and envelope functions. So, we obtained the band structure of InAs/GaSb for well widths of 1nm and barrier width of 8nm which all energy levels can be achieved simultaneously with this method. Then, based on the different thickness of the well (InAs) from 1 to 4 nm and fixed width of the barrier (GaSb) 8 nm, the energy of the first electron level (e1) and first heavy hole level (hh1) was calculated. Finally, the transition energies of this SQW for  $k_z=0$  were calculated and their variation for different well widths demonstrated.

### Keywords:

8-band k.p theory, Finite difference method, Band structure, Transition energy, Quantum well

## 열처리 온도가 digital alloy InGaAlAs multi quantum well의 광학적 특성에 미치는 영향

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### Abstract:

본 연구에서는 (InGaAs)<sub>0.4</sub>(InAlAs)<sub>0.6</sub> barrier 층과 (InGaAs)<sub>0.8</sub>(InAlAs)<sub>0.2</sub> quantum well 층을 디지털 합금(digital alloy: DA)방식으로 다중 양자우물 (multi-quantum well: MQW)구조를 형성한 샘플을 각각 700°C, 750°C, 800°C 그리고 850°C에서 열처리를 한 총 4가지 시료들을 photoluminescence (PL) 과 Photoreflectance (PR) 분광법을 통하여 열처리 온도가 MQW구조에 미치는 영향을 알아보았다. 저온에서 PL 실험 결과 700°C, 750°C, 800°C 시료에서 0.99 eV에서 MQW PL transition energy를 확인하였으며, 1.39 eV에서 InP 기판 신호가 관측이 되었다. 850°C 시료의 경우 MQW transition energy가 다른 시료들에 비해 0.03 eV 적색편이가 일어난 0.96 eV에서 관측이 되었으며, 1.39 eV InP 기판 신호가 관측되었다. 850°C 시료가 다른 시료들에 비해 MQW신호와 InP 기판 신호가 적색편이하는 경향을 보이고 있는데, 이는 열처리 온도에 의해 InAlAs 클래딩 층과 InP 기판 사이 계면에서 intermixing이 일어났으며 Ga증발이 일어나 Al 함량이 증가했기 때문이다. 또한, MQW의 PL신호가 열처리 온도가 증가함에 따라 반칙폭 (full width at half maximum: FWHM)이 증가하는데 열처리 온도가 증가함에 따라 MQW의 interdiffusion으로 인하여 균일도가 낮아졌기 때문이다. Interdiffusion과 intermixing에 대해 자세히 알아보기 위해 PR분광법을 진행하였다. PR 신호에서 PL신호에서 관측하지 못하였던 1.26 eV 부근에서 (InGaAs)<sub>0.4</sub>(InAlAs)<sub>0.6</sub> barrier 층 신호와 1.57 eV에서 InAlAs 클래딩 층의 신호를 관측하였다. 850°C 시료의 경우 barrier층의 신호가 다른 시료에 비해 0.2 eV 낮은 1.24 eV부근에서 관측이 되었으며, 1.51 eV에서 클래딩 층의 신호가 관측이 되었다. 앞에서 언급하였듯이 열처리 온도가 올라감에 따라 각 층의 계면에서 interdiffusion과 intermixing으로 인한 결과이다.

### Keywords:

photoluminescence, photoreflectance

# Phase Transitions and Critical Phenomena of the Square-Lattice Ising Model with a Ratio of 2:1 between the Nearest-Neighbor and the Next Nearest-Neighbor Interactions

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## Abstract:

The square-lattice Ising model with a ratio of 2:1 between the nearest-neighbor interaction and the next nearest-neighbor interaction interactions is exactly unsolvable. The exact integer values for the density of states of the square-lattice Ising model with a ratio 2:1 between the nearest-neighbor interaction and the next nearest-neighbor interaction was obtained on  $L \times 2L$  square lattices with free boundary conditions in the  $L$ -direction and periodic boundary conditions in the  $2L$ -direction up to  $L=12$ . The phase transitions and critical phenomena of the square-lattice Ising model with a ratio of 2:1 between the nearest-neighbor interaction and the next nearest-neighbor interaction interactions are investigated, based on its exact density of states.

## Keywords:

Phase Transitions and Critical Phenomena

## Direct measurement of correlation length for absorbing phase transitions

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### Abstract:

We introduce a quantity  $K(L,t)$  to measure the spatial correlation length in the one-dimensional contact process.

$K(L,t) = L\sigma^2 / \langle \rho \rangle^2$  is defined as a function of time, where  $L$ ,  $\rho$ ,  $\sigma^2$ , and  $\langle \rho \rangle$  are the system size, the particle density, the variance of  $\rho$ , and the ensemble average, respectively.

At the critical point,  $K(t)$  follows a power law of  $K(t) \sim t^{1/z}$  with  $z=1.5821(16)$ .

We estimate the correlation length exponent  $\nu_{\perp} = 1.1014(33)$  using the relation  $K_{\text{stat}}(p) \sim (p_c - p)^{-\nu_{\perp}}$  in the subcritical regime, where  $K_{\text{stat}}$  is the stationary value of  $K$ .

$K(t)$  is proportional to the correlation length therefore we could obtain the information of the correlation length directly using  $K(t)$ .

### Keywords:

Correlation length, Dynamic exponent, absorbing phase transition

## Functional connectivity and network analysis in a mouse model of mild traumatic brain injury

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### Abstract:

Mild traumatic brain injury (mTBI) is one of the most frequent neurological disorders. The criteria for characterizing temporary dysfunction of the brain are based on cognitive or neurological symptoms without a full understanding of the neuropathological basis for the outlook behaviors. From the neuropathological perspective of mTBI, most neuroimaging studies have focused on structural or functional differences in motor-related cortical regions but did not compare topological network properties between the post-concussion days. We investigated temporal changes of functional connectivity and evaluated network properties of functional networks in the brainstem. We found that functional connectivity and global and local network properties are decreased at post-concussion day 7 but normalized at post-concussion day 14. We also found that the local efficiency and clustering coefficient of the brainstem network were highly correlated with the anxiety-like behaviors at post-concussion days 7 and 14. The current study suggests that functional connectivity in the mouse brainstem may provide important recovery signs following mTBI.

### Keywords:

Mild traumatic brain injury, fMRI, Functional connectivity

## Numerical Analysis of Diffusive Epidemic Process

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### Abstract:

The Gillespie algorithm is the exact stochastic simulation method replicating continuous-time processes. Applying discrete-time approaches to continuous-time processes for the large values of the reaction rate affects the epidemics threshold leading to different results with the Gillespie algorithm [1]. In order to discuss this discrepancy issue, we consider the diffusive epidemic process (DEP) as one of continuous-time contagion processes. The DEP model is the simplest epidemic model allowing diffusion of particles and multiple occupancies. The most recent study [2] shows that the subdiffusive propagation of infection clusters is observed with the crossover scaling, which has never been seen with other numerical approaches. We discuss the effect of discrete-time approaches on spatio-temporal patterns of epidemic spreading, not only the critical threshold but also critical exponents. Finally, our study is extended to the universality class in the presence of the directional bias of particle diffusion.

[1] Fennell, P. G., Melnik, S., & Gleeson, J. P. (2016). Limitations of discrete-time approaches to continuous-time contagion dynamics. *Physical Review E*, *94*(5), 052125.

[2] Polovnikov, B., Wilke, P., & Frey, E. (2022). Subdiffusive Activity Spreading in the Diffusive Epidemic Process. *Physical Review Letters*, *128*(7), 078302.

### Keywords:

Gillespie Algorithm, Diffusive Epidemic Process, Continuous-Time Process, Spatio-Temporal Pattern, Crossover Scaling

## Activeness hinders accurate estimation of the extent of anomalous diffusion via thermodynamic uncertainty relation

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### Abstract:

Thermodynamic uncertainty relation (TUR) is a tradeoff inequality between dissipation and thermal fluctuation. Recently, TUR was successfully applied to bound the extent of anomalous diffusion, i.e., the timescale beyond which a system loses its anomalous kinetics. The crucial factor for the accurate estimation of the bound is tightness of the inequality. Here we investigate whether the extent of anomalous diffusion is tightly bound by TUR when the active noise or self-propelled particles are present in a dynamic system. For this purpose, we examine the Rouse and worm-like chains crosslinked with a self-propelled particle under a constant force and derive TUR for these active systems. We find that stronger activeness leads to lower TUR bound but larger diffusivity. This suggests that the activeness gives rise to a loose bound, thus, hinders the accurate estimation of the extent of anomalous diffusion.

### Keywords:

Thermodynamic uncertainty relation, active noise, anomalous diffusion, Rouse model, worm-like chain

## Excess defect kinetics in the two-dimensional ferromagnetic Ising model under slow cooling: Effects of nonlinear cooling protocols

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### Abstract:

We present an extensive simulation study that extends our recent work [Phys. Rev. E 99, 022113 (2019)] on the two-dimensional kinetic Ising model under a slow linear cooling. This study aims to systematically investigate how non-linearity of temperature cooling affects the non-equilibrium kinetics of excess defect generation and associated phase ordering. New interesting kinetic features are observed due to the nonlinear manner of coolings, and are found to be strongly constrained by the Kibble-Zurek mechanism. We find that via the Kibble-Zurek mechanism, one can engineer the nonequilibrium critical dynamics of the spin configurations in the two-dimensional Ising model such that a prescribed value of the critical dynamic exponent can be obtained by tuning the nonlinearity of slow cooling.

### Keywords:

Kibble-Zurek Mechanism, Ising model, Non-equilibrium system, Cooling system

## Excess defect kinetics in the two-dimensional ferromagnetic Ising model under Periodic Temperature

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### Abstract:

이전 연구인 비선형 온도 냉각 프로토콜이 도입된 2D-spin flip Ising model [Poster P1-st.006] 에서 확장하여, 온도 프로토콜이 냉각과 가열을 반복하는, 주기적인 온도 프로토콜을 도입하여, 잉여 흠 밀도 Excess defect density (EDD) 동역학을 살펴보았다. EDD dynamic scaling도 실시해보았다. 2차원 Ising model을 포함하여, 2차 상전이에서 온도 프로토콜에 의한 동역학은 Kibble-Zurek mechanism과 매우 강하게 연관되어있다. KZM 관점에서 EDD 동역학 해석을 하였으며, 이러한 주기적인 프로토콜에서는 비평형 정상 상태 NESS가 나타나며, 이 시스템에서의 NESS 특징을 살펴보았다.

### Keywords:

Non-equilibrium systems, Kibble-Zurek Mechanism, Ising model, Periodic Quench

## Nonequilibrium kinetics of excess defect generation and dynamic scaling in the Kawasaki Ising spin chain under slow cooling

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### Abstract:

We investigate the relaxation dynamics of a one-dimensional Kawasaki Ising chain via Monte Carlo simulations, when the system is cooled slowly from infinite temperature to zero temperature with different cooling protocols. The main quantity of interest is the excess defect density that represents the total defect density minus the equilibrium defect density at varying temperatures. We find that, for the classes of cooling protocols, the time dependence of the excess defect density for various cooling speed shows a dynamic scaling behavior that largely encompasses the Kibble-Zurek mechanism. Additionally, we confirmed the freezing effect of the defect density near zero temperature in one-dimensional conserved Ising model, and compared the conserved system with the nonconserved system of the previous paper [ 1 ]. We also checked that the Kibble-Zurek prediction emerges at zero temperature in the conserved system, and confirmed asymptotic behavior of excess defect density dynamic scaling.

### Keywords:

Kibble-Zurek mechanism, Kawasaki Dynamics, Kawasaki Ising model, Slow quench, Kibble-Zurek

## Revealing role of Korean Physics Society with keyword co-occurrence network

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### Abstract:

Science and society inevitably interact with each other and evolve together. Studying the trend of science is necessary not only for recognizing influential and rising topics for the next move but also for establishing better policies for the efficient distribution of the funds. Although several studies try to capture the trend of science leveraging scientific documents such as paper or patents, the sheer scope of the studies has been limited in the academic world, neglecting the interaction with society. Here we try to understand the trend of science along with society using a public magazine named "Physics and High Technology," published by the Korean Physics Society (KPS). We build the keyword co-occurrence for each time period and apply community detection to capture the keyword structure and track the structure's evolution. In the network, a research-related cluster is consistently dominant over time, and sub-clusters of the research-related cluster diverge to various fields of physics, suggesting specialization of the physics discipline. Also, we found that education and policy clusters appear consistently, revealing the KPS's contribution to science and society. Furthermore, we apply the PageRank algorithm for selected keywords ('semiconductor', 'woman', 'evading'...) to investigate the temporal change of the importance of keywords in the network. For example, the importance of the keyword 'woman' increases as time goes by, indicating that academia also pays attention to gender issues reflecting the social movement in recent years. Our bibliographical analysis of the public magazine can reveal diverse aspects of academia accompanying society.

### Keywords:

Keyword co-occurrence network, PageRank, Korean Physics Society, Physics and High Technology

## Demand prediction of public bicycle system through graph neural network

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### Abstract:

세계적으로 공공자전거의 사용이 늘어나고 있다. 하지만 자전거의 수요와 공급이 맞지 않아 이용자들의 불편함이 발생한다. 서울시 공공자전거도 수요와 공급의 불균형 문제를 가지고 있다. 이를 해소하기 위해 트럭으로 자전거 재배치를 하지만 인력과 비용이 발생한다. 이와 같은 문제들은 수요를 예측함으로써 해결할 수 있다. 본 연구는 어텐션 방법을 기반으로 하는 Graph Neural Network(GNN)를 활용하여 서울시 공공자전거 수요를 예측한다. 공공자전거의 수요는 주말 여부, 강우 여부에 따라서도 달라진다. 우리는 수요에 대한 정보뿐만 아니라 강수량과 주말에 대한 정보도 반영하여 더 높은 정확도로 예측을 한다. 정확도가 더 높아지는 것을 통해 외부 정보가 모델이 예측하는 데 있어 도움을 주는 것을 알 수 있다. 공공자전거 수요 예측 연구는 수요와 공급의 불균형 문제를 해결하는 것뿐만 아니라 노드의 정보가 시간에 따라 변화하는 것을 예측하는데 활용이 가능함으로써 여러 분야에 도움이 된다.

### Keywords:

Deep learning, Graph Neural Network, Traffic

## Roughening transition of information landscape on social networks

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### Abstract:

Halvorsen et al. [Phys Rev. E 103, 022303(2021)] 에서 제안된 정보 전달에 의한 influencer들의 경쟁 모형을 이용하여 정보 가치 landscape의 동역학적 특성에 대해 연구하였다. Linear dimension이  $L$ 인 구조가 고정된 정보교환네트워크를 가지는 influencer경쟁 모형에서 각 노드가 가지는 정보의 가치를 표면 성장 모형에서의 표면 높이  $\{h_i\}$ 로 mapping하면  $\{h_i\}$ 의 요동을  $W(L, t) = \langle (h - \bar{h}(t))^2 \rangle^{1/2}$  와 같이 나타낼 수 있다. 여기에서  $\bar{h}(t)$ 는 시간  $t$ 에서의 평균 높이를 나타낸다. 구조가 고정된 정보 교환 네트워크가 1차원 격자인 경우  $W(L, t)$ 는 항상  $W(L, t) = L^\alpha f(t/L^2)$ 의 축척 거동을 보임을 발견하였다. 반면, 정보 교환 네트워크가 2차원이 되는 경우 influencer의 정보 생산 확률과 follower의 정보 생산 확률에 따라  $\{h_i\}$ 의 landscape가 평평한 상에서 거친 상으로의 상전이가 일어나는 것을 발견하였다.

### Keywords:

Complex networks, Interface roughening

# Non-Gaussian to Gaussian crossover and ergodicity recovery of the random walk in spatially correlated annealed diffusivity fields

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## Abstract:

Fickian and Gaussian diffusion is a prototype of the diffusion dynamics driven by thermal fluctuation of the environment. In the past decade, however, the thermal dynamics of the particles in soft matter and biological systems have been spotlighted for their Fickian yet non-Gaussian diffusion. This new class of diffusion, the so-called Fickian yet non-Gaussian diffusion, features the linear growth of the mean squared displacement (MSD) and the non-Gaussian probability density function of displacements. The previous studies on the Fickian yet non-Gaussian diffusion focused on the short-time and the long-time limit of the system. Yet, the crossover timescale from the non-Gaussian to Gaussian distribution has not been studied. Furthermore, the role of the relative mobility of the environment to the diffusivity of the particle on the crossover timescale is still elusive. In this work, we study the crossover timescale from non-Gaussian to Gaussian diffusion and the effect of the mobility of the environment fluctuation on it via the annealed extreme landscape model. We propose an analytical method to estimate the crossover time and confirm our theory via the simulation. We speculate that in a quenched limit of our system, the diffusion of the particle inside the system is not ergodic while the diffusion becomes ergodic for a motile environment.

## Keywords:

Random walk, Non-Gaussian diffusion, Heterogeneous diffusion, Ergodicity breaking, Fluctuating diffusivity

## Investigation of the temperature dependence of Raman spectrum of anti-ferromagnetic CrPS<sub>4</sub>

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### Abstract:

Magnetic semiconductor CrPS<sub>4</sub> was first reported in 1977 [1]. CrPS<sub>4</sub> is an Ising-type antiferromagnet with the Néel temperature of 36 K in bulk [2,3]. In this work, the temperature dependence of the Raman spectrum of exfoliated CrPS<sub>4</sub> samples was investigated by polarized Raman spectroscopy with the 514.4 nm excitation source between 3.6 K and room temperature. The peak positions and the polarization dependences of the observed Raman modes are consistent with the previous report at room temperature [4]. However, at low temperature, there are some critical changes in the Raman spectra. The polarization dependence of the mode at 308 cm<sup>-1</sup> changed in the parallel configuration, whereas, new modes appeared, and the peak position and the intensity of some modes changed dramatically near the Néel temperature.

### References

- [1] R. Diehl *et al.*, Acta Crystallogr. Sect. B Struct. Crystallogr. Cryst. Chem. **33**, 1399 (1977).
- [2] A. Louisy *et al.*, Solid State Commun. **28**, 61 (1978).
- [3] H. L. Zhuang *et al.*, Phys. Rev. B **94**, 1 (2016).
- [4] S. Kim *et al.*, J. Phys. Chem. C **125**, 2691 (2021).

### Keywords:

Raman spectroscopy, CrPS<sub>4</sub>, Magnetic materials

## Magnetic ordering of NiPS<sub>3</sub> studied by Raman spectroscopy

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### Abstract:

Magnetic van der Waals materials are actively studied by researchers in various fields recently. Transition-metal thiophosphate (MPS<sub>3</sub>, M=Fe, Ni and Mn) is one of the magnetic van der Waals materials, which shows antiferromagnetic ordering in bulk below its Néel temperature [1-2]. NiPS<sub>3</sub> is an XXZ-type magnetic material showing antiferromagnetic ordering below the Néel temperature, which changes depending on the thickness of the material [2]. After the magnetic ordering of NiPS<sub>3</sub> in the 2D limit is reported, many interesting properties of 2D magnetic materials are studied. We conducted temperature-dependent polarized Raman spectroscopy of exfoliated NiPS<sub>3</sub> samples. We measured the Raman spectra of samples from 3.5K to room temperature and analyzed the changes of the peak positions and intensities of Raman modes as the temperature increases. From a bulk crystal sample, a low-frequency peak is observed at 10 cm<sup>-1</sup>, which is not due to an interlayer vibration mode. The intensity of this peak seems to correlate with the magnetic transition. The dependence of this peak as the thickness of the sample will be presented.

### References

1. J.-U. Lee *et al.*, *Nano Lett.* **16**(12) 7433 (2016).
2. K. Kim *et al.*, *Nature Comm.* **10** 345 (2019).

### Keywords:

van der Waals material, Raman spectroscopy, Magnetic van der Waals material, NiPS<sub>3</sub>

## Epitaxial ferroelectric Hf<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2</sub> thin films deposited by using pulsed laser deposition

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### Abstract:

The ferroelectric random access memory (FRAM) is a nonvolatile memory which allows a fast access time and a low power consumption. Most research activities for developing FRAM devices were focused on PbZr<sub>0.52</sub>Ti<sub>0.48</sub>O<sub>3</sub> (PZT) due to its large remnant polarization and low coercive voltage. However, scaling down of PZT thin film below 50 nm thickness led to large leakage current in a FRAM device, which is induced by low bandgap and sidewall problem. HfO<sub>2</sub>-related materials are considered to be emerging ferroelectric materials for FRAM devices due to their excellent compatibility with CMOS process. In this study, pulsed laser deposition (PLD) method is used to deposit 10-nm-thick Zr-doped HfO<sub>2</sub> (HZO) films and La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> (LSMO) bottom electrodes on the single crystalline SrTiO<sub>3</sub> (STO) substrates. The peaks from X-ray diffraction (XRD) demonstrated that the ferroelectric HZO film with orthorhombic phase is epitaxially grown on the STO substrate. The HZO thin film with very flat surface reveals large remnant polarization of up to 22 μC/cm<sup>2</sup> measured by using positive-up negative-down (PUND) pulsed method. Therefore, ferroelectric properties of HZO thin film provide an opportunity to overcome the scaling down problems in the FRAM technology.

### Keywords:

ferroelectric, thin film, PLD, epitaxial, HZO

## Effect of Hydrothermal Synthesis Conditions on The Structural and Electrical Characterization of Hydrothermally Deposited $\text{Bi}_{0.5}(\text{Na}_{1-x}\text{K}_x)_{0.5}\text{TiO}_3$ Films

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### Abstract:

The continuous environmental issue of the lead used in many ferroelectrics and piezoelectric materials has stimulated research into lead-free alternatives with comparable properties. Although, in many previous researches, the  $\text{Bi}_{0.5}(\text{Na}_{1-x}\text{K}_x)_{0.5}\text{TiO}_3$  (BNKT) among the BNT-based materials have reported the enhancing ferroelectric and piezoelectric properties in certain area called a morphotropic phase boundary (MPB) region, the information of BNKT film are still rare. Especially, the components of BNKT such as Bi, Na and K are volatile in thermal annealing process which is necessary in film fabrication process so that they can make the vacancies in materials. To manage these problems, we used the hydrothermal synthesis for fabricating a film. In this experiment, the alkalic solutions such as NaOH and KOH were used not only as mineralizer but also raw materials of Na and K to control the ratio of Na and K in BNKT. We controlled the ratio of NaOH and KOH ( $y = [\text{KOH}] / \{[\text{KOH}] + [\text{NaOH}]\}$ ,  $y = 0.75$  to  $1$ ) and synthesis time (4h to 24h). We observed that their structure by HR-XRD, XPS, FE-SEM and AFM and electrical properties by dielectric and PFM. The samples film synthesized for 4 to 24h show the BNKT (200) reflection near STO (200) peak and sharp shape of rocking curve with  $0.06^\circ$  width of BNKT film and  $0.04^\circ$  width of STO substrate at  $y = 0.75$  for 8h. The phi scan for (103) peaks of the BNKT film means in-plane orientation of the film. Also, the (103) peaks of the (001)-oriented BNKT film demonstrate 4-fold symmetry with an equal  $90^\circ$  interval as the same as that of the STO substrate which reveals epitaxial growth of the film along in-plane orientation. The calculated lattice constant  $c$  from RSM are 4.11 Å for  $y = 0.75$ . The atomic ratio by XPS shows the differences between synthesis time such as 80:20 for 8h to 25:75 for 16h. The morphology and thickness were observed by FE-SEM and AFM. Furthermore, the dielectric constant of BNKT on Nb:STO(100) is 138 at 10 kHz. In addition, we are able to observe their piezoelectric properties by PFM signal of in-plane and out-of-plane images.

### Keywords:

Hydrothermal synthesis, Ferroelectrics, Epitaxial film

## Modulation of MIT characteristics of tungsten-doped vanadium dioxide thin films via controlling composition gradation

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### Abstract:

Vanadium dioxide (VO<sub>2</sub>) is widely known for metal-insulator transition (MIT) phenomena triggered at the MIT temperature,  $T_{MIT}$ , of ~67°C. However, the  $T_{MIT}$  of VO<sub>2</sub> fairly above room temperature limits its introduction to real-world applications. Therefore, diverse physical and chemical methods to modulate  $T_{MIT}$  have been demonstrated. Above all, the cation substitution of V<sup>4+</sup> with W<sup>6+</sup> leads to efficient and stable lowering of  $T_{MIT}$ . Also, broadening the phase transition regime via the gradual doping inside VO<sub>2</sub> may lead to achieving the temperature resistance coefficients (TCRs) remarkably higher than those of conventional vanadium oxide structures. In this work, we have synthesized W-doped thin films where the W doping concentration varies monotonically in a direction perpendicular to as well as parallel to thin film surface. These two different types of compositionally graded VO<sub>2</sub> thin film structures would be of relevance to developing next-generation temperature sensors and heat detectors.

### Keywords:

vanadium dioxide (VO<sub>2</sub>), metal-insulator transition (MIT), substitutional doping, temperature resistance coefficient (TCR)

## Competing phases in epitaxial SnO<sub>2</sub> thin films deposited on sapphire(0001) substrates

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### Abstract:

Herein, the competitive crystalline phase between orthorhombic columbite (C-SnO<sub>2</sub>) and tetragonal rutile (R-SnO<sub>2</sub>) phases in SnO<sub>2</sub> thin films deposited on sapphire(0001) substrates was investigated. Off-specular X-ray diffraction analysis revealed that only the C-SnO<sub>2</sub> was formed initially; however, the growth of the R-SnO<sub>2</sub> dominated with increasing thickness. Both phases were epitaxial to the sapphire, and the directional relationship can be summarized as R[100]//C[100]//sapphire[0001] along the surface normal direction and R[010]//C[001]//sapphire[11 $\bar{2}$ 0] along the in-plane direction. In particular, a supercell structure was proposed to accommodate the lattice and symmetry mismatch between C-SnO<sub>2</sub> and *c*-plane sapphire. The electrical conductivity behavior indicated that the C-SnO<sub>2</sub> was metallic. As the film thickness increased, the optical bandgap gradually decreased from ~4.68 to ~3.56 eV owing to the increased amount of the R-SnO<sub>2</sub> in the SnO<sub>2</sub> thin films. Our results support the crossover of the dominant crystalline phase from the initial C-SnO<sub>2</sub> to the later R-SnO<sub>2</sub> during the sputter deposition of epitaxial SnO<sub>2</sub>/sapphire(0001) thin films, which significantly altered the electrical and optical properties.

### Keywords:

SnO<sub>2</sub>, orthorhombic columbite, tetragonal rutile, epitaxy, bandgap

## Effect of top electrode on ferroelectricity in hafnium-zirconium oxide thin film capacitors

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### Abstract:

Recently, HfO<sub>2</sub>-based ferroelectric materials have attracted a lot of attention due to many advantages such as high tolerance of read and write, CMOS capability, and very small critical thickness. Especially, hafnium-zirconium oxide (Hf<sub>1-x</sub>Zr<sub>x</sub>O<sub>2</sub>, HZO) is one of the extensively studied HfO<sub>2</sub>-based ferroelectric materials, since it has relatively wide dopant range ( $x = 0.3 - 0.5$ ) to exhibit ferroelectricity. RF sputtering method is a widely used deposition technique for HZO thin film capacitors due to better productivity and capability on current industrial deposition structure. However, sputtering technique has many process parameters, including RF power, argon flow rate, and operating pressure, and thus it is relatively difficult to grow high-quality HZO thin films. Also, it is well known that top electrode materials and annealing conditions strongly affect ferroelectricity of HZO thin film. In this work, we present our recent efforts to grow ferroelectric HZO thin film capacitors. We fabricated HZO thin film capacitors with varying HZO thickness, top electrode materials, and annealing temperature. We investigated the physical properties of the HZO capacitors using GI-XRD, polarization-voltage hysteresis, and so on. Especially, we discuss the effect of top electrode on ferroelectricity in HZO thin film capacitors.

### Keywords:

Ferroelectrics, Thin film, Sputtering, HZO, Top electrode

## Ferroelectric $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}$ synaptic barrister for energy-efficient convolution neural network

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### Abstract:

A convolutional neural network (CNN) is a representative deep learning network used in artificial intelligence (AI), which can learn and recognize diverse visual imagery with high accuracy and fault-tolerant. Since Y. Lecun *et al.* first proposed the CNN model in 1998 [1], it has been widely utilized in various AI applications including image learning, voice recognition, face recognition, and bio-signal analysis [2]. In this study, we designed and fabricated a ferroelectric  $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}$  (HZO) synaptic barristor and used it as a unit of the convolutional kernel for the CNN structure. The channel conductance corresponding to synaptic weight is controlled by the change of the Schottky barrier between graphene and semiconductors upon the electrostatic gating. This device is capable of several essential synaptic functions such as STP, LTP, and LTD. Furthermore, we fabricated a novel diagonal-gated crossbar array employing a ferroelectric HZO synaptic barristor and simulated the learning energy and the required number of data slidings for image recognition. Our result shows that our device system can minimize the required input data sliding and omit the pooling process in a conventional CNN structure, shortening the computation time and increasing energy efficiency.

## 고엔트로피 산화물(La-Ce-Nd-Gd-Y)에서 La<sub>2</sub>O<sub>3</sub>의 물리적 화학적 특성 분석

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### Abstract:

지금까지 재료 개발에 있어서 응용분야의 광범위한 확장을 위해 새로운 종류의 소재가 개발되어 왔다. 산화물을 이용한 소재 또한 다양한 방면으로 개발되어 왔다. 그 중 하나인 고 엔트로피 산화물은 높은 강도, 열적 안정성, 느린 확산 속도, 낮은 열전도도, 전기전도도 등의 우수한 특성을 가지고 있다. 이러한 특성 때문에, 배터리, 광전, 열전, 해양산업, 항공산업 등의 분야에서 많은 관심을 받고 있다. 본 연구에서는 화학적 공정인 졸겔 법 (Sol-gel method)을 이용하여 (La-Ce-Nd-Gd-Y)<sub>x</sub>O<sub>y</sub> 희토류 산화물을 합성하고, 1600°C에서 고온 열처리 한 후, 형성된 희토류 산화물의 특성을 비교 분석 하였다. 이렇게 합성된 (La-Ce-Nd-Gd-Y)<sub>x</sub>O<sub>y</sub> 복합체의 미세구조 및 물리적, 화학적 특성을 이해하기 위하여 XRD, XPS XAS 등을 이용하여 분석하였다.

### Keywords:

고엔트로피 산화물, La<sub>2</sub>O<sub>3</sub>, Sol-gel method, XPS분석

## Ultrathin skin-attachable $\text{TiO}_x$ synaptic array integrated with an organic photodiode for finger gesture recognition

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### Abstract:

Human gestures and motions recognition technology have attracted great attention with the growing industry of Metaverse platforms and robot technology that requires in-depth human-computer interaction. Among them, especially, finger gesture recognition has been becoming important due to its high degree of freedom for effective and direct communication between human (or disable) and computer. In this study, we designed and fabricated a stretchable and skin-attachable  $\text{TiO}_x$  synaptic array integrated with an organic photodiode (OPD) for finger gesture recognition. In this device system, the different output voltage features depending on finger motion written according to digit patterns can be generated via OPD under the green and red light. Then, these features can be directly delivered through the connection between OPD and synaptic array to reshape the intended finger motion, and the cumulative digit pattern is trained via the  $\text{TiO}_x$  synaptic array based on the backpropagation algorithm. Notably, each device component showed mechanically stable operation in the finger deformation range. For the free-standing OPD device, it showed ~80 % efficiencies of power conversion efficiency measured on a solid substrate. And, the  $\text{TiO}_x$  synaptic array fabricated on an ultrathin parylene/SU-8 based substrate showed a stable transition between long-term potentiation and long-term depression for 100 cycles even at 60 % strain. We also integrated these two device components in the low-density array form and investigated the signal transmission under the light. Based on these experimental results, we successfully modeled and calculated the recognition accuracy for the finger gesture according to the ternary digit patterns from different drawing trials.

### Keywords:

Flexible, Stretchable, Neuromorphic, Organic photodiode, Finger writing detection

## LaVO<sub>3</sub>/Si의 LaVO<sub>3</sub> 두께 변화에 따른 태양전지의 특성연구

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### Abstract:

LaVO<sub>3</sub>은 가시 광 영역에서의 높은 흡수율로 인해 태양전지 소재로 각광받고 있다. 본 연구에서는 스퍼터링 증착법으로 성장된 LaVO<sub>3</sub> 박막을 10 부터 100 nm까지 조절하여 Si 기판 위에 제작하였다. 최종적으로 LaVO<sub>3</sub>/Si 태양전지를 제작하기 위해 상/하부 전극으로는 Au/InGa 전극을 사용하였다. LaVO<sub>3</sub> 층이 존재할 경우 태양광 흡수도 증가 및 Si 표면 반사도를 감소시켜 LaVO<sub>3</sub>가 존재하지 않은 소자보다 광전변환효율을 향상시켰다. 또한, 태양전지 효율은 LaVO<sub>3</sub> 두께 변화에 크게 의존하였으며, 두께가 70 nm 일 때 5.15%로써 최대값을 보였다. 태양전지의 효율을 더 향상시키기 위해, Si 후면에 TiO<sub>x</sub> passivation 층으로 증착하여 효율을 최대 6.78%까지 더 증가시킬 수 있었다. 마지막으로, 소자의 태양광 안정성을 확인하기 위해 60°C 온도와 ~35 % 상대습도 하에 500시간동안 측정한 결과, 변환효율이 90% 이상으로 유지됨으로써 우수한 장기 안정성을 확인하였다.

### Keywords:

Oxides, passivation layer, sputtering, solar cell, photostability

## Artificial Neuron Based on Nanorod Structured Silicon Oxide Memristor for Probabilistic Inference Application

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### Abstract:

Memristor, which simply consists of a switching layer inserted between two electrodes, is one of the most strong candidates to become a device platform for imitating the principal characteristics of the biological neural network due to its nonlinear and dynamic electrical characteristics depending on the history of applied electrical programming [1-3]. In this study, we fabricated a silicon oxide ( $\text{SiO}_x$ ) nanorod memristor using E-beam evaporator with glancing angle deposition at the wafer-scale and utilized the device as an artificial neuron for probabilistic computing applications [4]. Notably, the  $\text{SiO}_x$  nanorod structure provides the random distribution of multiple nanopores all across the active area, capable of forming a multitude of Si filaments at many  $\text{SiO}_x$  nanorod edges after the electromigration process. This can facilitate probabilistic switching that can mimic integrate-and-fire signaling and the stochastic dynamics of biological neurons with a very high dynamic range ( $\sim 5.15 \times 10^{10}$ ) and low energy ( $\sim 4.06$  pJ). Different probabilistic activation (*ProbAct*) functions in a sigmoid form are implemented, showing its controllability with low variation by manufacturing and electrical programming schemes. Then, as a proof of concept, based on the suggested memristive neuron, we demonstrated the self-resting neural operation with local circuit configuration and revealed the probabilistic Bayesian inferences for genetic regulatory networks with low errors ( $< \sim 2.41 \times 10^{-2}$ ) with its robustness to the *ProbAct* variation. Taken all together, our study shows the availability of the designed  $\text{SiO}_x$  nanorod memristive neuron for probabilistic neural networks that can be efficiently used for a variety of uncertainty quantification problems.

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### Keywords:

Silicon Oxide, Memristor, Nanorod, Probabilistic computing, Artificial neuron

## 반투명 광검출기 소자를 위한 그래핀/LaVO<sub>3</sub>의 이종접합 구조의 광학적 및 전기적 특성연구

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### Abstract:

본 연구에서는 LaVO<sub>3</sub> 박막 위에 그래핀 투명 전도성 전극을 1 부터 3층까지 전사하여 그래핀/LaVO<sub>3</sub>이종 접합을 처음으로 제작하여 반투명 광검출소자를 적용하였다. 소자의 광전류 특성은 그래핀 층수 변화에 크게 의존하였다. 그래핀이 2층 일 때, 532 nm 조명 하에 0.1 AW<sup>-1</sup>의 반응도,  $7.4 \times 10^7$  cmHz<sup>1/2</sup>W<sup>-1</sup>의 검출능, 및 380 us 광반응 시간을 보였다. 더불어 가시광선 영역에서 평균 투과도가 63%로 반투명 소자임을 증명하였다. 반투명 소자의 광반응도를 향상시키기 위해, Si 반사 거울을 이용하여 투과된 빛을 소자에 재 흡수 시킴으로써 광반응도를 약 10% 향상시켰다. 상온에서 2000시간 동안 소자의 안정성을 확인한 결과 기존 광반응도의 86%를 유지할 정도로 우수한 안정성을 보였다. 본 연구에서는 실험적인 결과들을 토대로 광검출기 성능의 메커니즘을 규명하고자 한다.

### Keywords:

LaVO<sub>3</sub>, graphene, heterostructure, semitransparency, photodetector

## Optimization of the Wavelength and Intensity in Monochromatic X-ray to Minimize Radioactive Exposure

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### Abstract:

Medical diagnosis using X-ray has been the cutting edge technology. Instead of Polychromatic X-ray, Monochromatic X-ray is immune from the filters that elevates Beam Hardening Artifacts which mess the image quality. However, the question remains to choose which specific wavelength and intensity to be applied. X-ray is an Ionizing radioactive beam which can damage human body such as DNA alternating into cancer. If the wavelength is too short or of high intensity, radioactive exposure increases. On the other hand, too long or low Intensity will defect quality of image. Since there is a tradeoff, optimization shall be in progress with the cost function that can comprise quality of image; Signal to Noise Ratio(SNR), radioactive exposure calculation from Relative Biology Effect (RBE) considered doseage, etc. For a simple 2D plane of photon energy and doseage, numerical optimization was applied to search the pair.

### Keywords:

Radioactive Exposure, wavelength, intensity, Monochromatic X-ray

## 자가 배열된 AuNPs로 인한 국부형 표면 플라즈몬 향상과 LPEG 소자에서의 전기적 특성 분석

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### Abstract:

최근 화석 연료로 인한 탄소배출을 줄이기 위해 친환경 에너지 생산기술 중 하나인 energy harvesting 기술이 많은 관심을 받고 있다. Energy harvesting 기술은 버려지는 에너지를 수확하여 재활용하는 기술로 압전 (piezoelectric), 마찰 (triboelectric), 초전 (pyroelectric), 열전 (thermoelectric) 등의 다양한 방법으로 연구가 이루어지고 있지만, 본 연구에서는 전자기파의 입자성을 이용하여 복사압이 가지는 운동에너지를 전기에너지로 변환하는 소자(light pressure electric generator, LPEG)를 제작하였다. 이러한 소자는 전자기파가 존재하는 다양한 분야에 적용할 수 있는 방법이기 때문에 응용처가 무궁무진하지만 낮은 복사압의 세기를 증폭시키는 것이 중요하다.

낮은 복사압의 세기를 증폭시키는 대표적인 방법으로는 표면 플라즈몬 (surface plasmon)이 있다. 표면 플라즈몬이란 양의 유전율을 가지는 물질과 음의 유전율을 가지는 물질의 경계면에서 생성되는 전자의 집단적인 진동으로, 입사된 빛과 강하게 결합하여 국부적으로 빛이 증폭되는 표면 플라즈몬 폴라리톤을 형성한다. 표면 플라즈몬을 형성하는 다양한 방법이 존재하지만, 본 연구에서는 Au nanoparticles (AuNPs)를 자가 배열하는 방법을 선택하였다. AuNPs를 자가 배열시키기 위한 linker molecular은 APTMS를 사용하였고 incubating 시간과 AuNPs의 크기를 변화시켜가면서 최적의 플라즈몬 특성을 얻었다. 또한 제작된 소자를 one sun (1.5G) 하에서 측정하여 전기적 특성을 분석하였고 이를 Raman 분석을 통한 SERS 현상과도 비교 분석하였다.

### Keywords:

에너지 하베스팅, 표면 플라즈몬, 금 나노입자, 복사압, 압전물질

## Study of electronic structure of janus 2D metal monochalcogenides for valleytronics

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### Abstract:

Since the discovery of graphene, various two-dimensional (2D) materials have received a lot of attention from the scientific community because of their excellent atomic and electronic properties. Until now, 2D materials have shown outstanding potential for new devices based on their interesting electrical properties beyond conventional 3D materials. In recent years, many researchers have studied the valley degree of freedom in hexagonal 2D materials for valleytronics applications. In this study, we focus on two-dimensional (2D) metal monochalcogenides (MMCs) and janus 2D MMCs among hexagonal 2D materials for future valleytronic device applications using density functional theory calculations. Specifically, we investigate GaX and janus GaXY (X, Y = S, Se, Te) by considering spin-orbit coupling (SOC) effect. As a result, we identify the Rashba-type spin splitting in band structures of janus Ga<sub>2</sub>SSe and Ga<sub>2</sub>STe, while the Zeeman-type spin splittings at the K and K' valleys of GaX and janus Ga<sub>2</sub>XY show opposite spin contribution. Further, Berry curvatures of GaX and janus GaXY are calculated. Present studies would provide a deep understanding of janus 2D metal monochalcogenides for valleytronics and spintronics applications.

### Keywords:

janus, valleytronics, MMC, Berry curvature

## Neural Network Potential for Reaction in Atomic Layer Deposition Process

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### Abstract:

In recent years, the semiconductor industry is growing rapidly with the development of artificial intelligence. Atomic layer deposition (ALD) is one of the most important technologies for semiconductor processing due to its high aspect ratio. ALD process requires precursors that repeatedly react with each other for layer growth. However, the complex reaction mechanism of ALD makes it difficult to understand the exact reaction mechanism of many ALD processes.

As computing power increases, many researchers using artificial intelligence (AI) in many fields such as social science, engineering, physics, chemistry, and material science. In material science, AI techniques are used for physical property prediction, crystal structure prediction, machine learning potential and others. Machine learning potential (MLP) is one of applications that can compute as fast as classical force field with accuracy of ab initio computations. MLP can be used in many systems that are difficult to compute due to their high cost.

In our previous study, we simulated Kinetic Monte Carlo (KMC) of titanium nitride (TiN) atomic layer deposition because of its importance in semiconductor processing.  $\text{TiCl}_4$  and  $\text{NH}_3$  precursors were chosen for the simulation. Due to the complex local atomic environment, it is difficult to calculate all reactions of ALD on the table used in KMC. To overcome this problem, MLP can be used to accelerate event table creation due to its lower computational cost than ab initio computation.

In our study, we investigate reaction mechanism of TiN atomic layer deposition. Density functional theory (DFT) was used to calculate the reaction energies of probable paths for reaction in TiN ALD. Using results of DFT calculation, we trained machine learning potential with neural network model. Finally, the test set was used to verify the accuracy of neural network potential (NNP) in predicting reaction energy. These results help to create more accurate KMC simulation for ALD.

### Keywords:

Atomic Layer Deposition, Machine Learning Potential, Density Functional Theory

## Realization of High Color Rendering Index of Conventional White LED Lighting by Using Red Quantum Dot Films

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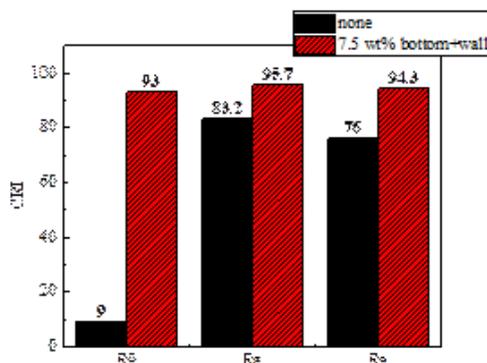
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### Abstract:

Conventional white LEDs used in the lighting market are easily fabricated by applying YAG( $Y_3Al_5O_{12}$ ) phosphors onto blue InGaN LEDs. However, in this case, the color rendering index (CRI) is relatively low due to the lack of deep-red component. One way to solve this problem is to use both green and red phosphors together, but thermal and optical trap problems due to reabsorption occur. This can be solved by applying quantum dots (QDs) in the desired wavelength region especially as a remote structure such as QD film or cap. In this study, a red QD film and a QD wall of a CdSe/ZnS core/shell structure with an emission wavelength of ~630 nm were fabricated and applied to conventional LED lighting.



[Fig.1] CRI of case of "none" and "bottom+wall" cases using the QD film and QD wall where the QD concentration is 7.5%.

We applied red QD films to a conventional 15 W white LED lighting having CRI~80 and CCT (Color Correlated Temperature) of ~5700 K. The red QD film and QD wall were synthesized by using QDs of a CdSe/ZnS core/shell structure. The QD wall was attached to a highly reflecting film. We tested six different configurations using a diffuser plate of thickness 2 mm. The "none" case is the one without any QDs; the "wall" case uses only QD wall; the "top" and the "bottom" cases denote the one where the QD film is attached on or below the diffuser plate, respectively. Especially, when comparing the top and the bottom cases, the CRI of the bottom case was higher. [Fig.1] shows that the CRI increases more substantially when QD wall is combined with the QD film. Interestingly, in the case of bottom+wall configuration, the CRI Ra increases to 95.7. In the case of bottom configuration, the light passes through the diffuser plate after red excitation via the QD film, which makes it more favorable to additionally utilize the unconverted blue light in the optical cavity. In this study, we clearly showed that the CRI can be increased by more than 90 through proper placement of the QD film in the conventional white LED lighting. Further improvement can be expected by applying the QD wall.

This research was supported by the Ministry of Trade, Industry & Energy (MOTIE), Korea Institute for Advancement of Technology (KIAT) through the program of Smart Specialized Infrastructure Construction (No. P0013743).

**Keywords:**

Quantum dots, Solid state lighting, Color Rendering Index

## 쌀겨를 이용한 바이오차의 합성과 물리화학적 특성 연구

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### Abstract:

섬유, 플라스틱, 인쇄산업 등 염색산업에서 배출되는 염색 폐수는 독성이 있고 색이 있는 고농도의 유기화합물을 함유하고 있기 때문에 환경오염에서 중요한 오염원이다. 염색폐수 처리의 여러 방법 중 활성탄을 이용한 흡착법이 가장 많이 사용되고 있지만, 활성탄의 경우 생산비용이 비싸다는 단점이 있다. 따라서 최근 이러한 단점을 보완하기 위하여 바이오차를 이용한 염료 제거에 대한 연구가 주목 받고 있다.

본 연구에서는 쌀겨를 이용한 바이오차의 합성과 물리화학적 특성에 대한 연구결과를 보고한다. 쌀겨를 석영관으로 밀폐된 전기로에 넣고 열분해 온도를 각각 300, 400, 500, 600, 700 °C에서 바이오차를 합성하였다. 열분해 온도가 증가할수록 바이오차의 수득율이 증가하였다. XRD, FT-IR, SEM-EDX, Raman 분광을 통하여 제조된 바이오차의 물리화학적 특성을 분석하였다. 300 °C에서는 탄소에 관련된 라만피크가 나타나지 않았으며 이는 아직 탄소가 형성되지 않았음을 의미한다. 400 °C부터 탄소의 D와 G에 해당하는 피크가 나타나기 시작했으며,  $I_D/I_G$ 의 크기는 열분해온도가 증가함에 따라 커지는 것을 알 수 있었다. 열분해 온도 변화에 따라 제조된 바이오차의 염료 흡착 특성을 Rhodamine B를 이용하여 측정한 결과 Rhodamine B의 흡착 효율은 열분해온도 600 °C에서 가장 크게 나타났다.

### Keywords:

바이오차, 고에너지 볼밀링(HEBM), 염료 흡착, 라만분광

# Investigation of polarization mode dispersion effect on optical signal to noise ratio measurement employing polarization vanishment

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## Abstract:

Measurement of optical signal to noise ratio (OSNR), a gauge of the performance of the optical transmission system for fiber optic communication, should be made by wavelength channel in future optical fiber networks capable of dynamic recombination. To this end, an OSNR measurement method of using the annihilation of light polarization using a polarizer was previously reported, which is inevitably affected by polarization mode dispersion present in an optical fiber link, resulting in a measurement error. In this study, the effect of polarization mode dispersion on OSNR measurement utilizing polarization vanishment is theoretically investigated via simulation and the results are analyzed.

## Keywords:

Optical signal to noise ratio, polarization mode dispersion, optical fiber networks

## **Study of impact of electronic amplifiers on pursuit of polarization modes for optical fiber communication**

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### **Abstract:**

In order to compensate for polarization mode dispersion (PMD), which is incurred by fiber link birefringence and induces impediment to and restricts data rate of fiber optic transmission systems, a method of pursuing in real time via reiterated feedback control two orthogonal polarization modes, which irregularly fluctuates over time, was reported. Electronic amplifiers can be used in the feedback process and can influence the polarization mode pursuit. In this work, the impact of the electronic amplifiers on two perpendicular polarization modes trailing is studied by way of theoretical simulation, and the analysis and discussion of the simulation results are presented.

### **Keywords:**

Polarization mode dispersion, electronic amplifier, optical fiber communication

## Characterization of Carbon Dots using Tobacco-ash by various solvent for solvothermal method

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### Abstract:

Tobacco is a narcotic preference food, and many people smoke despite having many harmful substances, such as nicotine and tar. Tobacco is made by processing tobacco leaves, which are the Solanaceae family plants. Often, the plant-ash is used as fertilizer but tobacco-ash cannot be used as fertilizer because it contains many chemical compounds, such as nicotine. As a result, burnt tobacco-ash is a cause of 2<sup>nd</sup> environmental pollution. In general, many studies have been synthesized on plant leaves as a precursor material for carbon dot. And as a result, many research results have been published. However, research reports on tobacco-ash classified as garbage have not yet been published.

In this work, we synthesized carbon dots with using wasted tobacco-ash by solvothermal method according to various solvents such as DI-water, EtOH, and 2-ProH, etc.. Their structures, luminescence, and morphology characterization synthesized carbon dots were investigated by using X-ray photoelectron spectroscopy (XPS), raman spectroscopy, Fourier-transform infrared spectroscopy (FT-IR), photoluminescence (PL) and high-resolution transmission electron microscopy (HR-TEM), respectively. For this results, the possibility due to the recycling of tobacco-ash is expected.

### Keywords:

carbon dot, tobacco-ash, solvothermal synthesis

## Tunable luminescence property and optical temperature sensing performance of Bi<sup>3+</sup> and Sm<sup>3+</sup> co-doped GdNbO<sub>4</sub>

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### Abstract:

In the field of optical thermometer, due to the influence of light radiation and sample size fluctuation, the single excitation optical thermometer has some limitations in practical use. However, there is a self-tuning principle in fluorescence intensity ratio (FIR) technology based on dual-emission centers, which can use the intensity ratio from two independent emission centers to achieve accurate temperature measurement and good spatial resolution. FIR model is considered as one of promising methods because of its advantages of fast response time and high sensitivity. It is generally believed that Bi<sup>3+</sup> ions can emit light of various wavelengths in diverse matrix environments. Different from lanthanide rare earth, the emission of Bi<sup>3+</sup> ions only come from s<sup>2</sup>-sp transition. Due to the rich color of Bi<sup>3+</sup> emission, Bi<sup>3+</sup> as a sensitizer and activators of phosphors have been widely concerned. Compared with Bi<sup>3+</sup> ions, the emissions of Sm<sup>3+</sup> are relatively simple, and most of them are red, which is due to the <sup>4</sup>G<sub>5/2</sub> → <sup>6</sup>H<sub>J</sub> (J = 5/2, 7/2, 9/2) transitions of Sm<sup>3+</sup> ions. In addition, Bi<sup>3+</sup> and Sm<sup>3+</sup> co-doped materials have been demonstrated the good temperature dependence luminescence.

In this work, GdNbO<sub>4</sub>:Bi<sup>3+</sup>, Sm<sup>3+</sup> phosphors were successfully synthesized by solvothermal reaction method. Based on energy transfer from Bi<sup>3+</sup> to Sm<sup>3+</sup> ions, the tunable luminescence properties were carefully studied.

### Keywords:

GdNbO<sub>4</sub>:Bi<sup>3+</sup>, Sm<sup>3+</sup>, Luminescence, Temperature sensing

## Luminescent properties of carbon dots derived from various paper

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### Abstract:

Carbon dots (CDs) have been researched as a new type of luminescent materials in next generation, due to their abundant source, high biocompatible properties, easy fabrication, hydrophilicity, high quantum yield, high photo-stability. Since the CDs are based on organic materials, organic based materials can be used as their precursor. For these reason, green synthesis of carbon dots, which use natural or wasted organic material as their precursor, have been studied. Among various organic materials, paper is generally used in print, package, art, etc. Although the annual consumption of paper is increased, their recycling have troubled, owing reduction of wasted paper price.

As the wasted paper was composed with cellulose, utilization of wasted paper as a precursor of CDs can be fabricate two dimensional hexagonal structure, which have advantages in high quantum efficiency, good chemical stability, hydrophilic properties in the CDs. Although the chemical composition of paper was based from cellulose, the chemical composition of paper is varies with their purpose. Since the chemical composition of precursor affect in the luminescent properties of CDs, the comparison of CDs derived from various wasted paper is demanded to control and optimize their characteristics.

In this study, the paper cup, A4 paper, newspaper, and box were utilized as precursors of CDs. The CDs were synthesized by using a hydrothermal method. To compare their characteristics, the structural, morphological, luminescent properties of the CDs was analyzed.

### Keywords:

carbon dot, paper

## Study of Morphology and Device Property of Quantum Dot Light Emitting Diode

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### Abstract:

Due to narrow bandwidth and easy wavelength range tuning by changing the size of the particles, quantum dot based light emitting diodes (QD-LED) have advantages over organic-based light-emitting diodes (OLED). In addition, some hole-transporting materials are mixed into the quantum dot (QD) emission layer (EML) to improve the efficiency of the QD-LED. Even though there is an optimized concentration of the hole-transporting materials in the efficiency, the relation of the morphology and efficiency is not yet known. In this work, we found that the efficiency of green QD-LED can be improved through the blending of hole transport material. In particular, the efficiency was enhanced by ~20% when we applied 4,4',4''-tris(N-carbazolyl)triphenylamine (TCTA), a representative small molecular hole transporting layer material. However, it was found that TCTA improves the hole transporting ability, but it also plays a role in blocking the flow of electrons coming from the cathode when it is blended at a certain ratio or more. Therefore, the efficiency increases over a certain percentage and then changes to a sudden decrease trend. It is interesting to note that TCTA and QD do not mix isotropically but rather create a specific structure having vertically aligned QD. To correlate the change in the properties of the material and the change in electrical properties, various x-ray analyses using synchrotron radiation were performed. From the grazing incidence small X-ray scattering (GISAXS) technique, we found no significant ordering change compared to the QD-only film for the QD mixed with 10 wt% of TCTA, which showed the best efficiency of the devices. The enhanced ordering deteriorates the efficiency characteristics of the devices, presumably due to a vertically layered structure of emitting layer which may cause a carrier leakage resulting in imperfect charge injection into a QD.

### Keywords:

Quantum dot light-emitting diode, Grazing incidence small X-ray scattering, Morphology-efficiency relation

## 콘쥬게이션 폴리머 코팅 조건에 따른 형광 소멸 정도의 차이 연구

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### Abstract:

Conjugated polymer의 일종인 PEE와 MEH-PPV 박막을 스펀코팅하여 폭발물 증기에 의한 형광 특성 변화를 관찰하였다. 박막의 SEM(Scanning electron microscope)과 AFM(Atomic force microscope) 측정을 통하여 박막의 두께와 균일성, 표면 형태를 확인하였으며, 박막의 PL(Photoluminescence) 세기가 TNT(Trinitrotoluene) 증기와 반응에 따라 감소하는 PL quenching 현상이 발생하는 것을 관찰하였다. 박막 코팅시의 용액 농도에 따라 PL 세기와 quenching 정도가 어떻게 의존하는지 연구하였으며, MEH-PPV와의 혼합 박막을 제작하여 PEE와 MEH-PPV 사이의 에너지 이동이 용액 농도에 따라 어떻게 변화하는지에 대해 연구하였다.

### Keywords:

Explosive detection, Fluorescence quenching, Conjugated polymers

## Vertical transistor synapse based on Schottky barrier height modulation with organic ferroelectric material

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### Abstract:

Development of artificial synapses is essential for highly-efficient neuro-inspired computing system [1]. Among the various structures for artificial synapse, the vertical three terminal structure not only enabled nondestructive weight-update behavior, which is attributed to the completely separated terminals for reading and writing but also can overcome the structural limitations of planer three terminal such as low array design and complex line design [2]. In this presentation, we will introduce vertical transistor synapse based on schottky barrier height modulation with organic ferroelectric materials. The vertical transistor synapse consists of indium gallium zinc oxide (IGZO) film deposited by RF sputtering system sandwiched by crossed Au electrode and patterned CVD graphene electrode. To modulate the schottky barrier height between the IGZO/graphene junction, organic ferroelectric material Poly(vinylidene fluoride-trifluoroethylene (PVDF-TrFE) was spin-coated as the gate dielectric layer. Finally, the photolithography process for Al gate electrode pattern was performed, and PGMEA was used as a solvent to prevent damage to PVDF-TrFE during the lift-off process. When apply the gate voltage, the device showed gradually conductance switching by modulating the schottky barrier according to the change in the polarization direction of PVDF-TrFE. Also, device can mimic the essential synaptic function, long-term potentiation (LTP), and long-term depression (LTD) with 60 state. Also, the vertical transistor synapse was achieved up to ~90 % recognition accuracy for MNIST patterns in conventional convolutional neural network structure for a 6-kernel with 3x3 size. These results demonstrate that the vertical three-terminal devices that exploit modulation of Schottky barrier height can be applied to artificial synapses in advanced neuromorphic computing.

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### Keywords:

neuromorphic, artificial synapse, schottky barrier modulation, vertical transistor

## Controlling evaporator temperature to improve carrier properties of crystalline organic semiconductor

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### Abstract:

Organic field-effect transistors (OFETs) are key electronic components for the flexible organic electronic devices of the future. In recent years, a lot of effort has been given to fabricating crystalline organic semiconductor thin films from solutions for use in OFETs. Several groups have focused on a soluble pentacene derivative, Bis(triisopropylsilylethynyl)pentacene (TIPS-pentacene), as the semiconductor material in organic FETs. Bis(triisopropylsilylethynyl)pentacene (TIPS-pentacene), as a typical p-type semiconductor, is widely used in OFETs. The hole mobility in TIPS-pentacene is highly dependent on the crystal orientation and crystal quality, the presence of cracks, and crystal size. In general, the highest field-effect mobilities are obtained from high boiling point solvents and slow crystal growth or from a binary mixture of solvents. We applied this effect to organic semiconductor devices by manipulating the crystal structure by controlling the evaporation temperature of organic semiconductors. Crystal morphology was observed using AFM and XRD. The effect of these properties on charge transfer in organic semiconductors was analyzed through the electrical properties of I-V, C-V, C-F measurements.

### Keywords:

TIPS-pentacene, Temperature, Crystalline, Organic double-layer diode, Crystal effect

## Eu<sup>3+</sup> 이온이 도핑된 CaTiO<sub>3</sub> 나노입자를 이용한 엑소좀 분리 연구

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### Abstract:

엑소좀(exosomes)은 바이오마커 및 약물전달매체로서 연구자들 사이에서 매우 큰 관심을 받아왔으나, 30~100 nm 크기의 엑소좀을 시료로부터 분리하고 분석하는데 분리시간, 분석시스템의 민감도 및 특이도 문제 등 여러 제약을 가지고 있다.

본 연구에서는 Eu<sup>3+</sup> 이온이 도핑된 CaTiO<sub>3</sub> 나노입자 (CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs)를 이용한 엑소좀 분리 연구결과를 보고한다. CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs 고에너지 볼밀링(High-energy ball milling, HEBM) 방법을 이용하여 합성하였고, XRD, SEM 측정을 통하여 나노입자의 결정구조와 표면형상 및 미세구조를 분석하였다. X-선 회절 패턴을 분석한 결과 합성한 CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs는 CaTiO<sub>3</sub>와 동일한 사방정계의 결정성을 나타냈으며, Eu<sup>3+</sup> 이온이 CaTiO<sub>3</sub>에 효율적으로 잘 도핑 되었음을 확인할 수 있었다. 본 실험에서는 인간배아 신장의 HEK 293 세포에서 유래한 엑소좀을 사용하였다. CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs 2 mg을 세포배양액 10 ml에 넣고 30분 동안 incubation 후 Western blot 분석을 통하여 CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs에 엑소좀이 흡착되었음을 확인하였다. CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs의 양과 incubation time에 따른 엑소좀 흡착율을 측정하고 결과 CaTiO<sub>3</sub>:Eu<sup>3+</sup> NPs 2mg, incubation time 5분에서 엑소좀의 흡착 효율이 최대가 되었음을 확인할 수 있었다.

### Keywords:

엑소좀(exosomes), 고에너지 볼밀링(High-energy ball milling, HEBM), CaTiO<sub>3</sub>:Eu<sup>3+</sup> 나노입자

## Bioelectronic nose with micelle-stabilized olfactory receptors based on CNT-FET for detecting buttery flavors

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### Abstract:

인간의 오감 중 하나인 후각은 많은 생명체의 삶에서 중요한 역할을 맡고 있다. 지금까지 후각을 모방하기 위해 다양한 시도들이 있어왔고, 특히 후각 리셉터를 활용하여 진행된 연구는 특이적인 냄새 감지를 달성하였다. 하지만 후각 리셉터를 발현시키고 안정화시켜 전기적 신호를 검출해내는 것에는 어려움이 있었다. 본 연구에서는 박테리아 발현 프로토콜을 활용하여 ODR-10 후각 리셉터를 저비용 및 고효율로 과잉 발현하였다. 높은 순수도의 ODR-10 리셉터는 micelle 구조를 통해 안정화 되었으며, 탄소나노튜브 전계효과 트랜지스터의 위에 화학적으로 고정되었다. 이를 활용하여 ODR-10과 특이적으로 결합하는 버터 향을 가진 다이아세틸을 검지하는 인공 전자 코를 제작하였다. 본 연구에서는 실제 맥주, 와인, 막걸리, 소주 등 상업적으로 판매되고 있는 주류에서 다이아세틸의 농도를 정량적으로 평가하는데 활용할 수 있다는 것을 보여주었으며, 또한, gas permeable membrane을 활용한 인공 전자 코 구조물을 제작하여 기상-액상 인터페이스를 통한 다이아세틸 기체 검출이 가능함을 확인하였다. 이러한 결과들은 우리의 센서가 다양한 종류의 음식 산업과 주류의 품질 확인 등에 활용될 수 있는 강력한 도구가 될 수 있다는 것을 시사한다.

### Keywords:

탄소나노튜브 전계효과 트랜지스터, 인공 후각, 가스 센서

## **Development of new electron Pair Distribution Function (ePDF) analysis software for future gravitational wave detector upgrades**

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### **Abstract:**

Since 2015, the Advanced LIGO (Laser Interferometer Gravitational-wave Observatory) detectors have been successfully detecting gravitational wave (GW) signals. To extend the detection range further to observe GW signals from different sources, it is critical to improve the sensitivity of detectors. Since the recent enhancement in quantum noise via squeezing, coating Brownian noise has emerged as the most critical noise source in Advanced LIGO's noise curve. In order to reduce this noise, a new research model was introduced: utilizing atomic structure characterization to optimize the target amorphous oxide coating material. ePDF (electron Pair Distribution Function) analysis was used to study various amorphous oxide coating material candidates. For efficient and effective analysis, we have developed a new python-based software: ePDFpy. In this poster, this newly developed software will be introduced, along with some preliminary data analysis for potential Advanced LIGO mirror coating candidates.

### **Keywords:**

Gravitational wave detectors, Advanced LIGO, amorphous material, atomic structure characterization, software development

## **Development of effective local atomic structure analysis method for amorphous coating materials for future gravitational wave detectors.**

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### **Abstract:**

The Advanced Laser Interferometer Gravitational-wave Observatory (aLIGO) detectors have successfully observed the gravitational wave (GW) signals since 2015. However, detectors' sensitivity is critically limited by coating Brownian noise, especially around 100 Hz frequency band, where the detector is the most sensitive. In order to enhance the capability of GW detectors, understanding the atomic structure of amorphous oxide coating materials is crucial to optimize the performance of future mirror coatings. To accomplish this goal, the electron pair distribution function (ePDF) analysis was introduced to get structural information in short-range order of amorphous materials, which is reported to have a strong correlation with the mechanical loss of mirror coating. In this poster, an introduction of acquiring efficient and effective ePDFs from amorphous materials and some preliminary analysis results of future GW detector mirror coating materials are presented.

### **Keywords:**

Gravitational wave detector, Advanced LIGO, Amorphous material, Atomic structure characterization, Electron pair distribution function

## The construction of a 2nd repump laser for laser cooling of MgF molecules

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### Abstract:

Ultracold molecules provide a next generation platform to explore quantum computing, quantum chemistry, and precision measurements. Some classes of diatomic molecules can be cooled down below 1 mK using laser cooling. Due to the light mass and the highly diagonal Franck-Condon factors (FCF), MgF is a suitable candidate for laser cooling. Only three lasers - main, 1st repumper, and 2nd repumper - are required to obtain about  $10^5$  photon scatterings, which is necessary to cool the molecules down to the Doppler limit temperature. Among the three transitions, the 2nd repump transition frequency has not been experimentally confirmed yet. We constructed an external cavity diode laser (ECDL) to first detect the 2nd repump transition and later to use it as a 2nd repump laser for the laser cooling.

The ECDL is constructed based on the Littrow configuration. The frequency of the ECDL is stabilized and controlled using a transfer cavity controlled by a Labview interface. The transfer cavity is referenced by the main laser at 359 nm, which is stabilized independently.

We plan to determine the 2nd repump transition frequency by observing the fluorescence from a MgF buffer-gas beam, and utilize this laser as a 2nd repump laser for laser cooling. In the poster, each of the components and the current performance of the ECDL will be presented in detail.

### Keywords:

laser cooling, ECDL, MgF, diatomic molecules

## Phase noise measurement of a Raman laser system with low-phase noise fiber lasers for an atomic quantum gravimeter

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### Abstract:

The laser linewidth has a significant effect on phase noise in an optical phase lock loop (OPLL) system. For phase locking with a diode laser, an additional configuration is needed to reduce the laser linewidth. We build a heterodyne method OPLL system with two DFB(Distributed feedback) fiber lasers which have narrow-linewidth of less than 0.1 kHz and low-phase noise of less than -120 dB rad/@1 kHz. We also utilize a digital phase detector, which is more perturbation resistant than an analog phase detector. However, due to the slow response of the piezo of the fiber laser, the phase-locking performance of lasers using intrinsic piezo for wavelength modulation is limited.

### Keywords:

Phase noise measurement

## Construction of a buffer-gas beam source towards a magneto-optical trap for MgF molecules

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### Abstract:

Neutral polar diatomic molecules are expected to be a next-generation quantum platform because of their abundant internal structures and intrinsic electric dipole-dipole interactions. To maximally utilize these merits, achieving ultracold temperature is a prerequisite. The final platform we aim for is an array of MgF molecules trapped in optical tweezers. MgF molecules have a favorable energy structure for laser cooling and a larger electric dipole moment of 3 debyes. The molecules also have a light mass and a short transition wavelength so they are expected to be very advantageous for laser cooling and trapping. As a first step to preparing ultracold samples of MgF, we are planning to trap the molecules in a magneto-optical trap.

We constructed a buffer-gas beam source that produces a cold MgF molecular beam. MgF molecules are cooled down below 4 K by collisions with cold He buffer-gases after being generated by ablations. About 30% of the produced MgF molecules are in  $v=0$ ,  $R=1$  state, which is the electronic ground state of quasi-cycling transition of MgF for the MOT. After we built the whole set-up, we performed absorption spectroscopy of  $7\text{Li}$  to verify the buffer-gas beam source. The overall design and the performance of the buffer-gas beam source will be presented in detail in the poster.

### Keywords:

MgF, diatomic molecule, magneto-optical trap, buffer-gas beam, absorption spectroscopy

## Parametric resonance of $^{85}\text{Rb}$ in Dual Magneto-optical Trap

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### Abstract:

We report the construction of the dual magneto-optical trap system for rubidium and cesium atoms to investigate an inelastic collision mechanism between nonlinear dynamics of two atomic species. The parametric resonance of  $^{85}\text{Rb}$  atom cloud is realized by modulating the intensity of lasers counter-propagating along the z axis of the anti-Helmholtz coils in phase. Furthermore we trapped the cesium atom at the same trap center, and will discuss theoretically what happen in an inelastic collision mechanism between a parametric resonant rubidium atoms and a magneto-optical trapped cesium.

### Keywords:

dual magneto-optical trap, an inelastic collision mechanism

## Towards the Creation of Degenerate Fermionic/Bosonic NaK Molecular Gases with Long-range Dipolar Interactions

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### Abstract:

Experiments with ultracold atoms probe quantum statistics and extreme phases of matter with unprecedented level of precision. However, since the interaction between a pair of atoms in these experiments is often limited to the isotropic and short-range contact interaction, we aim to create a quantum degenerate gas of dipolar  $^{23}\text{Na}^{40,41}\text{K}$  fermionic/bosonic ground state molecules that feature strong anisotropic and long-range dipolar interactions. The strong dipolar interaction between the molecules will give access to exotic many-body phases of matter such as topological superfluids and quantum crystals, and will also enable two-qubit gate operations required for quantum information processing schemes with molecular qubits.

In this poster, we present our recent progress in constructing the experimental apparatus (UHV, laser, magnetic coil systems). Once an ultracold mixture of Na and K atoms are prepared in an optical dipole trap, subsequent Feshbach association followed by a coherent two-photon STIRAP transfer will produce fermionic/bosonic dipolar molecules in their absolute ground state. The creation of quantum degenerate gases of NaK dipolar molecules will pave the way to perform quantum simulation of extended Bose/Fermi Hubbard models in optical lattices, and also serve as a promising starting point to develop a scalable quantum information processing platform through chemically stable dipolar ground state molecules.

### Keywords:

Ultracold quantum gases, ultracold molecules, dipolar interaction, quantum computing

# Analysis of high-harmonic generation in solids using diabatic basis

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## Abstract:

In many studies about high harmonic generation in solids, the Bloch or the Houston functions are used as the basis function. The former is used to get the total current only and the latter to get currents between bands to produce a specific plateau in the harmonic spectrum. In the Houston basis, if two energy bands having avoided crossings are treated as two independent ones, not one, then the infinite high frequency has occurred in the harmonic spectrum. The high frequencies are different from the plateau shown commonly in the HHG, and no physical interpretations are allowed. The abnormal behavior is cured by transforming from the adiabatic basis to the diabatic basis. As a result, it enables us to identify the currents inducing plateaus in the harmonic spectrum. This poster details the calculations using a diabatic basis. Besides, it proves that the high-frequency portion of the harmonic spectrum is induced by a surviving population from constant destructive interference while a laser pulse is applied.

## Keywords:

high harmonic generation, solids, diabatic basis

## Closed Triple Collision Orbits and Stability Matrix

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### Abstract:

헬륨과 같은 이-전자 원자의 광이온화 단면적은 에너지가 이중-이온화 문턱 에너지  $E = 0$  로 다가감에 따라 공명들 사이의 겹침과 상호 간섭이 많아짐으로 인하여 매우 혼돈한 요동을 보인다. 이러한 혼돈한 요동은 핵 근처에서 시작하여 다시 핵으로 돌아오는 닫힌 삼중충돌 궤도(closed triple collision orbit (CTCO))라는 고전적 궤도의 정보를 이용한 준고전적 방법으로 해석이 가능하다는 것이 알려졌다 [C. W. Byun, et. al. Phys. Rev. Lett. 98, 113001 (2007)]. 광이온화 단면적을 준-고전적으로 해석하려면 고전적인 궤도인 CTCO 그 자체 뿐만 아니라 그 궤도와 관련된 stability matrix를 수치적으로 매우 정확히 구해야 한다. 이 논문에서는 CTCO의 궤도와 그것의 stability matrix를 핵과 전자 사이의 이중 (binary) 충돌을 제거한 좌표계를 사용하여 수치적으로 매우 정확히 체계적으로 구하는 방법을 설명할 것이다. 또한, 전자의 전하  $Z > 9/4$ 인 경우 Wannier 궤도의 효과가 나타나는지에 대하여도 검증을 할 것이다.

### Keywords:

stability matrix, 준고전적 방법, closed triple collision orbits

## 광공진기 내부에 포획된 단일 중성 원자의 움직임 분석 Analysis on the motion of single trapped atoms in an optical cavity

KIM Donggeon \*<sup>1</sup>, LEE Dowon <sup>1</sup>, HA Taegyul <sup>1</sup>, NOH Changsuk <sup>2</sup>, LEE Moonjoo <sup>1</sup>

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### Abstract:

원자-공진기 시스템을 통한 빛과 물질의 상호작용은 현재 활발히 연구되고 있으며, 양자 네트워크 등 양자 정보 분야에서의 응용성으로 인해 그 중요성이 커지고 있다. 본 연구에서는 광공진기 내부에 포획된 단일 이준위 원자를 쌍극자 포획하는 원리와 갇힌 원자의 3차원 움직임에 대해 계산한다. 공진기 내 원자의 움직임은 원자-포획 레이저의 주파수 차이가 클 경우 보존적인 (conservative) 움직임에 의해, 주파수 차이가 상대적으로 작을 경우 자발 방출에 의한 확산적인(diffusive) 움직임에 의해 지배된다. 각 경우에 대해 본 연구팀에서 작동하는 광공진기[1, 2]에서 원자의 움직임을 예측한다. 또한 원자의 움직임을 3차원, 실시간으로 관측하기 위해 개발 중인 헤테로다인 광학계에 대해 소개한다.

[1] J. Kim\*, K. Kim\* et al., Sensors 21, 6255 (2021)

[2] D. Lee et al., Opt. Continuum, in press (2022)

### Keywords:

Optical cavity, Two-level atom, Dipole trap, Heterodyne detection, 3D motion

## Moving frame imaging of cold atoms in an optical dipole trap for coupling to nanophotonic devices.

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<sup>2</sup>Department of Physics, KAIST  
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### Abstract:

We introduce a moving frame imaging technique of optically trapped atoms that are transported by an afocal system.

The afocal system with a movable objective lens provides a moving focus position of an optical dipole trap beam without significant numerical aperture variation during transfer. Moreover, since the ODT focus position can be magnified with respect to a moving lens, the trapped atoms can be transported with a range spanning interconnected vacuum chambers. We superpose an absorption imaging system onto this moving-focus ODT system. The imaging beam propagates at an opposite direction to ODT beam sharing optical components, hence, the imaging system is always in-focus with the ODT providing in situ absorption images during transport. We image atoms being transported from a glass chamber to a nanofiber placed in a science chamber and measure the atom number, temperature, and potential depth of the cold atoms during transport.

## Identification of the number of graphene layers and absence of fluorine layer on fluorinated graphene with partially removed thin film via AFM

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### Abstract:

Graphene is in the spotlight as a nanomaterial due to its excellent electrical and physical properties. [1], these properties of graphene can be changed by doping. Control of the fluorine / carbon ratio of fluorinated graphene (FG) can open the bandgap and tune the electrical conductivity and optical transparency [2,3]. Accordingly, it will be important to accurately measure and classify the electrical and physical properties of samples using graphene in future nanotechnology. The number of graphene layers of FG and the presence or absence of fluorine thin film were distinguished via various modes of an atomic force microscopy (AFM) and machine learning. We mechanically removed fluorine thin films via a contact mode AFM from FG. Measurement of the AFM shows higher precision and accuracy for in fine areas due to better resolution than other optical measurement methods.

The AFM can measure various physical properties as well as topographic information of the sample. Because the AFM measure the change of the cantilever by the interaction from the sample surface, it is greatly affected by the cantilever and the surface conditions which cause the image noises. We additionally, investigate how to clean the obtained AFM images by using the machine learning method.

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[2] Y. Liu, J. Li, X. Chen, and J. Luo, Fluorinated Graphene: A Promising Macroscale Solid Lubricant under Various Environments. *ACS Appl. Mater. Interfaces* 11(43), [40470-40480](#) (2019).

[3] K.-I Ho, C.-H. Huang, J.-H. Liao, W. Zhang, L.-J. Li, C.-S. Lai, and C.-Y. Su, Fluorinated Graphene as High Performance Dielectric Materials and the Applications for Graphene Nanoelectronics. *Sci. Rep.* 4, 5893 (2014).

### Keywords:

Atomic force microscopy, AFM, Graphene, Thin film, Machine learning

## Magnetic Field Dependence of Modulation Transfer Spectroscopy for $^{87}\text{Rb}$ and $^{85}\text{Rb}$ Atoms

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### Abstract:

We study on magnetic-field enhanced modulation transfer spectroscopy (MTS) for  $^{87}\text{Rb}$  and  $^{85}\text{Rb}$  atoms. We have experimentally investigated the magnetic field dependence of modulation transfer spectroscopy (MTS) on the various magnetic field strength and on the different angle between the polarization direction and the magnetic field direction. The polarization of probe beam is aligned and fixed along the magnetic field direction, while the polarization direction of pump beam changes. We report how the amplitude and slope of the modulation transfer spectroscopy signal with each  $^{87}\text{Rb}$  and  $^{85}\text{Rb}$  atoms depends on the field strength and polarization angle.

### Keywords:

magnetic-field enhanced modulation transfer spectroscopy

# Estimating non-Gaussianity of a quantum state by measuring orthogonal quadratures

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## Abstract:

We derive the lower bounds for a non-Gaussianity measure based on quantum relative entropy (QRE). Our approach draws on the observation that the QRE-based non-Gaussianity measure of a single-mode quantum state is lower bounded by a function of the negentropies for quadrature distributions with maximum and minimum variances. We demonstrate that the lower bound can outperform the previously proposed bound by the negentropy of a quadrature distribution. Furthermore, we extend our method to establish lower bounds for the QRE-based non-Gaussianity measure of a multimode quantum state that can be measured by homodyne detection, with or without leveraging a Gaussian unitary operation. Finally, we explore how our lower bound finds application in non-Gaussian entanglement detection.

## Keywords:

non-Gaussianity, relative entropy, homodyne detection

## Hitting time in a point of view on a graph as an electric network

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### Abstract:

Hitting time in random walks on graphs is a substantial quantity for the classical and quantum study of Markov chains. And a point of view on graphs as electric networks has turned out to be useful in the analysis of quantum walk search. Recently, some literatures introduced a theorem on hitting times that is expressed in terms of physical quantities introduced in electrical networks as follow: the average hitting time  $H_{\pi, M}$  equals  $2WR_{\pi, M}$ , where  $W$  is the sum of conductance over edges,  $R_{\pi, M}$  the effective resistance between the stationary distribution  $\pi$  and the set of marked vertices  $M$ . However, any proof of the theorem has not been given yet. In this talk we present a proof of the theorem.

### Keywords:

hitting time, quantum walk search, electric network, Markov chain

## Compensating the drift of mode-locked lasers' repetition rate to drive trapped-ion qubits

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### Abstract:

이온 트랩 양자 컴퓨터에서 자주 사용되는 원소인  $^{171}\text{Yb}^+$ 는 공명 주파수 12.6 GHz의 초미세 전이선을 가진다. 큐비트를 이용한 게이트 연산을 위해 전이선을 모드락 레이저를 이용한 Raman 전이 방식으로 구동한다. 이를 위해 중심 파장 355 nm, 펄스 길이 15 ps, 펄스 반복율 약 118 MHz인 모드락 레이저를 사용하는데, 반복율이 시간에 따라 표류하는 것이 이온 전이선의 안정적인 구동에 문제가 된다. 본 발표에서는 상용 펄스 카운터와 field programmable gate array 프로그래밍을 이용하여 모드락 레이저 반복율의 주파수 표류를 보상하였다. 모드락 레이저의 반복율은 약 20분 동안 110 Hz 정도 표류함이 측정되었고, 레이저가 통과하는 음향광변조기에 같은 양 만큼의 주파수를 표류의 반대방향으로 가해 전체적인 Raman 전이는 일정한 주파수로 이루어지게 하였다. 본 발표에서 실험적인 세부 사항을 논의한다.

### Keywords:

iontrap

## **A concentric solid immersion lens shortening milling time and retaining photon collection efficiency for nitrogen-vacancy center.**

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### **Abstract:**

Quantum defects in solid are successful resources for quantum information, quantum computing and quantum sensing. As one of them, a nitrogen-vacancy center showed enormous improvement in these fields. Although a number of methods for increasing a photon collection efficiency, which is important for a readout fidelity and a quantum network, have been developed, further improvements for easier and faster to make should be done. Here, we demonstrate a new shape (we call concentric solid immersion lens) which is suitable for that uses and can be made by using focused ion beam milling directly on a commercial diamond surface. And we simulate milling volume, which is proportional to consuming time for making it, and photon collection efficiency compared with a case of just plane surface, and both of them get accomplished by experiments. The milling volume is lower to 16% compared with a hemispherical solid immersion lens which is adopted normally. The photon collection efficiency is more than 2.5 times higher than case of plane surface.

### **Keywords:**

NV center, focused ion beam, quantum defect, quantum information, quantum computing

## Observation of the photon statistics of single-atom superradiance

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### Abstract:

In a laser, the lasing threshold is a critical point above which the stimulated emission dominates over the spontaneous emission of excited atoms. Unlike the spontaneous emission, the stimulated emission has coherence among the emitting photons. The emission rate of the atoms increases above the lasing threshold by the coherence. There have been many efforts to lower the lasing threshold. By doing so, one can produce coherent light source even at very low output power. Recently, the energy transfer efficiency from total emission to a specific lasing mode, parameterized as  $\beta$ , greatly improved. It is achieved by reducing the size of a cavity down to subwavelength scale. This approach enhances the Purcell effect, lowering the energy loss of spontaneous emission. As  $\beta$  gets close to unity, the slope difference of the in-out power curve at the lasing threshold smoothly disappears. However, even in this case, it has been observed that the measured photon statistics below the threshold is not coherent: the laser behaves like a thermal light source. In this poster, we report a new type of coherent light source. Using superradiance, our laser keeps photon coherence at any input energy. It also exhibits output power increasing quadratically with respect to the number of emitters. This is a basic trademark of superradiance. Our ever-coherent light source shows no lasing threshold, or thresholdless. The photon statistics, or the second-order correlation function  $g^{(2)}(\tau)$ , is obtained by using the Hanbury-Brown-Twiss correlation measurement technique. Due to the remnant non-collective spontaneous emission, the  $g^{(2)}(0)$  does not exactly converge to unity. The observed lowest  $g^{(2)}(0)$  at the threshold is  $1.04 \pm 0.02$  with optimum experimental parameters.

### Keywords:

superradiance, laser, second order correlation, thresholdless

## Poling-driven modulation in structural and optical properties of $\text{Eu}^{3+}$ doped $(1-x)\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3-x\text{BaTiO}_3$

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### Abstract:

무연(lead-free) 압전체인  $(1-x)(\text{Na}_{0.5}\text{Bi}_{0.5})\text{TiO}_3-x\text{BaTiO}_3$ (NBT-BT)는  $\text{Pb}(\text{Zr}_{0.5}\text{Ti}_{0.5})\text{O}_3$ 와 같은 납이 포함된 상용 압전체를 대체하기 위한 물질로 연구되어 왔다. NBT-BT는 NBT와 BT의 특정조성에서 갖는 조성상경계(Morphotropic Phase Boundary,MPB)에서 2개 이상의 결정 구조를 갖는 것이 보고되어 있다. 또한 압전성능을 발현을 위한 분극 처리 과정에서 외부인가 전기장에 의한 비가역적 결정구조 변화를 나타냄이 앞선 연구들을 통해 보고되었다. 란타넘족 이온  $\text{Eu}^{3+}$ 는 주변결정장에 영향을 받아 발광특성이 변화한다.

$\text{Eu}^{3+}$ 는 주변결정장의 중앙대칭성이 감소할수록 f-f transition에 의한 발광이 강해진다. 본 연구는 외부자극을 통한 광방출 특성변조 조사를 목표로, 외부 전기장에 의한 NBT-BT의 결정구조변화를 유발하고,  $\text{Eu}^{3+}$  주변의 국소결정장 변화로 인한 발광특성이 변화함을 관측 및 해석하였다.

준비된 시편은 BT의 비율 0%, 2%, 4%, 6%, 8%의 조성의 5개 시편을 제작하였다. 첨가된  $\text{Eu}^{3+}$ 는 ABO<sub>3</sub> perovskite 구조의 A-site에 첨가하였으며 농도는 0.4%로 고정하였다. X-ray diffraction(XRD) 및 온도의존 유전상수, 압전계수, Photoluminescence(PL)를 측정하였다. 분극처리 전과 후의 결정구조 변화와  $\text{Eu}^{3+}$  이온의 발광특성 변화의 강한 상관관계를 확인하였다. 측정된 XRD 데이터를 Rietveld refinement 구조 분석 결과 NBT-xBT:Eu relaxor가 단사정계(monoclinic)과 능면체(rhombohedral), 정방정계(tetragonal)의 혼합으로 이루어져 있고 분극처리 후  $\text{Eu}^{3+}$  주변결정장의 중앙대칭성이 증가하며 PL의 세기가 감소했다. 분극처리 후 측정된 압전계수와 PL 감소율, 구조상의 변화율은 NBT-xBT:Eu의 BT의 비율에 따라 변했고 그 경향성은 서로 유사했다. 종합적인 결과로 NBT-xBT:Eu는 새로운 광전자 재료가 될 가능성을 시사한다.

### Keywords:

Pizeo-electrics,  $\text{Eu}^{3+}$ , Photoluminescence, NBT-BT, Rietveld refinement

## Study of electrical property changes of aligned PbTiO<sub>3</sub> nanotube synthesized by hydrothermal method

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### Abstract:

Ferroelectrics such as K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub>, BaTiO<sub>3</sub>, PbZr<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub>, and PbTiO<sub>3</sub> (PTO) are known to have unique electrical and dielectric properties at the one-dimensional nanoscale, and active research is currently underway. Among the methods for forming such nanostructures, research on synthesizing a vertically oriented ferroelectric nanotube through a low-temperature process called hydrothermal synthesis has been reported.

In this work, PTO nanotubes were prepared through Pb<sup>2+</sup> doping by putting anodized TiO<sub>2</sub> nanotubes into a hydrothermal synthesizer. Firstly, the number of anodization (one-step or two step) and the NH<sub>4</sub>F concentration in the electrolyte were adjusted to investigate the changes in the diameter, wall thickness, and distance between the nanotubes of the TiO<sub>2</sub> nanotube. The all structural changes were checked by FE-SEM. Therefore, we obtained the aligned nanotube arranged as the number of the anodization steps. Secondly, the hydrothermal synthesis time and TiO<sub>2</sub> template position of PTO were applied as variables. As a result of XRD and Raman spectroscopy, we confirmed the perovskite structure of PTO nanotube. The electrical properties ( $\epsilon_r$  & *P-E* loop) were measured. As the frequency increases (10<sup>2</sup> to 10<sup>7</sup> Hz), the  $\epsilon_r$  decreases linearly with half or more value until the 10<sup>7</sup> Hz (30–100). The  $\epsilon_r$  tends to increase in proportion to the hydrothermal synthesis time, which is considered to have a direct effect on the increased wall thickness. Through the *P-E* loop, the polarization did not reach a value of zero, that is, a residual polarization value can be observed. Consequently, we observed that the shape of nanotube can be controlled by synthesis condition and that it also can affect to their electrical properties.

### Keywords:

Hydrothermal synthesis, Ferroelectric, PTO nanotube, Nanostructure

## The interplay of oxygen vacancies and ferroelectricity in Ca-substituted super-tetragonal BiFeO<sub>3</sub>

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### Abstract:

Ferroelectricity is useful for applications in memories, actuators, ultrasonic transducers, and many more [1-2]. On these ferroelectric materials, oxygen vacancy defects have been suggested as one of the key factors in modifying resistance state [3], phase transition [4], and enhancing ferroelectric transition temperature [5]. But understanding the mechanisms of how oxygen vacancies affect ferroelectric properties is far from complete. Here, we report the interplay of ferroelectric mixed-phase domain structures with conductivity modulation in a Ca-substituted super-tetragonal (T phase) BiFeO<sub>3</sub> grown on LAO (001) substrate as a result of electric-field-induced oxygen vacancy migration. We present our observation of micron-scale domain textures characterized by piezoresponse force microscopy (PFM) and local conduction mapping taken by conductive AFM (CAFM) under sample-biased tip poling. The base material BiFeO<sub>3</sub> is a known ferroelectric material that can have R, T, S phases, and their variations [6]. R phase can be grown on a substrate with relatively well-matched lattice parameters such as SrTiO<sub>3</sub> and DyScO<sub>3</sub> with polarization along <111> direction. On the other hand, the T phase, which is highly elongated in <001> direction, can be stabilized on a substrate such as LaAlO<sub>3</sub> with a strong polarization along pseudocubic [001] and a weak polarization along <100> direction [7-9]. Although our experiments are similar to those in R-phase Ca-substituted BiFeO<sub>3</sub> [10], the observation in T-phase Ca-doped BiFeO<sub>3</sub> is a unique point of this study. The experimental results deepen our understanding of the interaction between oxygen vacancies and strained ferroelectrics.

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- Cell phone number: 010-5515-2689

### Keywords:

Ferroelectric, Oxygen vacancies, Defect, Strain, SPM

## Enhanced electromechanical response (111)-oriented perovskite ferroelectric oxides

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### Abstract:

The so-called morphotropic phase transition (MPT), compositionally induced change in a crystalline structure, is of great practical interest. In this presentation, we demonstrate the phase coexistence and enhanced piezoelectricity in a few tens of nanometers thick, Pb-free CaTiO<sub>3</sub> films via a thickness-driven phase transition. Due to the competition between interfacial and bulk energies, as film thickness increases, epitaxial CaTiO<sub>3</sub> films exhibit a ferroelectric-to-paraelectric phase transition that is concomitant with the rhombohedral-to-orthorhombic structural transition. We investigated this MPT in nanoscale CaTiO<sub>3</sub> films stems from the metastable nature of ferroelectricity. We visualize the resulting morphotropic phase boundary at the atomic scale in nanoscale CaTiO<sub>3</sub> films. We also show that this thickness-driven MPT could lead to reasonably good piezoelectricity at the nanoscale by piezoresponse force microscopy measurement. This study highlights the rich phase evolution of complex ferroelectrics as a novel platform to control the functionality of nanoscale electromechanical devices.

### Keywords:

morphotropic phase transition, morphotropic phase boundary, metastable ferroelectricity, piezoelectricity, epitaxial thin film

## Growth and atomically resolved polarization mapping of ferroelectric Bi<sub>2</sub>WO<sub>6</sub> thin film

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### Abstract:

Ferroelectric thin films are widely applied to various electronic devices such as capacitor or ferroelectric tunnel junction, due to their non-volatile electric polarization under zero-field. Bi<sub>2</sub>WO<sub>6</sub> (BWO), which is the simplest member of Aurivillius phase, triggered a lot of interest by its robust ferroelectric properties such as high Curie temperature ( $T_C \sim 950$  °C) and strong spontaneous polarization ( $\sim 50$   $\mu\text{C}/\text{cm}^2$ ). Most interesting property is that its ferroelectric domains are aligned along only the in-plane (IP) direction, forming 90° degree in total 4 directions, meaning no minimum thickness is needed unlike other conventional ferroelectric materials. Moreover, ferroelectric domains of BWO can be switched with low energy cost than other conventional ferroelectrics like PbTiO<sub>3</sub>. These properties are essential for realizing electric device applications with low energy and volume demand. Although BWO has such advantages, a systematic study focusing on the growth condition of BWO thin films, and experimental proof for origin of ferroelectricity is still missing. Here, we have grown epitaxial BWO thin films on (001)-oriented SrTiO<sub>3</sub> substrates via pulsed laser deposition (PLD). Various films are grown with tuning the two most important parameters, oxygen pressure and substrate temperature. Quality of crystal structure and surface of BWO films is confirmed by X-ray diffraction, atomic force microscopy and transmission electron microscopy and we got growth window for BWO thin film. Finally, we proved the ferroelectric properties and its origin in our BWO films using piezoresponse force microscopy and scanning transmission electron microscopy. Based on our observation, we conclude that W cations pure in-plane dislocation relative to Bi atomic arrangement cause ferroelectricity. We expect our study would contribute to the realization of BWO-based low-energy, space consuming electric device.

### Keywords:

Ferroelectric, Bi<sub>2</sub>WO<sub>6</sub>, pulsed laser deposition, Scanning Transmission Force Microscopy

## Synthesis, structure, and PL emission of Ce<sup>3+</sup> and Eu<sup>3+</sup> co-doped Sr<sub>2</sub>SnO<sub>4</sub>

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### Abstract:

Rare earth activated fluoride phosphors have attracted attention in recent years in the field of solid state lighting. In this work, RE (RE = Ce<sup>3+</sup>, Eu<sup>3+</sup>) doped/co-doped Sr<sub>2</sub>SnO<sub>4</sub> phosphor has been synthesized by a conventional solid-state reaction method. Photoluminescence (PL) properties of this sample were investigated by JASCO FT-8500 spectrofluorometer. The structural features of all the samples were analyzed by X-ray Diffraction (XRD), which showed that the samples were crystallized in a well-known tetragonal structure (PDF#89-0373). The excitation PL spectra of Sr<sub>2</sub>SnO<sub>4</sub>:Ce<sup>3+</sup> show a broad band in the range from 240 nm to 290 nm, which can be attributed to the transitions from the 4f ground state of Ce<sup>3+</sup> ions to the field splitting levels of the 5d state. The emission PL spectra, obtained under 255 nm excitation, feature a broad 5d→4f emission band in the ultraviolet/visible spectral range with the maximum peak located at around 385 nm. PL intensity depends on the content of Ce<sup>3+</sup> ions in Sr<sub>2</sub>SnO<sub>4</sub>. A broad PL excitation peak in the range of 220–350 nm is obtained by co-doping Ce<sup>3+</sup> with Eu<sup>3+</sup>. Strong red emissions were observed from Ce<sup>3+</sup> and Eu<sup>3+</sup>-codoped Sr<sub>2</sub>SnO<sub>4</sub> under 464 nm excitation. Excellent photochromism and luminescence modulation properties are found in Sr<sub>2</sub>SnO<sub>4</sub>: Ce, Eu ceramics.

### Keywords:

Sr<sub>2</sub>SnO<sub>4</sub>, Ce<sup>3+</sup>, Eu<sup>3+</sup>, photochromism, luminescence modulation properties

## Growth phase diagram of cobalt oxide thin films with control of oxygen vacancy

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### Abstract:

$AB_2O_4$  spinel oxides have various functionalities originated from their tetrahedral crystal field and spin configuration. The physical properties of these materials are diverse, for example, ferromagnetism, antiferromagnetism, spin-glass, and even superconductivity. Recently, the two-dimensional topological superconductivity has also been predicted at the antiferromagnetic/superconducting interface of spinel oxide structure [1]. However, a realization of this exotic phase requires a stable antiferromagnetic state, which is a hardship due to the subtle electronic structure and intrinsic geometrical spin frustration of spinel oxides [2]. The magnetic properties of these systems are governed by crystal field splitting with oxygen bonding; thus, the formation of oxygen vacancy ( $V_O$ ) plays an important role to utilize the physical properties of spinel oxides.

Control of  $V_O$  in this system is also important for the application. Among the spinel oxides, cobalt oxides have recently got much attention with their catalytic behavior for oxygen evolution/reduction reaction [3]. Since cobalt ion has multiple oxidization states, cobalt oxides can be rock-salt CoO and spinel  $Co_3O_4$ . The reduction/oxidization of cobalt oxides are very sensitive to temperature and pressure. This sensitivity makes cobalt oxides highly reactive. There have been extensive studies on the oxidization process in cobalt oxides from the bulk, nanoparticles, and thin films. Previous works have reported that the oxygen pressure is a key parameter to control the oxidization state of cobalt oxides thin films [4], while overlooking the possibility of  $V_O$  formation with their growth temperature.

Therefore, a comprehensive understanding of growth conditions including temperature and  $V_O$  formation in cobalt oxides is still required, particularly on thin films.

In this paper, we provide a detailed growth diagram of cobalt oxide thin films with  $V_O$  formation. We grew several cobalt oxide thin films on  $MgAl_2O_4$  (111) [MAO(111)] substrate by pulsed laser deposition (PLD) technique. MAO single crystal was used for the epitaxial growth since it has a similar lattice constant and spinel structure with  $Co_3O_4$ . Growth temperature and oxygen partial pressure [ $P(O_2)$ ] were the main variables. To distinguish the various oxidation states and  $V_O$  formation of cobalt oxide thin films, we performed X-ray diffraction (XRD) for the lattice structural characterization, and X-ray photoemission spectroscopy (XPS) for the core-level electronic characterization. We also conducted spectroscopic ellipsometry for the optical properties. Combining the experimental results, we obtained a comprehensive growth phase diagram. Even we used a single CoO compound as a target for PLD, we could obtain various oxidized phases of cobalt oxides. As a result, we could suggest a criterion for the growth and analysis of cobalt oxide thin films.

### Keywords:

Co<sub>3</sub>O<sub>4</sub>, Cobalt Oxide, Thin film

## Investigation of temperature dependent resistance of two-dimensional electron gas in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> hetero-interface

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### Abstract:

For the device application of SrTiO<sub>3</sub>-based two-dimensional electron gas, it is important to understand how to control the physical properties by applying back gate voltage. Here, we report that the hysteresis behavior in the temperature dependence of the resistance between cool-down and warm-up process was controlled by the back gate voltage in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> hetero-interface. The magnitude of hysteresis increased as the applied back gate voltage increased, and the hysteresis was observed only when the lowest temperature was 50 K or less in the temperature sweep experiment from room temperature to lowest temperature. To explain the hysteresis, we present a model including interplay between increase in dielectric constant of SrTiO<sub>3</sub> with decreasing temperature and electron trapping at impurity sites. Our results will play an important role in explaining hysteresis in the temperature dependent resistance in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> hetero-interface.

### Keywords:

hetero-interface, two-dimensional electron gas

## Magnetic octupole induced oscillation of Hall effect in an antiferromagnetic semimetal

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### Abstract:

Antiferromagnets (AFM) have recently attracted extensive interests as a platform for exploring prominent topological phases such as Weyl semimetal and Axion insulator. However, the intrinsic characteristics of AFM place the limitation on detecting predicted topological phenomena and make it difficult to manipulate them as futuristic low-power microelectronics devices. Therefore, to unlock the futuristic potentials of AFM, the manipulation of the magnetic ordering in AFM is the crucial key. Here, we demonstrate that magnetic  $T_1$ -octupole is generated in the antiferromagnetic  $\text{Nd}_2\text{Ir}_2\text{O}_7$  thin film by epitaxial strain and has additional topological contributions to the Hall effect. Particularly, the  $T_1$ -octupole induces additional sixfold oscillation in the Hall effect when magnetic field ( $H$ ) and current ( $I$ ) are rotated in the same plane. Moreover,  $T_1$ -octupole orderings induce anomalous field-dependent behaviors ( $H^3$  and  $H^4$ ) of Hall effect when  $H$  and  $I$  are parallel, in which the Hall effect should conventionally vanish. Our work provides a new strategy to engineer topological phenomena via magnetic octupole ordering in AFM, which would provoke novel spintronic devices in which the manipulation of magnetic octupole is desirable.

### Keywords:

magnetic octupole, antiferromagnet, topological physics

## Spectroscopic evidence for the metallic ground state of SrIrO<sub>3</sub> monolayer

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### Abstract:

We investigated the electronic structure of ultrathin SrIrO<sub>3</sub> film down to monolayer by angle-resolved photoemission spectroscopy. In order to prevent extrinsic charging effect of relatively resistive films, a recently reported 'charging-free heterostructure' system is utilized for photoemission measurements. [1] We observed that spectral weights remain distinctly at the X ( $\pi,0$ ) point of the Fermi surface of monolayer SrIrO<sub>3</sub>, which has not been reported in previous studies. The semi-metallic behavior of thick SrIrO<sub>3</sub> film was thought to be a result of large bandwidth of 3D material, and thus the Mott insulating Sr<sub>2</sub>IrO<sub>4</sub> like properties were expected in the case of reduced dimensions at the ultrathin limit. In our results, a gradual decrease in quasiparticle intensity was observed at the X point, but it could not finally match the electronic structure of Sr<sub>2</sub>IrO<sub>4</sub>. We also performed K dosing on the surface of monolayer SrIrO<sub>3</sub>, and it became more metallic after several steps of dosing. Our results suggest that dimensionality is not the only origin of the metallicity of SrIrO<sub>3</sub> but that other origin, such as octahedral rotation angles, could be one of them.

[1] B. Sohn, et al., Nat. Commun. 12, 1-8 (2021)

### Keywords:

ultrathin film, Metal-insulator transition

## Transition of temperature dependent resistivity behavior in SrTiO<sub>3</sub>/SrIrO<sub>3</sub>/SrTiO<sub>3</sub> depending on the thickness of the SrIrO<sub>3</sub> film

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### Abstract:

When SrIrO<sub>3</sub> film is grown on the SrTiO<sub>3</sub> substrate by using PLD method, the temperature dependent resistivity behavior changes into "insulator-like", "metal-like" and "intermediate" depending on the growth condition. Among them, we focused on the "insulator-like" growth condition and observed the changing of the temperature dependent resistivity behavior by growing SrTiO<sub>3</sub> capping layer where the SrIrO<sub>3</sub> film has the "insulator-like" property. When the thickness of the SrIrO<sub>3</sub> film becomes less than a certain thickness, we observed that the sample's temperature dependent resistivity behavior changes into "metal-like". We deposited SrIrO<sub>3</sub> and SrTiO<sub>3</sub> films on the SrTiO<sub>3</sub> substrate by using PLD method, and we also controlled the thickness of the film by a unit cell by using RHEED(Reflection High-Energy Electron Diffraction). To find out the critical thickness where the temperature dependent resistivity behavior changes, we fixed the thickness of SrTiO<sub>3</sub> capping layer and made a variation of the thickness of the SrIrO<sub>3</sub> film. As a result, the temperature dependent resistivity behavior of the sample was found to be "insulator-like" in the case of SrIrO<sub>3</sub> film thickness 9~20 unit cell, "intermediate" in 7,8 unit cell, and "metal-like" in the case of SrIrO<sub>3</sub> film thickness in 1~6 unit cell.

### Keywords:

transition metal oxide, PLD, thickness of film

## Correlation between the magnetic exchange energy and Neel temperature in pyrochlore ruthenates

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### Abstract:

Transition-metal pyrochlore oxides provide a rich platform for exploring diverse states of matter due to the unique crystal structure and chemical versatility. Specifically, pyrochlore ruthenates, a family of strongly correlated 4d materials, houses a wide range of interaction between spin, orbital, and lattice degrees of freedom. Rare earth pyrochlore ruthenates are generally known to be spin-1 Mott insulators that display antiferromagnetic ordering of Ru ions below the Neel Temperature ( $T_N$ ), with  $T_N$  strongly depending on the size of the rare earth ions.

In our study, a series of polycrystalline pyrochlore powder samples  $RE_2Ru_2O_7$  ( $RE = Y, Nd, Sm, Eu, Ho, Er$ ) was synthesized and temperature dependent Raman spectroscopy measurements were performed. Our results concisely show a strong positive correlation between the one-magnon excitation energy and  $T_N$  of each compound, varying from  $T_N = 80K \sim 150K$ . Also, a new low-energy mode that hints of a Higgs-type fluctuation, reported in our separate study on single-crystalline  $Nd_2Ru_2O_7$ , was shown for all the measured compounds. Additionally, we will address the spin-phonon coupling displayed in the Raman spectrum.

### Keywords:

pyrochlores, one-magnon, Raman Spectroscopy

## Changes in physical properties of nickelate thin film due to pulsed laser irradiation

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### Abstract:

When a metal oxide single crystal is irradiated with a laser, oxygen vacancy or structure transition occurs and the physical properties are changed. In the case of SrTiO<sub>3</sub> single crystal, when irradiating laser, If the laser intensity exceeds a certain level, oxygen vacancy occurs. Due to this, it turns into metal and ferromagnetism properties. If the physical properties are changed using laser like this, patterning using a mask is possible. so we will be able to manufacture various semiconductor devices. In this experiment, we deposited (Nd<sub>0.8</sub>Sr<sub>0.2</sub>)<sub>4</sub>Ni<sub>3</sub>O<sub>10</sub> thin film on SrTiO<sub>3</sub> substrate using pulsed laser deposition. After that, we irradiated the pulsed laser to the thin film in various environments. We first measured the resistivity of the thin film. When the thin film was irradiated with a laser of strong intensity, the resistivity was greatly increased. Then, we measured XPS and XRD to find out why the resistivity changed.

### Keywords:

nickelate, metal oxide, laser irradiation, pulsed laser

## Manifestation of Hund's rule effect in the optical conductivity near the metal-insulator transition of NiS<sub>2</sub>

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### Abstract:

In recent decade, the effect of Hund's coupling  $J$  in multi-band system has been studied with much attention. Hund's coupling affects the energy scale of the system by nature, as can be understood from that it determines the energy scale of spin Kondo screening. This phenomena was prominent in non-half-filled and non-singly-filled multi-orbital case, but recently, the similar Hund's physics has also been observed evidently in half-filled NiS<sub>2-x</sub>Se<sub>x</sub> system. It was demonstrated that the kink in the spectral function is produced by Hund  $J$ , and it is closely interconnected to the quasiparticle coherence-incoherence crossover temperature. [1] Here, we will present our study of pressurized NiS<sub>2</sub>, in correlated metallic phase, to investigate the Hund's physics in half-filled multi-band system. We will visit how the energy scales are determined, and in particular we will examine how Hund's effect is manifested in the optical conductivity. The anomalous frequency dependence away from the Drude behavior was observed, and it is produced by the kink in the spectral function. Our results propose that half-filled multi-band system can be also a good ground to study rich fundamentals such as the Hund's physics.

[1] Bo Gyu Jang, *et al.*, *Nat. Commun.* **12** 1208 (2021)

### Keywords:

metal-insulator transition, Hund's physics, optical conductivity

## The Exciton-Phonon Coupling in the Critical Temperature $T_c$ of Excitonic Insulator State in $\text{TiSe}_2$

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### Abstract:

The Bose-Einstein condensation of electron-hole pairs produced a new state of matter known as an excitonic insulator.  $\text{TiSe}_2$  is the typical material exhibiting the excitonic insulator state among the possible candidates mentioned. The critical temperature  $T_c$  measured of  $\text{TiSe}_2$ , below which an excitonic insulator exists, is around 200K with an energy gap of 74 meV. Our theoretical study of the excitonic insulator of  $\text{TiSe}_2$  is based on the effective mass model for valence and conduction band electrons interacting via a statically screened Coulomb potential in 2D and 3D. We compute  $T_c$  as a function of the energy gap, which is assumed to be controlled by pressure, and the strength of exciton-phonon coupling by solving the linear exciton gap equation. The nonlinear exciton gap equation is employed to calculate order parameters quantitatively. We also illustrate how the change of the electron effective mass resulting from the spin-orbit coupling in electronic structure affects the  $T_c$  of excitonic instability. The calculation shows that the Coulomb interaction alone accounts for most of the measured  $T_c$ , 136K, and 208K in 2D and 3D, respectively. While the exciton-phonon coupling contributes slightly, increasing the value of  $T_c$  by 4 to 6K. Furthermore, the frequency of L1 phonon mode in  $\text{TiSe}_2$  as a temperature function is obtained from the model, and it is qualitatively consistent with experimental results.

### Keywords:

excitonic insulator,  $\text{TiSe}_2$ , critical temperature, exciton-phonon coupling, effective mass model

## Electrical and Thermoelectric Properties of Gamma-GeSe

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### Abstract:

Group-IV monochalcogenides have recently emerged as layered structures with great potential in ferroelectric and thermoelectric properties. Here, we report the experimental investigation on the electrical and thermoelectric properties of recently identified polymorphs of GeSe, gamma-GeSe. Temperature dependent electrical measurement confirms that gamma-GeSe have conductivity of approximately  $10^6$  S/m with high carrier concentration above  $10^{21}$  cm<sup>-3</sup>. The temperature-dependent Seebeck coefficient of gamma-GeSe is also experimentally measured, which is found to scale linearly with temperatures. The measured power factor at room temperature is approximately  $50 \mu\text{W/mK}^2$ .

### Keywords:

GeSe, IV-VI compounds, Group-IV monochalcogenides, thermoelectric, Seebeck coefficient

## Analysis of Photoelectrochemical (PEC) property and APXPS of Strontium Titanate Oxysulfide (STO-S)

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### Abstract:

Photoelectrochemical property of oxysulfide is of great interest for water splitting and hydrogen production applications due to its tunability of bandgap from ultraviolet to visible-light region and high reactivity for redox reaction [1,2]. Understanding the interaction between oxysulfide surface and water is essential to enhance catalytic performance. However, fundamental understanding during catalytic reactions at the interface have not been remained in its infancy yet. Ambient pressure X-ray photoemission spectroscopy (AP-XPS) is useful to investigate chemical bonding characteristics of the solid surfaces exposed with various gas environments, such as water (H<sub>2</sub>O), up to a few millibar pressure [3]. Here, we examined surface bonding characteristics of both SrTiO<sub>3</sub> (STO) and sulfur-doped SrTiO<sub>3</sub> (STO-S) in H<sub>2</sub>O gas environment using the AP-XPS. We revealed that surface oxygen states (O<sub>2</sub><sup>-</sup>) is a dominant constituent at STO-S surface when H<sub>2</sub>O gas is adsorbed on the surface. Our results suggest that the active surface states are largely enhanced in the STO-S compared to the STO and propose potential application of STO-S for the photocatalytic applications.

[1] S. Perera *et al.*, Chalcogenide perovskites – an emerging class of ionic semiconductors, *Nano Energy*. **22** (2016) 129–135.

[2] Q. Wang *et al.*, Oxysulfide photocatalyst for visible-light-driven overall water splitting, *Nat. Mater.* **18** (2019) 827–832.

[3] N. Domingo *et al.*, Water adsorption, dissociation and oxidation on SrTiO<sub>3</sub> and ferroelectric surfaces revealed by ambient pressure X-ray photoelectron spectroscopy, *Phys. Chem. Chem. Phys.* **21** (2019) 4920–4930.

### Keywords:

Strontium Titanate Oxysulfide, Photoelectrochemical property, APXPS

## Charateristics of Interlayer Excitons in $WS_2/PbI_2$ Heterostructures

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### Abstract:

2 차원 전이금속 디칼코게나이드 (transition metal dichalcogenides; TMDCs)는 상온에서도 엑시톤이 안정적으로 결합하는 특징이 있다. 특히, 서로 다른 2차원 TMDCs의 단일층끼리 접합된 heterostructure의 밴드구조가 type-II로 형성이 되었을 때, interlayer excitons (IXs)을 관측할 수 있고 IXs는 강한 Coulomb 상호작용과 긴 수명 등의 특성으로 광전자소자와 벨리트론닉스, 양자정보소자로 응용 가능하다. 본 연구에서는 2차원 TMDCs 중 하나인  $WS_2$  단일층과 2차원 반도체인 요오드화 납 ( $PbI_2$ )을 이용하여 heterostructure를 제작하였다.  $SiO_2/Si$  기판에  $PbI_2$  precursor 용액을 이용하여  $PbI_2$  nanoflakes를 성장시켰고, 그 위에 단일층의  $WS_2$ 를 박막분리 후 트랜스퍼 하였다. 극저온(3 K)에서  $WS_2$  neutral exciton과 trion에 의한 photoluminescence (PL) peak가 각각 593, 604 nm에서 관찰되었다.  $WS_2/PbI_2$  heterostructure의 이종접합 경계면에서 IXs에 의한 PL을 688 nm에서 관측하였다. 또, 온도와 레이저 세기에 따른 PL 스펙트럼을 분석하였다. Time-resolved PL 실험을 통해 IXs의 평균수명이 4.3 ns인 것을 측정하였고, 단일층  $WS_2$ 의 평균수명에 비해 긴 수명을 갖는다는 것을 확인하였다.  $WS_2/PbI_2$  heterostructure의 exciton 특성을 저온 PL 실험결과로 논의한다.

### Keywords:

Interlayer exciton,  $WS_2$ ,  $PbI_2$

## Observing phase degradation of NCM materials over cycling via Simultaneous EDS-EELS tomography.

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### Abstract:

Long life and high capacity are important conditions for good battery performance. Lithium nickel cobalt manganese oxide (NCM) is one of the most promising cathode materials, providing these crucial conditions. However, the NCM material is still susceptible to structural degradation caused by repeated charging and discharging cycles of the battery. Although such degradation can negatively affect the battery life and capacity, the mechanism of structural degradation remains largely unknown. In this research, we simultaneously combined energy dispersive x-ray spectroscopy (EDS) tomography with electron energy loss spectroscopy (EELS) tomography to measure the 3D distribution of the composition of transition metals and their oxidation states over battery cycling. Simultaneous EDS-EELS tomography allows us to obtain the 3D information regarding both elemental distribution and oxidation states while minimizing beam damage. This allows us to observe the 3D migration and phase changes of each chemical element over cycles, which will ultimately help us to understand the lithium ion battery degradation mechanism.

### Keywords:

EDS tomography, EELS tomography, Lithium transition metal oxides

## Low temperature characteristics of interlayer excitons in MAPbI<sub>3</sub>-perovskite/CdSe-ZnS-QD hybrids

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### Abstract:

페로브스카이트(perovskite)는 높은 전력변환효율과 긴 엑시톤(exciton) 수명(lifetime)과 같은 특성 때문에 다양한 광전자 소자에 응용되고 있다. CdSe 기반 무기물 양자점(quantum-dot; QD)은 크기를 변화시켜 밴드 갭을 조절할 수 있고, 양자효율이 높은 특성 때문에 첨단 디스플레이 발광 소재로 응용되고 있다. 본 연구에서는 페로브스카이트 물질 중 하나인 메틸암모늄 요오드화납(methylammonium lead iodide; MAPbI<sub>3</sub>)을 반응매 방식(anti-solvent method)을 이용하여 성장시킨 후, 기능이 부착된 셀렌화 카드뮴-황화 아연의 코어-셸 구조 양자점(functionalized CdSe-ZnS-QD)을 MAPbI<sub>3</sub>의 표면에 도포하여 이종접합(heterojunction) 하이브리드 시스템을 제작하였다. 상온에서 3 K까지의 광범위한 온도 영역에서 광발광(photoluminescence; PL) 스펙트럼을 고해상도 레이저 공초점 현미경(laser confocal microscope; LCM)을 이용하여 측정, 분석하였다. 저온(160 K 이하)에서의 LCM PL 스펙트럼을 분석한 결과, CdSe-ZnS-QD은 약 1.97 eV, MAPbI<sub>3</sub>는 1.66 eV와 1.60 eV에서 엑시톤(exciton) 특성 peak을 관찰하였다. 두 물질의 계면에서는 각각의 엑시톤보다 에너지가 낮은 약 1.38 eV에서 층간 엑시톤(interlayer-exciton; IX)에 의한 peak을 관찰하였다. IX의 특성을 확인하기 위하여 온도 및 여기(excitation) 레이저의 세기에 대한 의존성과 시분해 광발광(time-resolved PL; tr-PL) 스펙트럼을 측정, 분석하였다. 온도변화에 따른 각 엑시톤들의 PL peak 위치는 red 변위와 blue 변위의 다른 특성이 관찰되었다. IX은 여기 레이저의 세기가 증가할수록 에너지의 크기가 증가하였고(약 1.38 eV에서 1.40 eV), 평균 엑시톤 lifetime은 IX가 약 4.91  $\mu$ s로 CdSe-ZnS QD가 약 0.70 ns로 MAPbI<sub>3</sub>가 약 18.5 ns로 측정되어서 IX의 수명이 긴 것으로 확인하였다.

### Keywords:

interlayer exciton, photoluminescence, perovskite, quantum dot

## 개방형 공초점 공동을 활용한 전기적 패브리-페롯 간섭계

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### Abstract:

공초점 공동(Confocal cavity)은 광학계에서 안정적이면서 높은 큐 공진기를 만들기 위해 사용된다. 이 연구에서는 2차원 전자계 소자로 전자를 이용한 공초점 공동을 구현하였다. 전기 전도도 실험을 통해 공초점 공동내에서의 패브리-페로 간섭을 측정하였고, 이 간섭효과가 열린 전자계에서 이뤄짐을 확인하였다. 또한 전기적 퍼텐셜을 인가함으로써 전자들의 파장이 세밀하게 조절하는 것을 관측했으며, KWANT를 이용한 컴퓨터 시뮬레이션에서도 이러한 현상이 재현됨을 확인하였다. 전자계에 수직방향으로 자기장을 걸어줄 경우 간섭무늬가 사라짐을 보았는데, 이는 전자들이 공동을 빠져나가는데 파동함수의 공간적인 분포가 영향을 미치는 것으로 예상된다.

### Keywords:

패브리-페롯 간섭계, GaAs/AlGaAs, 양자점, 공동모드

## Coexistence of Surface 2DEG and Topologically Protected Surface states in Topological Insulator Nanowire

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### Abstract:

Topological insulators (TIs) are materials with an insulating bulk gap and gapless surface state, indicating that electrons can only transport along the surface of the materials. For instance, TIs have symmetry-protected Dirac fermions at the surface, so-called the topologically protected surface state (TSS). Because of the surface band-bending effect for highly doped TIs, it has been known that two-dimensional electron gas (2DEG) can coexist with the TSS. In this study, we observed beating patterns in the Aharonov-Bohm (AB) oscillations for Sb-doped Bi<sub>2</sub>Se<sub>3</sub> TI nanowires under varying magnetic fields. We propose that it is due to the coexisted states (TSS and 2DEG).

### Keywords:

Topological insulators, Aharonov-Bohm oscillation, topologically protected surface state

## Blue-Shift of Oxygen-Hydrogen Stretching Mode in Nano Films of Glycerol Bounded by Interfaces

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### Abstract:

Growth of films on a liquid substrate has been adapted in a number of applications taking advantage of a unique functionality due to interactions with liquid interface in the initial stage of the film growth. Nevertheless, fundamental understanding of the structural and chemical reactions which may occur during the formation of the solid-on-liquid interface has not been well established. In this study, we discuss molecular configuration of thin glycerol films utilizing Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy. The glycerol films are spin-casted on silicon dioxide substrates, followed by vapor deposition of thin Parylene-C films. In case of pure Parylene-C films, with no hint of oxygen related absorption peak, characteristic peaks associated with aromaticity in the polymer chains are found at  $\sim 3000$ ,  $1500$ , and  $1050\text{ cm}^{-1}$  corresponding aromatic CH, C-C stretching and Cl mode, respectively. Infrared absorptions for OH stretch mode at  $3290\text{ cm}^{-1}$  followed by double peak corresponding CH stretch mode are observed when a drop of glycerol is placed on the ATR crystal (bulk glycerol). When glycerol a thickness of  $\sim 30\text{ nm}$  is spread onto  $\text{SiO}_2$  surface, the OH stretch mode shifts to a higher wave number to  $3332\text{ cm}^{-1}$ , while the position of CH stretch mode remains the same. The OH stretch peak is further blue-shifted to  $3369\text{ cm}^{-1}$  when the glycerol film is bounded by a thin Parylene-C film. Shift of OH stretch mode in water molecules adsorbed on silicon ( $\text{SiO}_2$ ) interface is known to occur in decreasing wavenumbers. The red-shift which has been commonly interpreted due to the formation of more ordered bonding network in the vicinity of the water/ $\text{SiO}_2$  interface is just opposite to what we have observed in glycerol/ $\text{SiO}_2$  and Parylene-C/glycerol/ $\text{SiO}_2$  interfaces.

### Keywords:

FTIR, Blue-Shift, OH Stretching

## Cryogenic voltage sampling for a $10^6$ Hz signal propagating in a 2DEG channel

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### Abstract:

Recently, with the increase of interest in quantum information, various quantum technologies for quantum devices such as solid-state qubits have been developed. One of performance indices in quantum operation is the operation speed that is normally demanded in a range of  $10^6$ - $10^9$  Hz. In this high-speed operation region, the waveform of input signals could be deformed while being transmitted in quantum devices, operated at low temperatures. To guarantee such high-speed operation, it is important to check if the high-speed signal maintains the initial waveform. However, it is hard to use a commercial oscilloscope to directly detect the waveform travelling in a device located at a low temperature. Here, we demonstrate a cryogenic voltage sampling by using a Schottky barrier gate on a surface of two-dimensional-electron-gas (2DEG) channel based on GaAs/AlGaAs heterostructure to investigate deformation of waveform in a frequency range of  $10^6$ - $10^7$  Hz. The voltage sampling was conducted by applying a pulse wave to the Schottky gate, which allows a partial transmission of the test signal only in the gate pulse region in a time domain. Then, we measured a current as a function of a delay time,  $I(t_d)$ , between the pulse and test signals.  $I(t_d)$  corresponds to the waveform of test signal at the Schottky gate location after travelling from the incident point. Finally, we confirmed that a signal of  $10^6$  Hz range keeps the initial waveform, which travels through a one mm long 2DEG channel.

### Keywords:

Cryogenic voltage sampling, GaAs/AlGaAs, 2DEG, Schottky-barrier gate

## Studies on the response of NEOS-II Detector

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### Abstract:

The NEOS searches for sterile neutrinos by detecting reactor antineutrinos at a very short baseline in Korea. The NEOS detectors (1-ton GdLS) were deployed at the tendon gallery of the Hanbit reactor unit 5 (2.8 GW thermal power), 24 m away from the reactor core. In NEOS-I, the prompt energy spectrum from inverse-beta-decay was measured using 180 live-days of reactor-on data, which clearly showed the "5 MeV excess". To understand the "reactor antineutrino anomaly" and the origin of the "5 MeV excess", NEOS-II has recorded 388 (112) live-days of reactor-on(-off) data from September 2018 to October 2020, covering a whole burnup cycle of the reactor. In this work, we report studies on the response of the NEOS-II detector, results of event reconstruction, and related corrections, e.g., for the change of the detector characteristics with time. A simulation was developed and compared with the data energy spectra of beta and gamma events, validating how simulation fits data well.

### Keywords:

Reactor Neutrino Experiment, Liquid Scintillator, Geant 4 Simulation, Calorimeter, Inverse-beta-decay

## Lowering the energy threshold to 0.5 keV in NaI(Tl) scintillation detectors using SiPMs

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### **Abstract:**

NaI(Tl) scintillation detectors with photomultiplier tubes (PMTs) are widely used for radiation measurements. Instead of PMT, a silicon photomultiplier (SiPM) that has lately developed can be used, with advantages such as low bias voltage, compact volume, improved radiopurity, high gain and cost effectiveness.

In this poster, we will show the result of SiPM characterization at various low-temperature points and describe ongoing analysis work that can lower the energy threshold to 0.5 keV with simple variables.

### **Keywords:**

Dark Matter, SiPM, Particle Experiment, Detector

## The status of AMoRE-II background simulation.

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### Abstract:

The Advanced Mo-based Rare process Experiment (AMoRE) is an underground experiment searching for the neutrinoless double beta decay of  $^{100}\text{Mo}$  isotopes using  $^{100}\text{Mo}$ -enriched-crystal-contained cryogenic detectors. We are preparing the next phase experiment, AMoRE-II, at the Yemi underground Laboratory (Yemilab) located at the Handuk mine in Yemi mountain. In order to reach the background goal of  $10^{-4}$  events/keV/kg/year, various shield materials will be installed. To estimate the background conditions in the AMoRE-II, we performed simulations with the GEANT4 Toolkit. We simulated the background from external shield materials and materials in the nearby detector systems. Details of the various background simulations and estimated background levels in the region of interest (ROI) will be presented.

### Keywords:

Underground experiment, Geant4 simulation, AMoRE, double beta decay

## Performances of R&D crystal detectors for AMoRE-II at IBS HQ

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### Abstract:

The Advanced Mo-based Rare process Experiment (AMoRE) is an international experiment searching for the neutrinoless double-beta decay of  $^{100}\text{Mo}$  using molybdenum-based crystals with a cryogenic sensor. The AMoRE is considering lithium molybdate crystals for its phase-II experiment. We have tested the lithium molybdate crystal detector with various conditions such as individual detector mass and surface treatment. The new results of the detector test will be presented in the poster.

### Keywords:

AMoRE experiment, neutrinoless double beta decay, MMC

## Study on Hue-wavelength Relationship Using Digital Photo Image for Liquid Scintillator

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### Abstract:

이 포스터는 LED source를 사용하여 색조-파장(Hue-wavelength)의 관계에 대해 연구하고 이를 형광이미지 분석에 적용할 수 있는 가능성을 제시하였다. 색조-파장 관계를 통해 Liquid Scintillator 샘플에 용해된 flour 성분의 스펙트럼을 추정하기 위해 색상 공간에 디지털 사진 이미지 분석을 도입했다. 컬러 이미지 재구성과 디코딩에는 Bayer color filter array CFA) 와 demosaicing 을 적용한 Complementary Metal Oxide Semiconductor(CMOS) 이미지 센서를 활용했다. 샘플의 사진 이미지는 CMOS 센서 CFA 기반의 디지털 카메라로 촬영되었다. 색조와 파장은 밀접하게 관련이 있다. 현재까지 특별히 파란색 또는 UV 영역에 가까운 H-W 관계 측정에 대한 문헌 보고서는 전혀 없다. UV 영역에 가까운 H-W를 연구한 목적은 연구에 사용하는 photomultiplier tube(PMT)의 최대 양자 효율성(QE)가 약 430nm이기 때문이다. PMT 기반 실험에서 이러한 영역대의 파장 재현을 잘 이해하는 것이 필요하다. H-W 관계를 알고 나면 이미지를 분석하여 dominant wavelength를 확인할 수 있다. CMOS Bayer CFA 접근법은 값비싼 분광광도계를 사용하지 않고도 LS 샘플의 flours 스펙트럼을 추정할 수 있다.

### Keywords:

Hue, wavelength, photo image, PMT, Liquid scintillator

## Estimating various uncertainties in the Hue-Wavelength relationship using a CMOS sensor with CFA-based digital images

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### Abstract:

LS(Liquid Scintillator)는 pseudocumene, LAB등의 유기 solvent를 기반으로 만들어진 액체에 p-terphenyl, PBD, PPO, POPOP등의 형광물질을 섞어서 만들어진다. 입자가속기 내부에서 LS와 입자가 부딪혀 scintillation이 일어난다. 이때 LS에서 방출된 빛은 PMT를 통해 검출되는데 PMT마다 최대의 양자효율(QE)을 가지는 파장이 존재한다. LS에서 빛의 파장을 변환하기 위해 LS에 적절한 형광물질과 wavelength shifter가 요구된다. 기존에는 이러한 LS의 특성을 실험하기 위해 spectrometer를 사용했으나 비용적인 부담이 커서 비용절감 차원에서 LS를 CMOS 센서 기반의 카메라로 촬영해 색상을 분석해 파장을 확인하려 한다. 이 포스터에서는 색상과 파장간의 관계식을 분석하고 노출시간, 거리등에 따른 불확실성에 대해 조사해 보았다.

### Keywords:

Liquid Scintillator, Hue, Wavelength, CMOS, digital image

## Radioactivity levels in lead shields for experiments of rare process events

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### Abstract:

Experiments searching for rare process events such as neutrino-less double beta ( $0\nu\beta\beta$ ) decay and dark matter interaction require low radioactive background environment. AMoRE-II (Advanced Mo-based Rare process Experiment II) is an experiment investigating the  $0\nu\beta\beta$  decay of  $^{100}\text{Mo}$  with a Q-value 3034 keV. The experimental setup is under construction at a new underground laboratory, Yemilab, which has 1000 m overburden. Lead is the most popular materials to shield gamma rays from the external environment, such as rocks in the cave. However, the radioactivity of the lead is difficult to measure, because of the screen effect by its high effective Z number. Especially, the high energy gamma emitted from  $^{214}\text{Bi}$ , such as 3054 keV with gamma intensity 0.0209 %, can cause critical signals on the 3034 keV region and be merged with 3034 keV signals. Even more, high level of  $^{210}\text{Bi}$  (corresponds to  $^{210}\text{Pb}$ ) in the lead generate high level of bremsstrahlung up to 1162 keV and it makes trouble not only for low energy study, but also for the ROI by coincidence event. We measured the activity levels in several lead candidates for AMoRE-II setup obtained from various suppliers using an array of fourteen HPGe detectors named CAGE.

### Keywords:

Lead shield, Radioactivity, HPGe detector, Neutrinoless double beta decay, Dark matter

## **R & D of water Cherenkov detector as a muon veto detector for AMoRE-II.**

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### **Abstract:**

The water Cherenkov detector is one of the muon veto detectors for the AMoRE-II experiment. We have developed a prototype water Cherenkov detector. Different tests have been conducted to check its performance; this includes the light yield test, the use of 4-MU as wavelength shifter (WLS) material, and its stability in water with time. We present the design and results of the performed tests.

### **Keywords:**

AMoRE-II, Cherenkov, 4-MU

## AMoRE-I multiple hit study

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### Abstract:

AMoRE(Advanced Mo-based Rare process Experiment) is an experiment to search neutrinoless double beta (0vbb) decay of  $^{100}\text{Mo}$ . AMoRE-I detector has been composed of thirteen  $\text{Ca}^{100}\text{MoO}_4$  crystals and five  $\text{Li}_2^{100}\text{MoO}_4$  crystals(a total  $\sim 3$  kg of  $^{100}\text{Mo}$ ) within an assembly of four towers. This structure is proper to understand the background contribution by multiple events to searching for the 0n bb decay of  $^{100}\text{Mo}$ , even for an individual study about the excited states of the 2nbb decay of  $^{100}\text{Mo}$  through the measuring of the multiple gamma-rays and beta particles simultaneously. Moreover, the excited state study can provide experimental data which can be used to test and calibrate theoretical models needed to calculate 0nbb Nuclear Matrix Elements(NME), which have significant uncertainty depending on the theoretical models.

Here, I present the simulation and analysis study progress about the 2nbb excited state decay using the AMoRE-I detector.

### Keywords:

double beta decay, Multiple hit,  $^{100}\text{Mo}$ , AMoRE, Simulation

## Status of plastic scintillator detector development for AMoRE-II muon veto system

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### Abstract:

The AMoRE experiment is a neutrinoless double-beta decay search of CUP, IBS, using  $^{100}\text{Mo}$ , and AMoRE-II, 2nd phase of this experiment, will begin soon. This experiment is aiming to reach zero-background, and one of the ways is cosmic ray background rejection. For this reason, it is planned that the muon veto detector system for AMoRE-II will be operating in Yemi-Lab, and their development is ongoing now.

The muon veto system is divided into 2 types, which are a Plastic Scintillator for the 1st floor, and a Water Cherenkov detector for the 2nd floor. For the plastic scintillator part, we will install about 130 plastic scintillator detector boxes outside of the 1st-floor wall, and the mass production of these detector boxes was finished recently. In this poster, the status of plastic scintillator detector development so far will be presented.

### Keywords:

AMoRE-II, AMoRE, Muon Veto detector, Plastic scintillator

## Application of photopolymerized tissue equivalent plastic scintillator for use as a dosimeter in radiotherapy

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### Abstract:

최근 기존 선량률보다 매우 높은 선량률로 방사선치료를 하였을 경우 암환자의 치료효과가 개선되었다는 연구가 보고되었다. 하지만 기존에 표준으로 사용 중인 선량 측정 장비 ion chamber는 선량률이 너무 높은 경우 측정 한계를 초과하기 때문에 고선량률 방사선 선량 측정에 문제가 있다. 본 연구에서는 고선량률 방사선치료 선량계로서 조직등가 플라스틱 섬광체를 개발하고 방사선치료 선량계로서의 가능성을 확인하고자 하였다. PMMA를 플라스틱 베이스로 하고 유기 섬광체로 PPO 0.2 wt%와 파장이동체로 POPOP 0.01 wt%로 하였으며 인체와 유효원자번호( $Z_{\text{eff}}=7.42$ )를 유사하게 하기 위하여 triphenylantimony를 0.12 wt% 첨가한 후 광계시제로 Irgacure 819를 0.2 wt% 첨가하여 광중합법으로 조직등가 플라스틱섬광체를 개발하였다. 제작된 직경 5mm, 길이 2cm의 PMMA 플라스틱섬광체를 광케이블에 광학적 결합 및 광차폐한 후 광전자증배관과 결합하여 플라스틱 센서를 제작하였다. 개발된 조직등가 플라스틱 섬광체는 CLINAX IX 의료용 선형가속기에 대하여 ion chamber와 교차검증을 통하여 방사선치료용 선량계로서의 가능성을 확인하였다.

### Keywords:

Plastic scintillators , photopolymerization , tissue-equivalent , dosimetry

## R&D of the NaI(Tl) crystal encapsulation for the NEON experiment

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### Abstract:

NEON (Neutrino Elastic-scattering Observation with NaI) aims an observation of a coherent elastic neutrino-nucleus scattering (CEvNS) using reactor anti-electron neutrino with NaI(Tl) crystal detectors at Hanbit nuclear power plant in Yeonggwang. The NaI(Tl) crystal should be encapsulated by copper shielding for blocking moisture because the crystal is hygroscopic. The NEON experiment uses the liquid scintillator(LS) to select multiple tagging events to veto background events. However, noise is generated when NaI(Tl) detector is installed in LS. Noise is distributed at high energy as well as low energy, hard to discriminate signal events, and degree of vulnerability to noise generation depends on encapsulation design. So we tested and developed an encapsulation design to prevent noise generation. In this poster, encapsulation design, noise generation ,and how to upgrade encapsulation will be introduced.

### Keywords:

Neutrino, NEON, NaI(Tl), noise, Encapsulation

## Report of the neutral particle identification for searching a weakly interacting dark matter

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### Abstract:

We have studied about a dark matter, especially Weakly Interaction Massive Particle (WIMP) that is one of the most probable non-baryonic dark matter, using a direct detection method for several decades. In direct detection method, a Pulse Shape Discrimination (PSD) method is one of the major technology to identify the WIMP dark matter. The PSD methods were introduced and developed in several ways from 1960's.

Here, we report a progress about our study to discriminate the neutral particles with pulse shape induced through the elastic scattering between target and incident particles.

### Keywords:

dark matter, PSD, WIMP

## Implementation of magnetic monopole physics in GEANT4 and simulation results

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### Abstract:

Korea Experiment on Magnetic Monopole (KAEM) searches for elementary magnetic monopoles, which have been a question of electromagnetism for the last 150 years. People have searched for monopoles in the large mass, large magnetic charge region during the long period, but without success. Therefore, we assume that monopoles may exist in a region smaller than the mass and charge of electrons and designed an experiment for monopoles.

In GEANT4, we perform simulations for these monopoles and implement new physics and particles. This presentation will show how to configure monopole physics on GEANT4 and show the result of simple simulation by applying it.

### Keywords:

Magnetic monopole, GEANT4

## Performance of the Dilution Refrigerator System for AMoRE-II

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### Abstract:

The AMoRE experiment aims to search for the neutrinoless double beta decay of  $^{100}\text{Mo}$  using cryogenic calorimeters operating at 10 mK. The experiment requires an extensive refrigerator system to cool a detector assembly with a mass load of about 4 tons, including an inner Pb-Cu shield and the crystal detector modules. We report the performance of the dilution refrigerator designed for AMoRE-II. The refrigerator system is now installed at the IBS Center for Underground Physics headquarter lab. We made a successful cooling test that reached the mixing chamber temperature as low as 5.2 mK. We discuss the measured values of the base temperature and the cooling power of the dilution refrigerator with the performance required for the experiment. Moreover, we discuss the precooling method of using liquid nitrogen to expand it for the realistic load to the system when installed at Yemilab.

### Keywords:

Neutrinoless double beta decay, Dilution refrigerator

## Neutrino event reconstruction in Korean Neutrino Observatory (KNO) detector

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### Abstract:

The KNO project has been proposed as a next-generation water Cherenkov neutrino detector. We expect to make important discoveries such as CP violation, proton decays as well as observe neutrinos from supernovae. In order to understand the detector performance, we are developing a neutrino event reconstruction tool that simultaneously reconstructs event parameters, such as vertex and direction. In this presentation, we introduce the current status of the neutrino event reconstruction tool and plan to improve it.

### Keywords:

Korean Neutrino Observatory, KNO, Neutrino, Cherenkov, Simulation

## Geant4 simulation of 3-gamma annihilation of positronium for KAPAE detector

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### Abstract:

In particle physics, the search for positronium rare decays in 3- $\gamma$  annihilation such as milli-charged particle, mirror world, new light X-boson and extra dimensions can be performed by the KNU Advanced Positronium Annihilation Experiment (KAPAE). The ground state of positronium (Ps) has two possible configurations based on the relative spin orientations, the triplet state ( $^3S_1$ ), ortho positronium (o-Ps), and the single state ( $^1S_0$ ), para positronium (p-Ps). Due to C-parity conservation, p-Ps and o-Ps decay to even and odd numbers of gammas, respectively. In this study, the pure quantum electrodynamics (QED) of Ps annihilation is considered and the 3-gamma annihilation is simulated for the KAPAE by utilizing the Geant4 simulation toolkit. We report our simulation results and discuss the angular distribution of 3- $\gamma$  annihilation.

### Keywords:

positronium, Geant4, simulation, annihilation

## Study of cosmic-ray muon trajectories with plastic scintillator panels and silicon photomultipliers

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### Abstract:

Atmospheric muons are useful to measure their fundamental properties such as the flux and lifetime. We have constructed a scintillation panel detector using polystyrene-based extruded plastics. The detector is read out by 56 optical fibers coupled with 28 silicon photomultipliers. Main goal of the prototype is to identify muon's entry positions and therefore eventually its directions. We find that our experimental setup has ability to measure the cosmic-ray muon's trajectory.

### Keywords:

Cosmic muon, silicon photomultiplier

## Reconstruction Tool for Low Energy Neutrino Event at KNO

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### Abstract:

The KNO (Korean Neutrino Observatory) project has been proposed as a next-generation neutrino experiment that will lead out neutrino physics. Detecting low energy neutrino signals is important to clarify physics of sun, galactic center, supernovae collapse, and many others. The KNO software group has been developing a reconstruction tool for low energy neutrino. In this presentation, we report the status of the reconstruction tool development and the future plan.

### Keywords:

KNO, Water Cherenkov Detector, Reconstruction Tool

## Search for Pauli Exclusion Principle violation in an NaI(Tl) crystal

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### Abstract:

The Pauli exclusion principle (PEP) is the very basis of quantum mechanics for explaining states of fermions.

However, the correctness of PEP in an atom has not been widely and directly tested in an experiment. NaI(Tl) crystals in the COSINE-100 dark matter experiment have a large number of iodine nuclei that can be used to search for X-rays produced when anomalous electronic transitions happen.

Using the crystal background data spectrum, we fit for a process of the PEP violation where three electrons with a pair of the same spins exist in a K-shell of the nuclei.

We report the status of the analysis in this conference.

### Keywords:

COSINE-100, Pauli exclusion principle, NaI crystal

## Alpha signal modeling for the NaI(Tl) crystals in COSINE-100

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### Abstract:

COSINE-100 is a dark matter search experiment based on low background NaI(Tl) crystals, the same target material as DAMA collaboration experiments. Alpha signals are easily distinguished from gamma/beta signals because the attenuation length of alpha particles is relatively short within the detectors. From the alpha energy modeling, we can get the strict constraint of radioactive contaminants of the crystals. In this poster, we will elucidate the process of the alpha analysis and compare the quantity of the radioactive contaminants from this analysis with existing results.

### Keywords:

alpha, simulation, COSINE-100

## 3 MeV, 350 MHz RFQ 설계 비교 연구

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### Abstract:

100 MeV 양성자가속기에 사용되는 3 MeV Radio-frequency Quadrupole (RFQ) 은 2005년에 개발을 완료하여 운영중에 있으며, 현재 노후와에 따른 성능개선을 고려하고 있다. 3 MeV RFQ는 350 MHz의 운전주파수를 가지며, 4 배인 구조이다. 총 길이는 3.2 m로 개발 당시 진공 브레이징 접합이 가능한 80 cm 길이로 이루어진 섹션 4개로 구성되어 있다. 장 분포 안정화를 위한 방법으로 dipole mode separation을 위한 dipole rod와 quadrupole mode 안정화를 위한 resonant coupling 구조를 갖고 있는 것이 특징이다. 성능개선을 위하여 번처 에너지, 운전 빔 전류 등 주요 설계 변수에 따른 비교 연구를 수행하였다. 본 연구에서는 RFQ 운전 현황과 성능개선을 위한 설계 비교 연구에 대해서 논한다.

\* 본 연구는 과학기술정보통신부 연구비 지원을 받았음.

### Keywords:

양성자가속기, Radio-frequency Quadrupole

## Development of Artificial Neural Network Model for the Low Energy Beam Tuning in the KOMAC Proton Injector

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### Abstract:

A proton injector system produces a high-current and low-energy proton beam and makes beam parameters - such as beam centroid, and beam emittance - matched to a subsequent accelerator such as the radio-frequency quadrupole (RFQ). Beam parameters are generally unpredictable and time-varying, so beam tuning is often required to improve beam transport. Artificial neural network (ANN) is effectively utilized for nonlinear regression of the low energy beam tuning problems in the KOMAC proton injector. The ANN-based prediction model is created based on numerous datasets from beam dynamics simulations, according to various initial beam conditions and magnet control. This study presents the ANN model and application results for controlling the proton injector.

### Keywords:

Proton injector, Low energy beam tuning, Artificial Neural Network (ANN), Prediction model, Beam dynamics simulation

## Formation characteristics of magnetized Plasma Dipole Oscillation

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### Abstract:

Plasma dipole oscillation (PDO) is produced because of the wave breaking generated by two detuned lasers. The magnetic field advances the wave-breaking time, causing the breaking thresholds to decrease. The force balance model parameterized by pulse shape is used to derive dipole fields, which is not a major variation from the non-magnetized PDO. The circulation of Lorentz force, on the other hand, highlights the mode transition. When the magnetic field is increased to suppress the longitudinal electric field, the oscillating modes of charged particles are split into the X-mode cutoff, right circular mode (R), and left circular mode (L). A circulating single particle clump formed of X-mode emits electromagnetic radiations with the same spectra.

### Keywords:

Plasma dipole oscillation (PDO), wave-breaking, magnetic field

## Beam Error Analysis and Orbit Correction Simulation Studies at KOMAC

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### Abstract:

100 MeV proton linac at Korea Multipurpose Accelerator Complex (KOMAC) has been operated and provided beam services to users from basic sciences, bio-medical and semiconductors. To transport the beam without any beam loss through the linac at KOMAC, we have carried out the orbit correction studies on the distorted beam based on the transverse misalignment simulations. There are various sources of transverse misalignment. Here, transverse displacement error of the machine will be looked closely. In the work, we will show the simulation results of the beam dynamics of the error analysis and the corresponding orbit correction. And the future plans on the orbit correction in the real system will be present.

### Acknowledgement

This work has been supported through KOMAC (Korea Multi-purpose Accelerator Complex) operation fund of KAERI by MSIT (Ministry of Science and ICT).

### Keywords:

error analysis, orbit correction

## Drift tube linac의 빔집속을 위한 영구자석 기반 사극전자석 설계

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### Abstract:

한국원자력연구원에서 운영 중인 100 MeV 양성자가속기의 초기 20 MeV 구간은 3 MeV RFQ(Radio-Frequency Quadrupole)과 4 대의 DTL(Drift tube linac) 탱크로 구성되어 있으며, DTL 탱크 내부에는 빔 집속을 위한 사극전자석을 포함하는 150 여개의 드리프트 튜브가 설치되어 있다. 현재 운영 중인 20 MeV 드리프트 튜브용 사극전자석은 변압기 권선용 코일을 사용한 전자석을 사용하므로 운전 상황에 따라 전자석의 세기를 조절할 수 있다란 장점을 지니나, 장기간 운전에 따른 노후화로 인해 전자석의 파손으로 사용이 불가할 경우, 이의 유지 보수에 상당한 시간과 노력이 필요하다란 단점이 있다. 사극자석을 영구자석 기반으로 변경할 경우, 전자석 전원이 불필요하며 수명이 반영구적이므로 유지 보수가 간편해진다. 본 연구에서는 방사선에서 안정적인 SmCo 계열의 영구자석을 기반으로 20 MeV DTL의 설계값인 1.75 T의 적분자장을 가지는 사극자석 설계에 대해 발표한다.

본 연구는 과학기술정보통신부 연구비 지원을 받았음.

### Keywords:

DTL, Quadrupole, Magnet, KOMAC

## High-Order Harmonic Generation with Two-Color Laser Field for Warm Dense Matter Research

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### Abstract:

In the femtosecond Ti:Sapphire laser system with 800 nm wavelength, high-harmonic generation (HHG) can only generate odd harmonics for 1.55 eV. The interval between two adjacent is 3.1 eV. In order to narrow the spectral interval of HHG, even-order harmonics are also required. Using a beta barium borate (BBO) crystal installed before the HHG system, the second-harmonic laser field (400 nm wavelength) is produced with 90 degree rotated polarization of fundamental laser field. Even-order harmonics can be observed when the two-color laser field consisting of the fundamental and the second-harmonic fields passes through the HHG system. The characteristics of full integer-order harmonics with the interval of 1.55 eV will be presented.

This work was supported by Institute of Basic Science (IBS-R012-D1) and National Research Foundation of Korea (NRF-2019R1A2C2002864) of Korea.

### Keywords:

warm dense matter, high harmonic generation

## Electronic Structures and Atomic Bonding of the Warm Dense Carbon Plasma

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### Abstract:

A carbon under the high temperature and density condition, which is called as warm dense matter, is generated by exposing few tens of nm thick amorphous carbon (aC) and diamond sample with an intense ultrashort laser pulse. The electronic and atomic bonding structures of warm dense carbon (WDC) is measured with time-resolved x-ray absorption spectroscopy station constructed in the 150 TW area of CoReLS. A Ta laser-plasma, which produces broadband x-ray in the range of 250 – 500 eV, is used for x-ray source and it is resolved by the grazing incidence flat-field soft x-ray spectrometer, which has high resolution of 0.5 eV around carbon K-edge. Under the ambient condition, aC is composed with the mixture of *sp*<sup>3</sup> and *sp*<sup>2</sup> hybridization and diamond is dominantly composed with *sp*<sup>3</sup> hybridization. After the exposing of intense laser pulse, portion of *sp*<sup>1</sup> and/or *sp*<sup>2</sup> hybridization increases instantly in both carbon samples. The detailed temperature and pressure condition deduced by 1D hydrodynamic calculation with MULTI-fs will be presented.

This work was supported by Institute of Basic Science (IBS-R012-D1) and National Research Foundation of Korea (NRF-2019R1A2C2002864).

### Keywords:

warm dense matter, laser-plasma x-ray source, time-resolved x-ray absorption spectroscopy

## Development of ISOL Control System for the Production and Transportation of Rare Isotopes

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### Abstract:

Rare Isotope Science Project (RISP) at Institute for Basic Science (IBS) is carried to construct a Rare Isotope (RI) production facility dedicated to the production of neutron-rich radioactive nuclei. Isotope Separation On-Line (ISOL) is a large research complex system including a proton driver, target ion source, mass separators, beam transport system, diagnostic, and data acquisition equipment with the highest levels of safety.

Although safety and ISOL control system closely interact, they are usually implemented as independent subsystems because of different requirements. Therefore, both systems are managed by dedicated control devices.

The ISOL facility adopted Experimental Physics and Industrial Control Systems (EPICS) as general frame for the control system. It has to integrate into a common frame work from the control of different subsystems by providing a unique model of graphic user interface and a common set of utilities for data archiving and analysis.

Some of local control systems (LCS) such as EBIS, RFQCB, CLS, MMS, and Cyclotron can have their own supervisor for diagnostic purpose or even for routine operation. They will make their data available to the higher level supervisor to allow a coherent analysis of all parameters relevant for the overall facility operation.

In this presentation, we present the status of the ISOL Control System and overall architecture/hardware platform foreseen for an effective solution for exchanging data among control devices.

### Keywords:

Isotope Separation On-Line (ISOL), Control Program, PLC and EPICS, Rare Isotope (RI)

# High laser intensity, THz emission from plasma dipole oscillations by tunneling ionization effect in neutral gas

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## Abstract:

In this presentation, we introduce about the method of high THz generation emission of radiation. Traditionally, in plasma physics through laser-plasma interaction, several types of radiation sources have been studied. Such as radiation source base on solid-state medium. But unlike other methods this mechanism readily obtain the THz emission of radiation. Assume that ions are fixed, two high intensity of ultrashort laser pulse are colliding in plasma. the beat wave of slightly detuning by Ponderomotive force are trapped electrons. Trapped electrons are produced moving potential train. The trapped electrons produced a moving potential train, which oscillates like an electric dipole. which mechanism is called plasma dipole oscillation(PDO) [1]. In general, most PDO use only the plasma. However, this presentation introduces PDO using neutral gas. Through PIC simulation of our group, it was confirmed through 2D-simulation that stronger terahertz radiation was emitted by tunneling ionization effect in neutral gas than the PDO that generated terahertz radiation in plasma.

## Reference

[1] Kwon, K. B., Kang, T., Song, H. S., Kim, Y. K., Ersfeld, B., Jaroszynski, D. A., & Hur, M. S. (2018). High-energy, short-duration bursts of coherent terahertz radiation from an embedded plasma dipole. *Scientific reports*, 8(1), 1-9.

## Keywords:

THz emission of radiation generate, laser-plasma interaction , field-ionization

## Enhanced THz radiation from nanoplasma by oblique-collision of two-laser pulses

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### Abstract:

Terahertz (THz) imaging and sensing has identified its potential in biomedical research, security applications, and other fields. With these needs, the development of highly-efficient compact THz sources has been one of the focal points in THz research. A two-dimensional (2D) particle-in-cell (PIC) simulations analysis of beat-frequency radiation (lies in THz range) by oblique-collision of two-detuned laser pulses with a nanoplasma sheet is presented. It is generated due to the strong plasma current produced by the ponderomotive force (due to the beating of both laser pulses) near the colliding point, which is emitted into the vacuum from the front and back surfaces of the plasma sheet and is well synchronized with the driving laser pulses. The laser-to-THz energy conversion efficiency is significantly improved in a two-detuned laser pulse system, and a narrowband beat-frequency spectrum is also obtained compared to a single laser pulse system (providing a broadband frequency spectrum).

### Keywords:

Laser, THz, Nano-plasma-based structure, PIC simulation

## Raman amplification in plasma created by ionizing pulse

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### Abstract:

Energy loss of pump pulse is inevitable before delivering energy to the seed pulse as the pump pulse passes through the plasma field during the Raman amplification. This study implements Raman backscattering with the plasma generated from the gas by seed pulse to reduce the energy loss [1]. Hydrogen gas is loaded with picosecond pump pulse and femtosecond seed pulse using cplPIC particle-in-cell code. As a result, plasma creation by ionizing pulse is more effective on the growth rate of seed pulse than loading plasma directly. Therefore, this method reduces the energy loss of the Raman amplification.

### Reference

[1] A. A. Balakin, G. M. Fraiman, D. S. Levin, and S. A. Skobelev, Phys. Plasmas **27** 053106 (2020)

### Keywords:

RAMAN BACKSCATTER

## Development of smoothed particle hydrodynamics code for inverse bremsstrahlung absorption of laser energy in plasma

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### Abstract:

In the interaction between collisionless coronal plasma and high intensity laser beam, the laser energy is deposited to the plasma via inverse bremsstrahlung absorption. This phenomenon occurs in the underdense plasma, i.e. plasma with electron density lower than the critical density determined by the laser frequency. Here, we present our progress in developing a smoothed particle hydrodynamics (SPH) code intended for simulating aforementioned inverse bremsstrahlung absorption in laser-plasma interactions. Electron-ion collision frequency, which not only governs heat transfer and electron-ion heat exchange but also the laser energy absorption coefficient, is calculated by interpolating the values from classical plasma model and electron-phonon model. To our knowledge, this is the first SPH-based code to model high intensity laser-plasma interaction without relying on prescribed heat transfer coefficients.

### Keywords:

smoothed particle hydrodynamics, inverse bremsstrahlung absorption, laser plasma interaction

## Study on the erosion rate with solid metallic cathode of MEVVA ion source

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### Abstract:

금속 증기 진공 아크 (Metal Vapor Vacuum Arc, MEVVA) 이온원은 진공아크 방전을 이용하여 금속 플라즈마를 발생시키고, 금속 이온빔을 인출하는 금속 이온원이다. 이온원 내부에서 발생하는 진공 아크 방전은 높은 전류밀도 특성을 가지며, 따라서 기존 금속 이온원에서 인출이 어려웠던 고용점 물질이나 반도체 물질의 이온빔 인출이 가능하다는 장점을 가진다. MEVVA 이온원은 일반적으로 고체 금속 캐소드를 사용하며, 진공 아크방전은 캐소드 표면으로 유도되어 표면을 국부적으로 녹여 증기화 후, 이온화를 통해 금속 플라즈마를 생성한다. 따라서, 아크방전이 지속됨에 따라 금속 캐소드는 점차 소모된다. 본 연구에서는 먼저 MEVVA 이온원의 전원특성 및 안정성을 측정하여, 진공 아크방전 중 금속 이온원의 특성을 측정하였으며, 금속 이온빔 인출 후 캐소드 표면 변화 관측을 통해 적정 캐소드 사용시간을 유추한 결과에 대해 보고한다.

### Keywords:

MEVVA ion source, Vacuum Arc discharge, Cathode spot, Erosion rate

## Surface treatments of an ODS steel for a hydrogen-isotope permeation study in fusion structural materials

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### Abstract:

Development of fusion blanket materials, which are used in extreme environments such as high temperatures, high-energy neutron irradiations, and severe corrosions, requires the database of hydrogen-isotope permeation in materials on various parameters. In this study, we performed surface treatments using an oxide-dispersion-strengthened (ODS) steel, one candidate of the blanket structural materials, in order to obtain high-quality experimental results of hydrogen permeation in the ODS sample. We chemically polished the surface of a disk-shaped ODS sample (supplied by the Korea Atomic Energy Research Institute with a diameter of 20 mm and a thickness of 1.6 mm) and coated its surfaces with palladium by using argon-ion sputtering to minimize the effect of its native oxide layer on the surface. Hydrogen-isotope permeation experiments were measured using a custom-built hydrogen permeation measurement system at Dankook University. The results will be presented and compared with previously reported results.

### Keywords:

hydrogen-isotope permeation, ods steel, fusion structural material, nuclear fusion

## Development of Thermal Desorption Spectroscopy to measure quantitatively deuterium retention in Plasma-Facing Material

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### Abstract:

In nuclear fusion, hydrogen isotopes are used as fuel of fusion reaction. As consequently hydrogen isotopes are inevitably retained at material. This is reason that hydrogen isotopes retention is to be monitored and measured. Thermal desorption spectroscopy (TDS) method belongs to the group of techniques in which an event that takes place at the surface of solid substance is monitored which the loaded sample is heated with a certain temperature ramp in vacuum and the released gas is recorded by residual gas analyzer (RGA) [1]. TDS system is especially developed to measure quantitatively focused on deuterium. TDS system consists of furnace, vacuum chamber, and a sensitive residual gas analyzer (RGA, Extorr 300). Total volume of TDS system is roughly  $2400 \text{ cm}^{-3}$ . The background pressure in the UHV chamber during a measurement with furnace is in general  $1 \times 10^{-6}$  mbar, however, background pressure in UHV chamber equipped RGA is the  $10^{-9}$  mbar. Calibration on RGA and temperature were carried out. Firstly, the RGA signal for mass 4 ( $\text{D}_2$ ) were calibrated by using helium gases. A certain constant gas flow was introduced into the TDS system and the RGA signal was measured until the RGA reading was constant. This procedure was repeated for three different flow levels and the linearity was checked. The relationship between the measured RGA signal for M4 and a certain leak rate for externally introduced He gases was very close to 1 And then determination for heating rate is an important, because the dependence of the furnace temperature on time is determined by the selected heating rate. At low furnace temperature the sample temperature shows a significant lag compared with the furnace temperature during high ramping rate case. Using a temperature ramp of 6 K/min, thus, temperature was heated up to 1250 K. The D retention of plasma facing components will be reported by using TDS system.

### Keywords:

TDS, Tungsten, Deuterium retention

## Anomalously High Electron-neutral Collision Frequency Observed from the THz-based Plasma Diagnosis

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### Abstract:

For the past two decades, THz-based plasma diagnosis has been investigated in the hope of being employed in fusion plasma diagnostics. So far, many of the published THz plasma diagnosis works have been focusing on the plasma with a negligible electron-neutral collision frequency. For the THz-based diagnostics to be successfully employed in fusion plasma diagnostics, however, the method should be able to give accurate particle collision rate, electron and ion temperature, and electron density. In this regard, we report how the collision and electron density can be measured through the THz-plasma interaction. For this work, the variation of THz waveform during the THz-plasma interaction was studied by simulation using the plasma model derived from the Drude model. Results show that THz-based diagnostics can show anomalously high electron-neutral collision frequencies. Discussion on the THz-plasma interaction to explain this abnormality will be presented.

### Keywords:

Laser-plasma, Terahertz, plasma diagnostics, inductively coupled plasma

## 대기압 플라즈마의 조절변수에 따른 표면처리 효과 연구

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### Abstract:

대기압 플라즈마는 저온에서 동작하고, 라디칼이 풍부하기 때문에 열에 민감한 재료의 표면 처리에 활용될 수 있다. 본 연구에서는 폴리카보네이트, 폴리프로필렌, 폴리아크릴레이트 등에 저온 플라즈마를 처리하여 표면 변화를 관찰하였다. 수십 kHz에서 동작하는 pulsed-DC 전원 공급 장치로 DBD 타입의 젯에 전압을 인가하여 헬륨 플라즈마를 발생시켰다. 표면 처리에 앞서, 플라즈마 조절변수에 따른 플라즈마의 전기적, 광학적 특성을 조사하였다. 플라즈마 조절 변수 중에서도 듀티 비(5~50%)를 변화시켜 가며 처리시간에 따른 재료에서의 접촉각 변화를 관찰하였다. 플라즈마 처리한 모든 고분자 재료에 대하여 접촉각의 크기가 1~10초 사이에 급격히 떨어졌으며, 처리시간이 증가할수록 점차 감소하는 특징을 보였다.

### Keywords:

저온 대기압 플라즈마, 표면 개질, 친수성

## 아르곤-헬륨 플라즈마 내의 아르곤 준안정 준위 밀도 지속시간 측정

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### Abstract:

차세대 고출력 레이저 기술로 연속발전 다이오드 펌핑 불활성기체 레이저(diode pumped rare gas laser, DPRGL)가 활발히 연구되고 있다. DPRGL은 헬륨을 완충 기체로 사용한 불활성 기체 플라즈마를 이득 매질로 사용하는 방식의 레이저이다. 아르곤 플라즈마를 활용한 DPRGL의 경우 안정적인 연속발진을 위해서 아르곤  $1s_5$  준안정 준위 원자밀도가  $10^{12}\text{cm}^{-3}$  이상으로 유지되어야 한다고 알려져 있다. 본 연구에서는 DPRGL기술에 활용 가능한 이득 매질을 개발하기 위해 소형 펄스 방전 시스템을 설계 및 제작하였다. 레이저 흡수 분광법을 활용하여 아르곤/헬륨 플라즈마 내의 아르곤  $1s_5$  준안정 준위 원자밀도를 측정하였으며, 펄스폭, 펄스 반복율, 펄스 전압 등 플라즈마 동작 조건을 변화시키며 펄스 방전 중에 준안정 준위 원자밀도가 유지되는 시간을 측정 및 분석하였다.

### Keywords:

Laser absorption spectroscopy, diode pumped rare gas lase, Plasma diagnostics, Metastable atom

## Building a Neural Network Model of Linear MHD Stability Calculation for Pedestal Stability Analysis

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### Abstract:

Pedestal stability is one of the crucial keys in achieving high-performance tokamak plasma. Ideal MHD stability code MISHKA is frequently used to predict the onset of edge-localized mode(ELM), which causes the breakdown of the pedestal. However, calculations for the analysis of the pedestal stability by MISHKA usually take time order of several hours, which can be quite a burden for the real-time integrated tokamak modeling.

In this research, a new neural network(NN) model MISHKA-NN has been trained to replace MISHKA in these kinds of pedestal stability analysis. MISHKA-NN is a regression NN model which predicts the growth rate outputs of MISHKA. After the proper validation process, the applicability of the NN model has been tested by implementing it into the EPED1 model-based pedestal structure predicting tool. Implemented in the tool, MISHKA-NN reduces the analysis time from several hours to seconds with reasonable accuracy, suggesting the NN approach can be a new method to resolve both the numerical burden and accuracy issues in pedestal plasma physics.

### Keywords:

Pedestal, Tokamak, EPED1 model, MISHKA, Neural Network

## A Study on the Measurement of Plasma Density through Power Measurement of Reflective Signal

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### Abstract:

As plasma is widely used in the semiconductor process, research on plasma is being actively conducted to control the process process and predict the result in the semiconductor industry. Accordingly, in order to understand plasma, the importance of diagnostic technology capable of measuring plasma parameters and analyzing characteristics is increasing. Existing research on plasma diagnosis has only been conducted in a local range, and probe-type diagnosis, which is widely used to measure plasma, has the advantage of being able to measure various plasma variables, but it is measured by directly inserting a probe into the plasma. Therefore, there is a disadvantage of causing perturbation in the plasma.

The propagation characteristics of electromagnetic waves in plasma are affected by the dielectric constant that changes according to the plasma density. In this paper, the plasma density is measured by composing a reflectometer and an interferometer using the electromagnetic wave resistance of plasma. In addition, the experiment was conducted by comparing the measured density with the plasma density measured with a single langmuir probe, which is a diagnostic method used in the past.

### Keywords:

Microwave, Plasma diagnostic, Plasma cutoff frequency, Reflectometer, ICP plasma

## Effect of changing structure of diverter and PFC material in KSTAR

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### Abstract:

According to the computational simulation and actual operation results of the small-angle-slot (SAS) structure conducted in DIII-D, the heat flux or particle flux differed from several to several tens of times. In addition to this, a previous study conducted in tokamak devices around the world showed that the diverter region plasma and neutral particles react very sensitively to the diverter structure. In the same vein, we conducted a study applying the SAS structure in KSTAR, and obtained similar results. Previous research was applied to the central diverter of KSTAR, and this study tried to analyze the effect of changing the structure of the outer diverter. In addition, the analysis was conducted by changing the PFC material to carbon and tungsten. The study was conducted with the SOLPS-ITER computational simulation package.

### Keywords:

SOLPS, KSTAR, divertor, SOL, detachment

## Increase of Neutral Helium Metastable States Densities in an Atmospheric Pressure Plasma Jet by Laser-induced Plasma

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### Abstract:

Atmospheric pressure plasma jet (APPJ) is a plasma source produced at atmospheric pressure where driven gas flowing in the APPJ was mixed with ambient air. Laser-induced plasma (LIP) is a phenomenon in which substances are ionized by a focused high energy laser beam as the vaporization and excitation source. APPJ based on dielectric barrier discharges configuration was assembled by a quartz tube and a single ring electrode. Atmospheric pressure plasma was generated by applying a square pulse with the frequency of 5 kHz, the amplitude of 10 kV<sub>p,p</sub>. Helium metastable states densities along the APPJ were diagnosed by laser absorption spectroscopy method using two lasers with the absorption wavelengths of 1083 nm and 396 nm. A high power Nd:YAG pulse laser at the wavelength of 1064 nm was focused on the plasma plume of the APPJ to increase the helium metastable states. The helium metastable states densities increased  $\sim 10^2$  times after the laser pulses were focused on the plasma plume. Mechanism of the increase of helium metastable states in the APPJ by LIP was discussed.

### Keywords:

Atmospheric pressure plasma jet, laser-induced plasma, helium metastable states.

## 변수 랜덤화 플랫폼을 이용한 온라인 기반 일반물리학 평가 방법에 대한 학생들의 인식 조사

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### Abstract:

언컨택트 시대의 도래에 맞춰, 비대면 및 대면 강의 모두에서 활용이 가능한 온라인 기반 시험 및 자동채점 변수-랜덤화 플랫폼을 개발하였다. 이에 따라 본 연구에서는 이 플랫폼을 활용한 일반물리학 교과목을 수강한 학생들에 대해 온라인 평가 방법의 선호도와 만족도, 교육 효과성을 설문하고 분석하였다.

그 결과 온라인 평가의 선호도 측면에서, 지면 평가를 선호하는 가장 큰 이유는 지면 시험이 익숙하기 때문이고, 온라인 기반 평가를 선호하는 큰 이유는 응시 방법의 편의성, 결과의 즉각적 확인 그리고 시험지 제출의 편리성과 신속성 때문으로 나타났다. 온라인 평가 만족도 측면에서, 온라인 기반 평가 방법 도입을 과반 수 이상이 긍정적으로 평가하였다. 또한 온라인 평가의 교육 효과성 측면에서, 온라인 기반 평가 플랫폼을 이용한 수시평가나 과제물 부여가 학습 동기 유발과 성적 향상에 실제 도움이 되었다고 응답하였다.

이 연구의 결과는 온라인 기반 시험 및 자동채점 시스템이 일반물리학 교육에 활용되어 학생들의 만족도와 학업 성취도, 모두를 향상시킬 수 있을뿐만 아니라 새롭고 효과적인 교육 수단으로서 확대될 수 있는 가능성을 보여준다.

### Keywords:

물리교육, 변수 랜덤화 플랫폼, 온라인 기반 평가, 일반물리학

## 인공위성은 왜 떨어지지 않고 지구 주위를 계속 돌 수 있을까?

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### Abstract:

지구를 도는 위성은 앞으로 계속 나아가려는 관성과 지구와 위성이 서로 잡아당기는 뉴턴의 만유인력 때문에 끊임없이 돌고 있다. 공을 던지면 바로 땅에 떨어지는데, 인공위성은 왜 떨어지지 않고 지구 주위를 계속 돌 수 있을까? 이것은 많은 학생들이 인공위성에 대해 가지는 의문일 것이다. 한편, 컴퓨터의 발달과 보급이 가속화되면서 복잡하고 비가시적인 물리적 상황에 대한 학습자의 이해에 도움을 줄 수 있는 Computer Simulation이 유용한 학습 도구로써 주목받고 있다. 이에 본 연구에서는 인공위성 원리의 이해를 돕기 위한 교수-학습의 한 방법으로 Simulation을 활용하는 방법을 제시하고자 한다. 물리 교수-학습 활동에서 Simulation이 효과적으로 활용되기 위해서는 Simulation tool 자체도 중요하지만 Simulation tool의 사용설명서나, 물리 개념을 올바르게 이해하는데 결정적 도움이 되거나 개념을 바르게 이해하고 있는지 확인할 수 있는 적절한 질문지를 Simulation tool과 병행하여 활용하는 것이 매우 중요할 것이다. 본 연구에서 사용한 Simulation tool은 설명 동영상과 Worksheet도 함께 웹 사이트에 공개되어 있어, 사용설명서는 물론 Simulation을 통하여 무엇을 학습해야 하는지 명확하여 스스로 학습할 수 있다는 장점이 있어 수업시간이나 과제로 사용하기에 매우 유용할 것으로 판단된다. 인공위성의 원리를 뉴턴의 사고실험인 Newton's Cannon에서 출발하여, 수평방향으로 던져진 발사체가 중력에 의해 떨어지면서 지구 주위를 돌게 되는 것을 설명하고자 한다. Worksheet에 주어진 질문(Challenging and Interesting Questions) 외에 Simulation을 수행하면서 개념을 정확하게 이해하는데 도움이 될 만한 새로운 질문을 개발하여 추가함으로써, Simulation 수행과 함께 질문에 답을 하면서 자연스럽게 인공위성의 원리를 쉽게 이해할 수 있는 효과적인 학습방법이 될 것으로 기대한다.

### Keywords:

인공위성, 원운동, Newton's Cannon, Simulation

## 고등학생의 과학실험 그래프 작성 오류 유형의 위계 분석

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### Abstract:

우리는 고등학생들이 물리학 실험 결과를 그래프로 그릴 때 나타나는 오류들을 조사하고, 각기 다른 오류들 간에 위계가 존재하는지 분석해 보았다. 선행연구에서, 고등학교 2학년 111명을 대상으로 실험 그래프를 작성하도록 하고 동시에 과학실험 그래프 작성에 대한 이해도를 평가해본 바 있다. 여기서 나타난 오류들을 11가지 항목으로 분류하고 이해도 평가에서 오답인 경우를 12번째 항목으로 추가하여, 총 12가지 그래프 오류들 서로 간의 위계를 분석하였다. 위계분석 방법으로는 Hasse 다이어그램을 사용하였다. 그래프 작성 오류들의 위계와 과학실험을 통해 이론이 만들어지는 과정에 연관성이 있는지도 알아보았다.

### Keywords:

그래프 작성

## The aesthetics of science with a focus on quantum mechanics and its role in scientific discovery

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### **Abstract:**

The significant change in physics were emerged circa 2000, advocated by Max Planck, Niels Bohr, Werner Heisenberg, and others. The establishment of quantum mechanics showed up a drastic change in terms of philosophy compared to the classical mechanics. Even a number of experimental results brought about brand-new theories and principles. However, different viewpoint about aesthetic nature of science played a significant role in developing them in mathematical ways. In this study, I investigated how physicists contributing the emergence of quantum mechanics advocated genuine ideas in relation to the personal preference of aesthetic science.

### **Keywords:**

Aesthetics of science, Quantum mechanics, Copenhagen interpretation, Werner Heisenberg, Simplicity

## 학교 밖 과학 수업 개선을 위한 과학 전문 강사 연수 운영의 분석

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### Abstract:

4차 산업 혁명에 적합한 미래 인재를 양성하고, 과학 문화 대중화를 실현할 수 있는 학교 밖 과학 수업을 효율적으로 운영할 수 있도록 맞춤형 학교 밖 과학 전문 강사 연수 프로그램을 운영을 하기 위하여 학교 밖 과학 전문 강사의 수업 참여 운영 현황을 분석하고 맞춤형 학교 밖 과학 전문 강사 연수 프로그램 개발을 통하여 학교 밖 과학 수업 운영의 개선과 강사의 역량 강화를 하도록 개발하였다.

집합식 연수 프로그램을 이론과 실험으로 구성하여 실시하였으며, 집합식 연수를 이수한 후에 전국의 권역별로 실습을 실시하였다. 연수에 대한 만족도 설문 조사를 통하여 학교 밖 과학 전문 강사들의 강사 연수에 대한 요구를 조사하고 분석할 수 있었다. 고경력 및 신규 강사의 분포가 많았으며, 과학 기술 융합형 콘텐츠 개발과 지속적인 연수 운영의 지원을 요구하였다.

### Keywords:

과학 강사 연수, 학교 밖 과학 수업, 비형식 과학 교육