Highly Tunable Molecular Rectifier Realized by Interfacial Design in Molecular Heterojunction with Two-Dimensional Materials

Jaeho Shin[1,†], Seunghoon Yang[1,†], Yeonsik Jang[2], Jung Sun Eo[1], Tae-Wook Kim[3], Takhee Lee[2], Chul-Ho Lee[1,*], and Gunuk Wang[1,*]

[1]KU-KIST Graduate School of Converging Science and Technology, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Korea
[2]Department of Physics and Astronomy, and Institute of Applied Physics, Seoul National University, Seoul 08826, Korea
[3]Functional Composite Materials Research Center, Institute of Advanced Composite Materials, Korea Institute of Science and Technology, Jeollabuk-do 55324, Korea

2020 KPS Spring Meeting

2020.07.13–15

Korea Univ.

Jaeho Shin

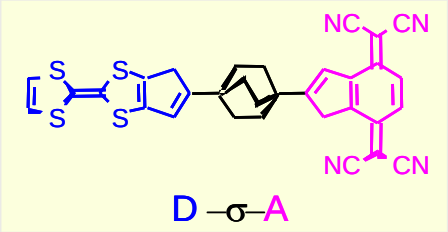
Colloborators

Korea Univ. : Prof. C.-H. Lee (2D materials)
SNU: Prof. T. Lee (Transport Mechanism)
KIST: Dr. T-.W. Kim (Transport Mechanism)

Brief Introduction : Molecular Electronics (ME)

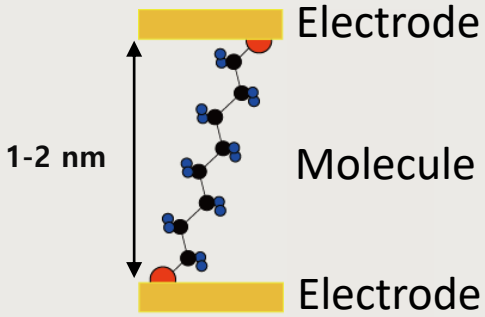
Beginning of Molecular Electronics

"Donor-Acceptor" molecule
acts as **P-N junction diode**

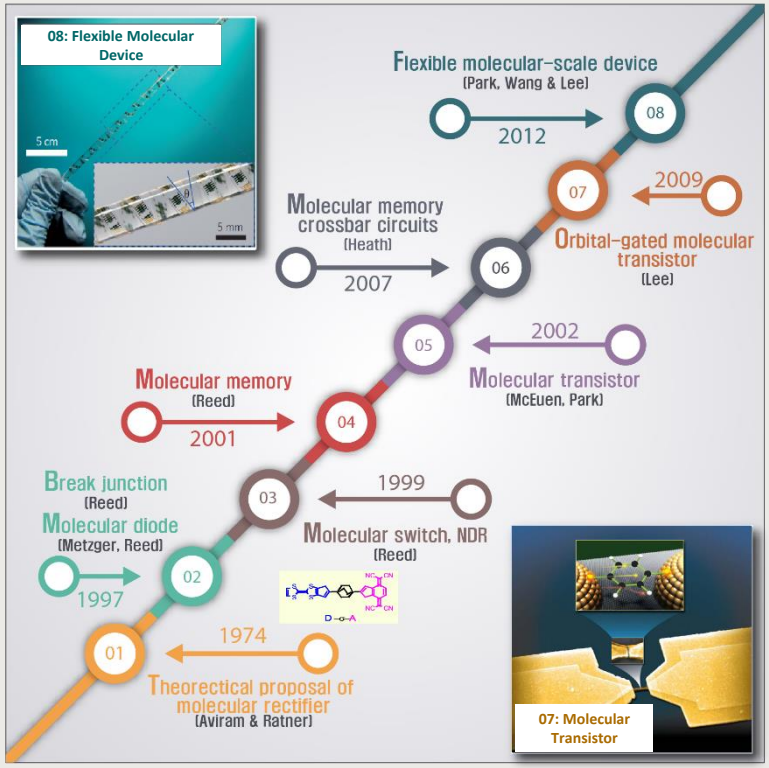


Aviram and M. Ratner,
Chem. Phys. Lett. 29, 277 (1974)

Molecular Junction



Development of ME



Advantages

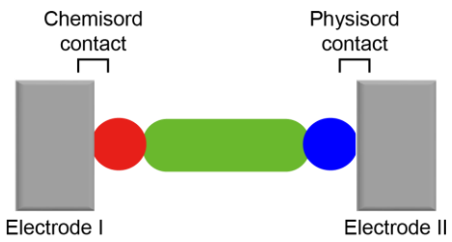
- Low cost & Low Temp.
- Low energy & High Density
- Molecular Functionalities
- Self-Assembled Monolayer

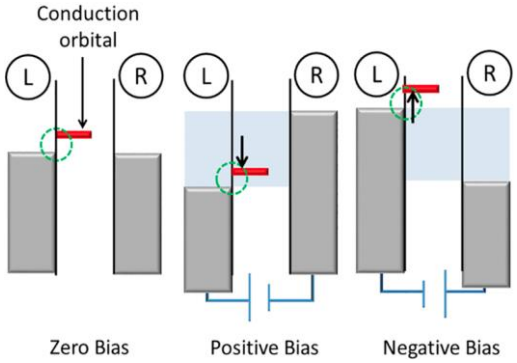
Challenges

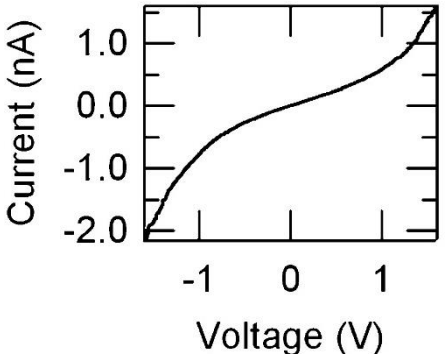
- Synthesis of Functional Molecules
- Stability & Yield
- Device Platform
- Integration/Addressability

Previous Research: Molecular Rectifier

Type 1.



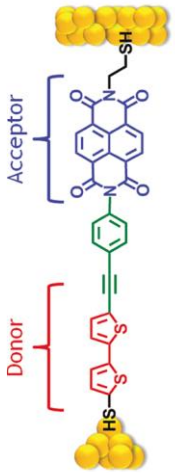


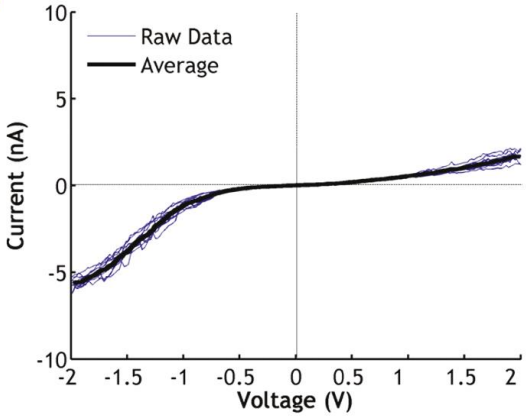


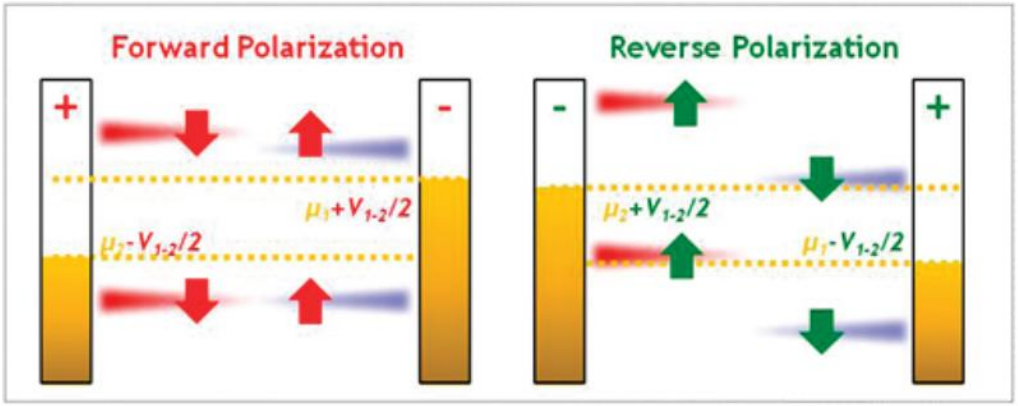
- **Molecular-scale diode by using asymmetric molecule-metal coupling in the molecular junctions.**
- **Owing to the asymmetric molecule-metal coupling, the MO mainly follows the Fermi level of the one electrode.**
- **The average rectification ratio at a 1.5 V bias is about one.**

***ACS Nano**, 2, 827-832 (2008)*
***Sensors**, 17, 956 (2017)*

Type 2.





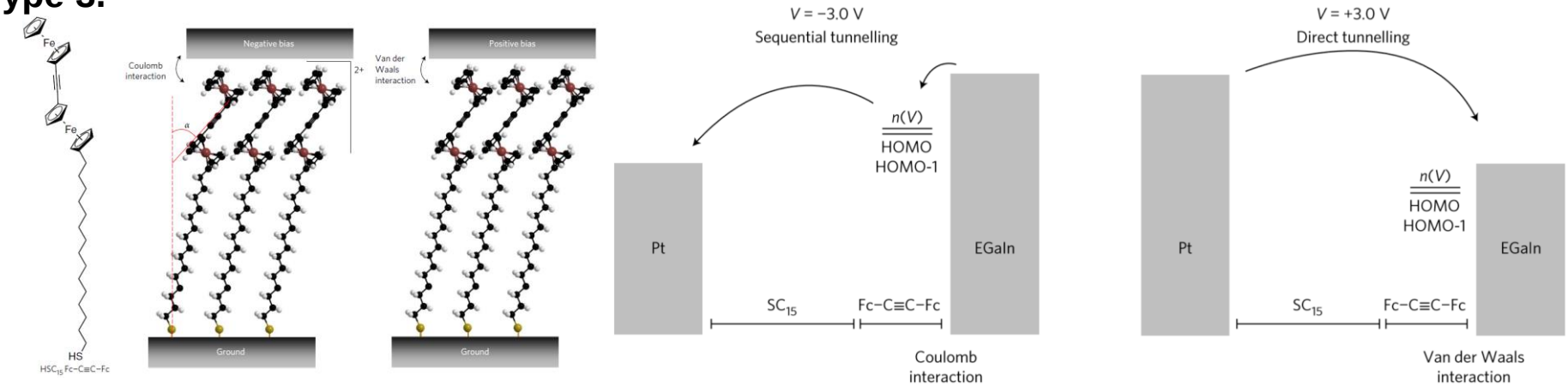


- **STM-BJ based molecular-scale diode, where an acceptor moiety covalently connected to a donor moiety.**
- **This molecular junctions resemble the Aviram-Ratner model molecule.**
- **The average rectification ratio at a 1.5 V bias is about five.**

***Nat. Chem.** 1, 635-641 (2009)*
***ACS Nano**, 5, 9256-9263 (2011)*

Previous Research: Molecular Rectifier

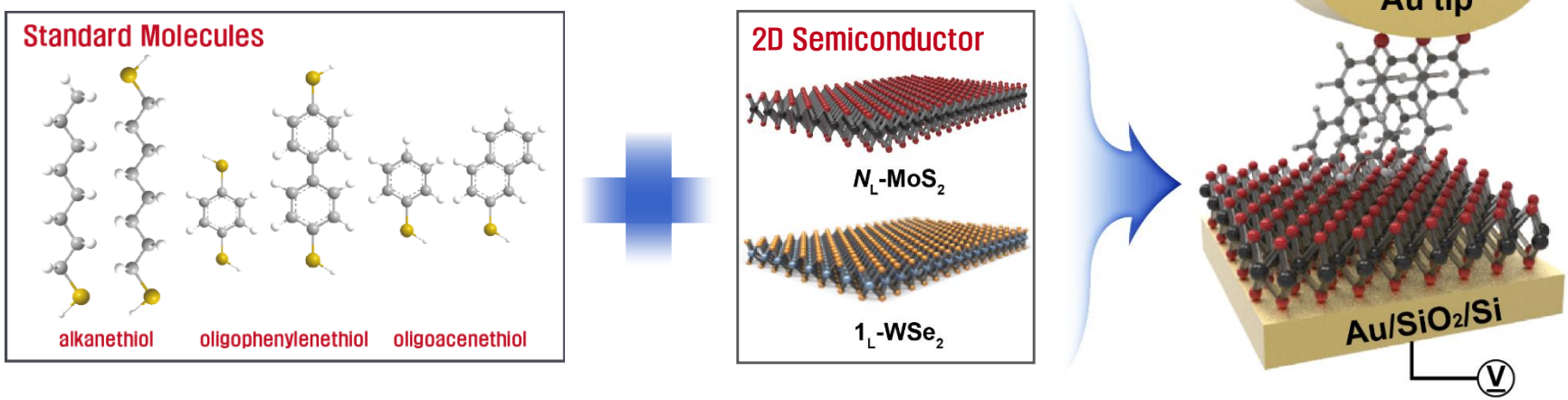
Type 3.



- **Two-level diode derived from EGaIn/SC_{15}Fc-C≡C-Fc/Pt molecular junction.**
- **Rectification ratio of 6.3 x 10^5 which is the results of a mechanism of rectification based on an increase in the number of conducting molecules in only one direction of bias driven by electrostatic interactions.**

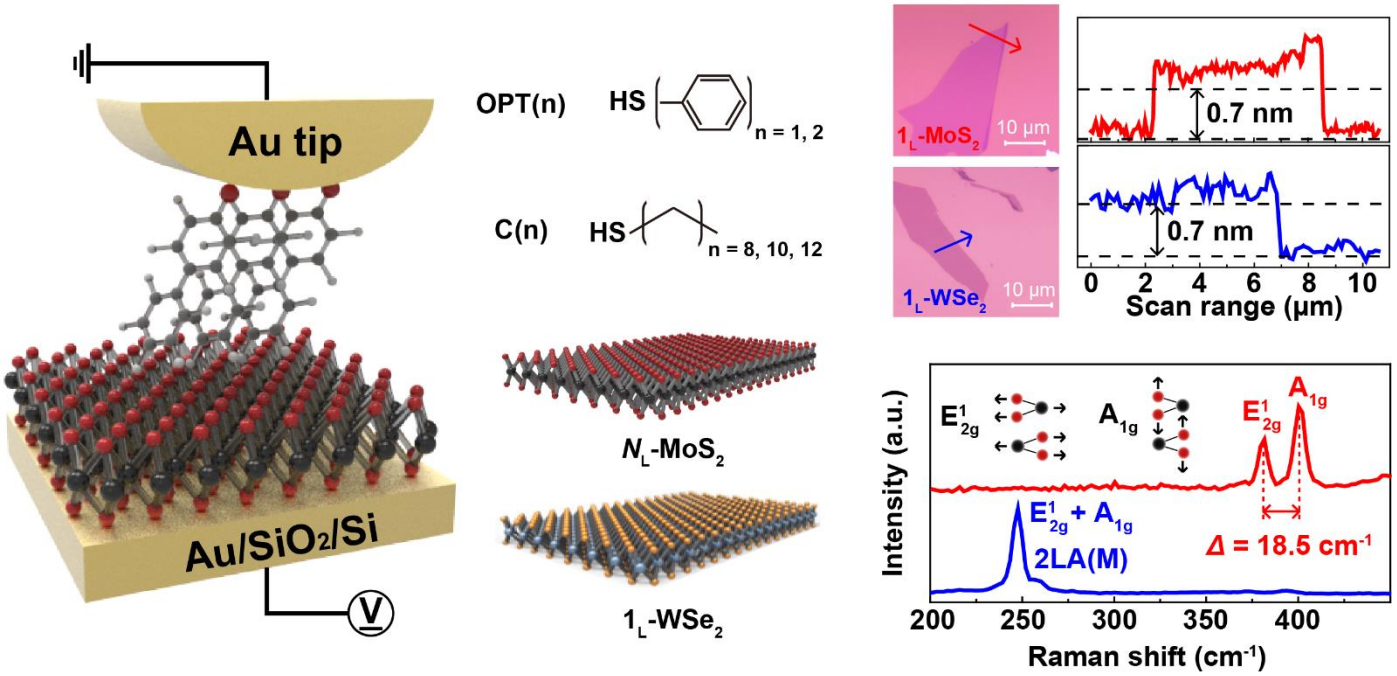
Nat. Nanotech. *12, 797-803 (2017)*

Molecular heterojunction



J. Shin *et al.* *Nature Communication,* 11, 1412 (2020)

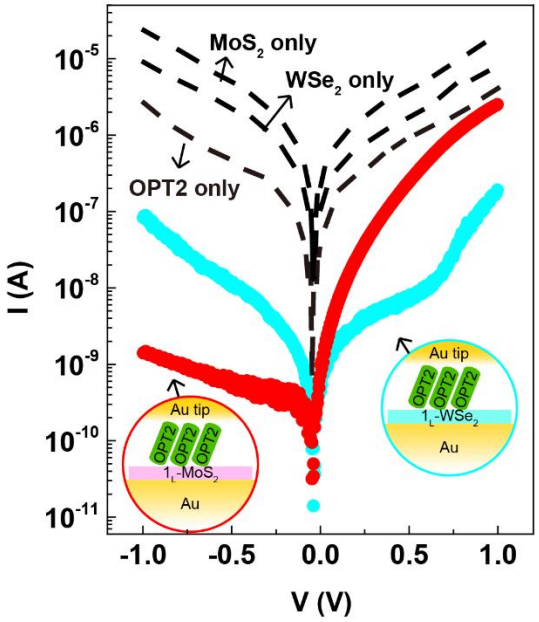
Molecular Heterojunction System

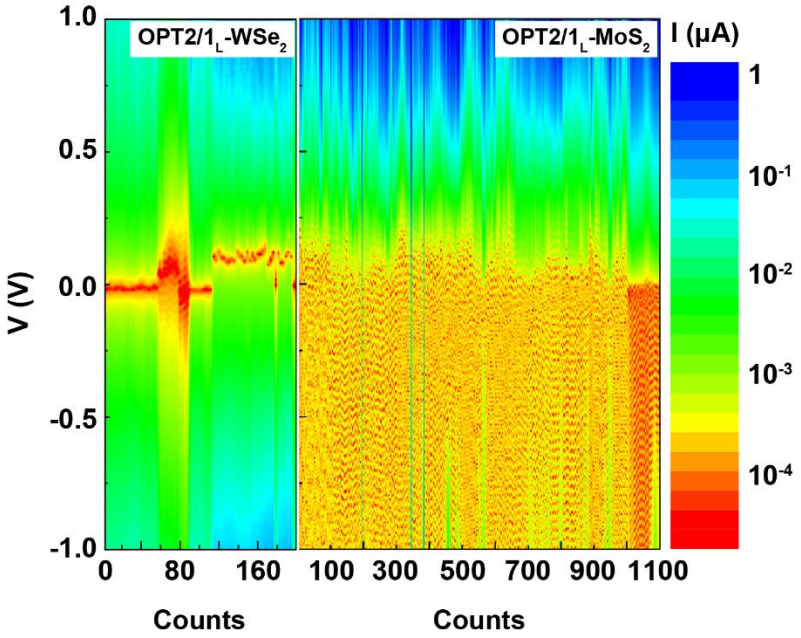


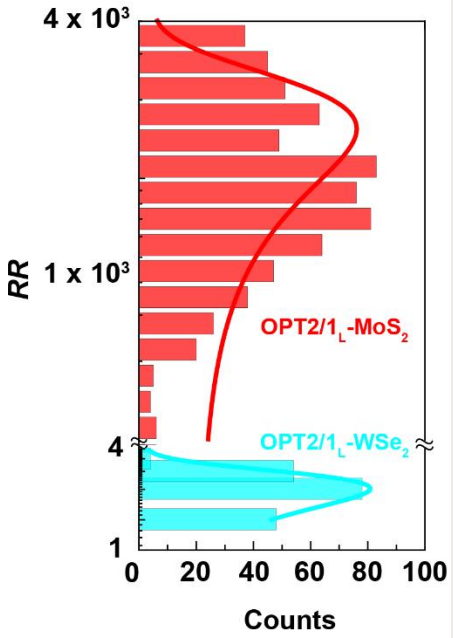
- Tip-loading force is set as 1 nN → To fix the interfacial coupling
- *n*-type MoS_2 / *p*-type WSe_2
- Different HOMO-LUMO gap (alkyl- or conjugated-based)

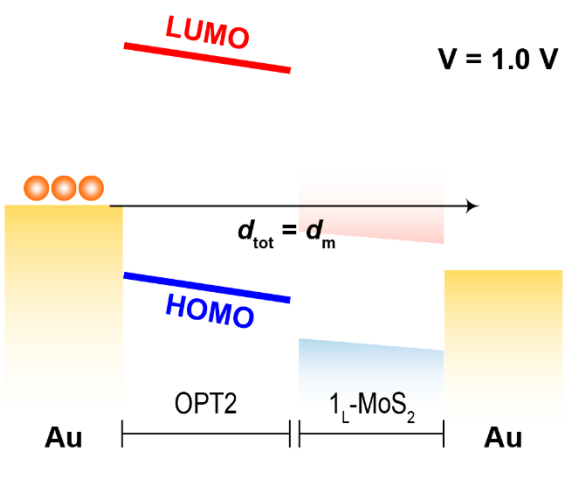
I. Type of 2D semiconductor-dependence (MoS_2 or WSe_2)
II. Number of MoS_2 layers-dependence (1_L-/2_L-/3_L-MoS_2)
III. Molecular length-dependence

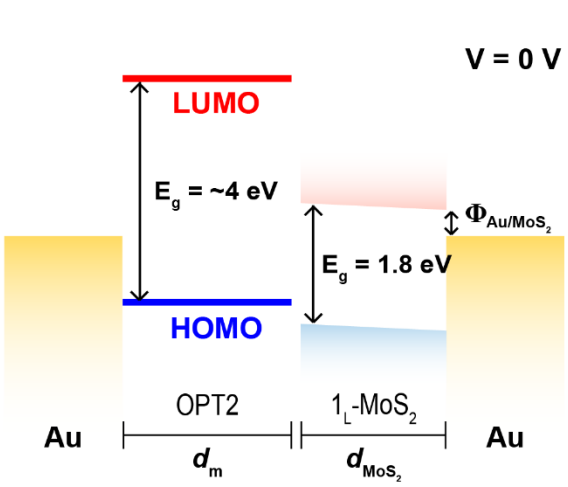
Electrical Characteristics for Molecular Heterojunction

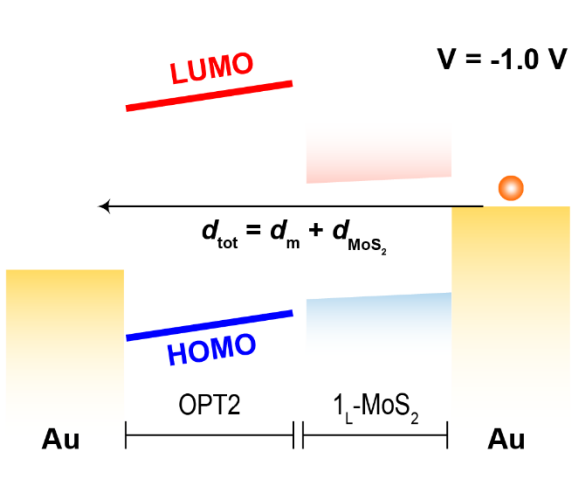




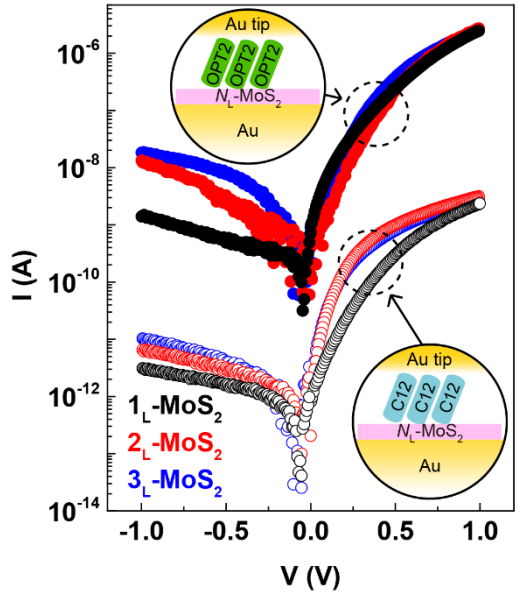


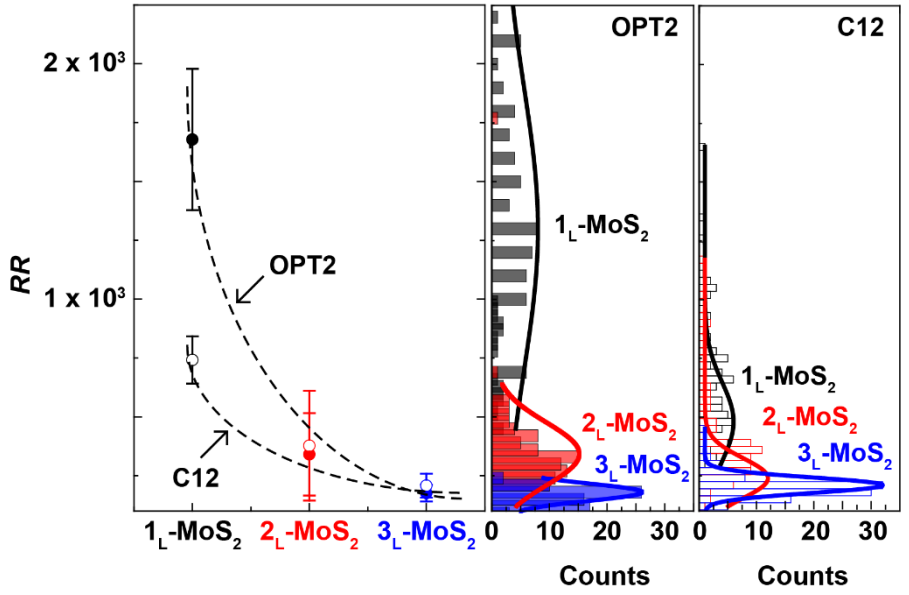


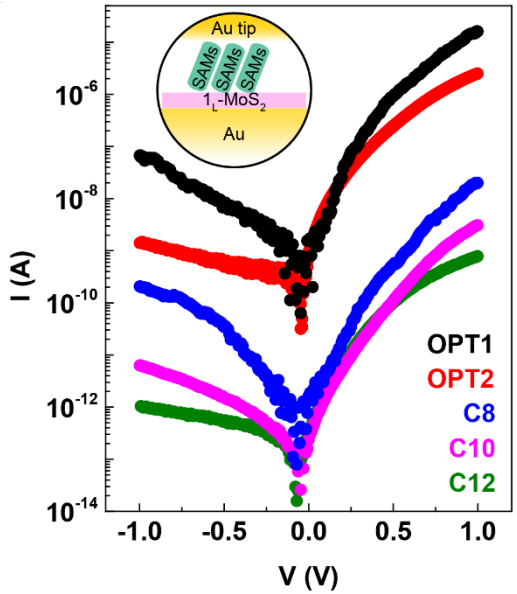


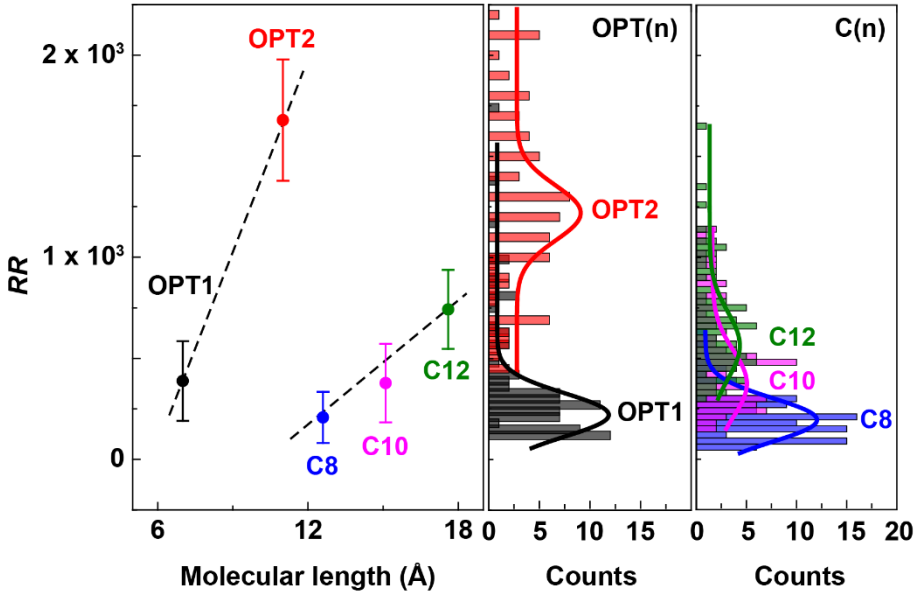


Tunable Rectification of Molecular Heterojunction System

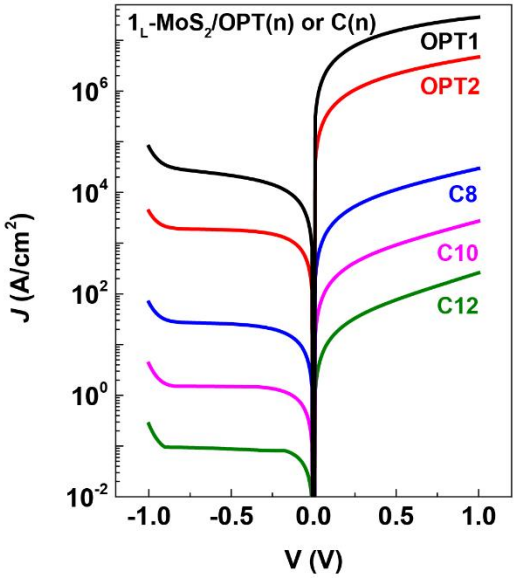


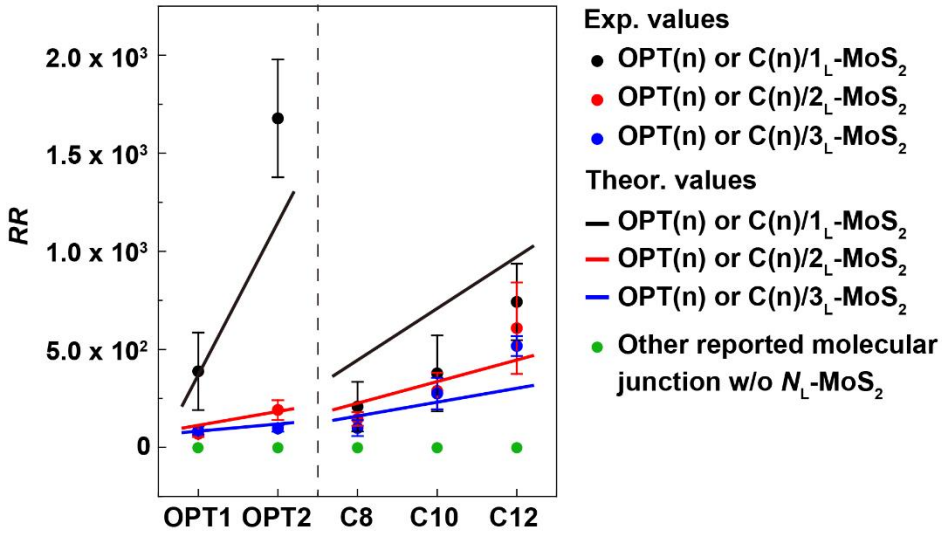


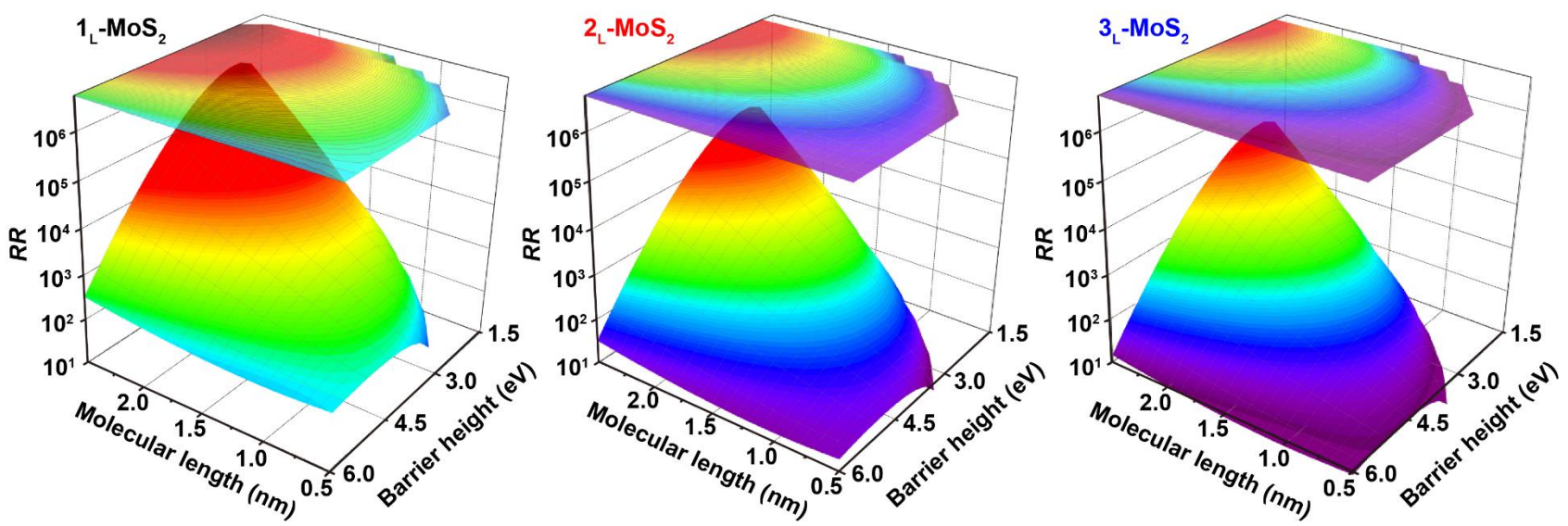




Charge Transport Model



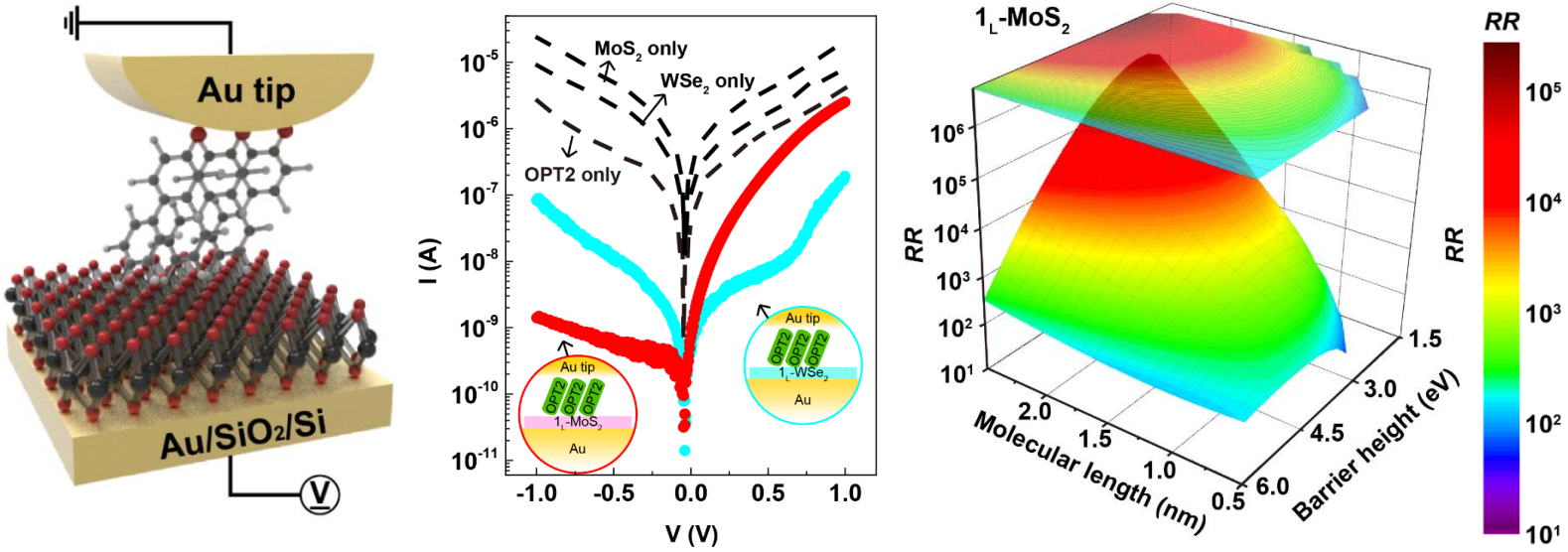




J. Shin *et al.* *Nature Communications* 11, 1412 (2020)

Summary

Conclusion



- We simply introduce a two-dimensional (2D) semiconductor (MoS_2 and WSe_2) as a rectifying designer at the alkyl or conjugated molecules/Au interface under 2 nm scale.

- These rectifying characteristics can be understood by the activation of different transport pathways depending on the voltage polarities through the different energy band alignments at junction interfaces.

- Notably, the rectifying characteristics can be largely tuned from 2.46 ± 1.42 to (1.38 ± 0.73) × 10^3 by changing the junction constituents such as molecular species, the type and number of 2D semiconductor layers.

J. Shin *et al.* *Nature Communications* 11, 1412 (2020)