Center for Artificial Low D Electronic Systems

2023 IBS-CALDES Seminar

- ✓ **Date & Time:** 4:30PM, September 26 (Tues), 2023
- ✓ **Venue:** IBS POSTECH Campus Bldg. 104 (Auditorium)
- ✓ **Speaker:** Prof. Myung Joon HAN (KAIST)
- ✓ **Title:** First-principles-based study of correlated transition-metal dichalcogenides

Organized by Prof. Han Woong YEOM(yeom@postech.ac.kr, 054-260-9000)
Dr. Jhinhwan LEE (jhinhwan@ibs.re.kr, 054-260-9014)

- **4:30PM~**

First-principles-based study of correlated transition-metal dichalcogenides

Mung Joon HAN
Department of Physics, Korea Advanced Institute of Science and Technology (KAIST)

In this talk, I will present our recent efforts of understanding the correlated electron physics in transition-metal dichalcogenides. By combining conventional density functional theory (DFT) with an appropriate form of many-body techniques, we try to investigate some key aspects that can be hardly accessible solely from experiments. Through its practical total energy formulation, the standard spin-polarized DFT method enables us to make extensive material simulation and direct comparison with experiments. Based on our recent calculation results of VTe2, I will discuss the role of 'hidden' magnetic order coupled with charge density wave (CDW) [1, 2]. In the case of VSe2, we adopted the standard formulation of so-called DFT+DMFT (dynamical mean-field theory) to describe the phase competition between CDW and ferromagnetic order. With the aid of this unbiased temperature-dependent calculation, we were able to estimate the magnetic order parameter and found that the ferromagnetic order can stabilize without CDW deformations [3]. Finally, I will introduce the concept of GW+ extended DMFT. We used this elaborate computation scheme to understand the gap formation of TaS2. Our calculation result indicates Mott gap is well developed in the realistic parameter regime [4]. I will try to discuss difficulties as well as differences when this series of methods is applied to real material issues.

References

[1] Won, Kiem et al., Adv. Mater. 32 1906578 (2020)
[2] Kiem et al., Nanoscale 14 10009 (2022)
[3] Kim et al., 2D Materials 5 035023 (2020)
[4] Kim et al., iScience 26 106681 (2023)