Interfacial magnetic coupling in vdW heterostructures with defective TMD

Meng-Chien Wang[1], Ching-Ray Chang[1, 2*]
[1]National Taiwan University, Chinese Taipei
[2]Chung Yuan Christian University, Chinese Taipei

Recently, 2D van der Waals magnetic systems have attracted much research attention because of their fruitful physics and application potential in low-power devices. As an example, chromium triiodide (CrI_3), one of the first isolated magnetic monolayers, is widely studied for its interesting layer-dependent and stacking-dependent magnetism. In addition to the properties of magnetic material itself, its interface with other materials also plays a key role in the behavior and performance of practical devices. Monolayer transition metal dichalcogenides(TMDs) are another group of 2D materials that have been intensively studied. Individually, they display intriguing electronic and optic properties. Also, the application of TMD for modulating spin transport in adjacent materials is explored. Most TMDs are known as nonmagnetic. However, previous theoretical and experimental studies have found that vacancy defects can induce magnetic moment and even long-range magnetic order in some TMDs. For example, Molybdenum diselenide ($MoSe_2$) with Mo vacancies is predicted to be a half metal. It is also reported that platinum vacancies are responsible for the long-range magnetic order in platinum diselenide ($PtSe_2$) at low temperatures. In this presentation, we study the interface between chromium triiodide(CrI_3) and two transition metal diselenides ($MoSe_2$, $PtSe_2$) using first principle calculation. We focus on the interlayer magnetic coupling between magnetic CrI_3 and defect induced magnetism in $MoSe_2$ and $PtSe_2$. In particular, $MoSe_2$ and $PtSe_2$ have 2H and 1T crystal structures, respectively. We study the effect of vacancy position on interlayer magnetic coupling and also discuss the influence of crystal structures. The study of defect-induced magnetism and associated interfacial effect is vital since defects are inevitably present in real materials.

*Corresponding author	Ching-Ray Chang
Affiliation	National Taiwan University
E-mail address	crchang@phys.ntu.edu.tw