Contribution ID: **214**

Type: **Contributed Oral**

First-Principles Study of Multiferroicity in 1T-$FeCl_2$/Bilayer-GaSe Heterostructure

Wednesday 3 December 2025 12:15 (15 minutes)

Multiferroic materials have gained significant attention as promising candidates for next-generation electronic applications due to their ability to exhibit multiple ferroic orders simultaneously, including ferromagnetism and ferroelectricity [1]. Importantly, controlling magnetism by switching polarization states of ferroelectric materials offers more flexibility for information storage and processing in high-performance electronic devices [2]. Here, we employ first-principles density functional theory (DFT) calculations to investigate the binding energies, electronic, magnetic, and ferroelectric properties of a two-dimensional van der Waals multiferroic heterostructure composed of 1T-$FeCl_2$ and bilayer GaSe. While pristine 1T-$FeCl_2$ exhibits half-metallicity with robust ferromagnetism, bilayer-GaSe remains a semiconductor with sliding ferroelectricity. The electronic band structure retains its half-metallic character in the spin-up channel, while in the spin-down channel, significant contributions from bilayer GaSe appear at the conduction band minimum and valence band maximum at the heterostructure interfaces. The ferroelectric polarization in the GaSe bilayer significantly modulates the magnetic anisotropy energy of the heterostructure compared to the free-standing $FeCl_2$ monolayer. The charge transfer from the GaSe bilayer to the ferromagnetic monolayer is facilitated by their work function difference, 5.35 eV and 4.98 eV, respectively. This is also confirmed by studying the differential charge densities and Bader charges of the heterostructures. The contact interface forms Ohmic contacts, enabling sufficient charge transfer between the layers. This study presents a theoretical framework for designing artificial multiferroics, paving the way for controlled magnetism with switchable polarization states in next-generation devices, including non-volatile memory and spintronic applications.

Reference:
[1] X. Feng, J. Liu, X. Ma, and M. Zhao, Physical Chemistry Chemical Physics 22, 7489 (2020).
[2] K. F. Mak, J. Shan, and D. C. Ralph, Nature Reviews Physics 1, 646 (2019).

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Session Classification: Condensed Matter & Materials

Track Classification: Topical Groups: Condensed Matter & Materials