Magnetic and Electronic Properties of Fe_3GeTeX (X = S, Se) Janus/Germanene Heterobilayers

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Abstract

Two-dimensional (2D) magnetic materials have garnered significant attention due to their potential applications in spintronics and nanoelectronics. Among them, Fe_3GeTeX (X = S, Se) Janus structures, derived from Fe_3GeTe_2, exhibit unique properties due to their intrinsic asymmetry, which can enhance spin-orbit coupling and introduce novel electronic and magnetic characteristics. Meanwhile, germanene, a 2D material analogous to graphene, features a tunable bandgap and strong spin-orbit coupling, making it an excellent candidate for integration into heterostructures. Combining Fe_3GeTeX with germanene offers a promising platform to explore the interplay between magnetism, spin-orbit interactions, and electronic properties in 2D systems.

In this study, we employ density functional theory (DFT) calculations to investigate the structural, electronic, and magnetic properties of Fe_3GeTeX/germanene heterobilayers. We analyze the stability of the heterostructure, interlayer coupling effects, modifications in the electronic band structure, and changes in magnetic anisotropy induced by germanene. Our results reveal how the Janus nature of Fe_3GeTeX influences the heterobilayer's electronic and magnetic properties.

The findings contribute to the fundamental understanding of 2D magnetic heterostructures and their potential applications in next-generation spintronic devices. By demonstrating the impact of Janus engineering in magnetic materials, this study provides insights into designing novel heterostructures.

This work is supported by the FLAG-ERA grant MNEMOSYN, by The Scientific and Technological Research Council of Turkey (TÜBİTAK) under project no. 221N400 and Y.M. acknowledges financial support from the Outstanding Young Scientist Program of the Turkish Academy of Sciences (TÜBA-GEBİP).

References

[1] Li, X., Li, D., Duan, S., et al. (2022). Magnetic properties and electronic structures of Fe_3GeTe_2-based heterostructures. Physical Chemistry Chemical Physics, 24, 19412–19418.
[2] Deng, Y., Yu, Y., Song, Y., et al. (2018). Gate-tunable room-temperature ferromagnetism in two-dimensional Fe_3GeTe_2. Nature, 563, 94–99.

Figures

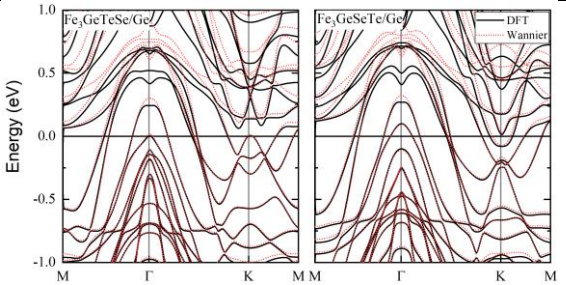

Figure 1: Electronic band structures of Fe_3GeTeX/Ge heterobilayer