Magnetic and Chiral Properties of 2D Janus VXY (X= Cl, Br, I; Y= S, Se, Te) Monolayers

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Abstract:

We present a comprehensive density functional theory (DFT)-based study of the two-dimensional ferromagnetic Janus VXY (X = Cl, Br, I; Y = S, Se, Te) structures (Figure 1), focusing on their dynamical, thermal, and electronic properties [1]. Our investigation explores the stability of all possible VXY configurations in both 1T and 2H structural phases. Among these, only the 1T phases of VBrS, VIS, and VISe monolayers are stable, exhibiting semiconducting behavior with significant spin-orbit coupling (SOC)-induced valley splitting, particularly reaching 0.1 eV in the VISe monolayer. We utilize first-principles calculations and anisotropic spin models to evaluate the magnetic properties of these monolayers, determining the exchange interactions between vanadium atoms and estimating the Curie temperature (T_C) using Green's function and Monte Carlo simulations, which are found to be around 100 K for all three stable structures.

All stable monolayers are identified as ferromagnetic semiconductors with spontaneous valley splitting in the out-of-plane magnetization direction, proportional to the SOC strength. Additionally, the absence of inversion symmetry in Janus VXY structures results in a significant Dzyaloshinskii-Moriya interaction, enabling the formation of chiral magnetic structures. At 0 K, these monolayers exhibit nonzero topological charge (Q), indicative of spin frustration. Under an out-of-plane magnetic field of ~0.7 T, skyrmion formation is observed, with the VISe monolayer displaying a skyrmion lattice at ~0.1 T that disappears at higher fields. At 5 K, VIS shows chiral magnetic structures, while VBrS and VISe exhibit Néel-type domain walls. In the presence of an in-plane field, bimerons form around 0.5 T due to the in-plane easy axis of these monolayers. Our findings highlight the potential for controlling magnetic skyrmions in 2D Janus structures and pave the way for further research in this field.ONE page abstract format: including figures and references.

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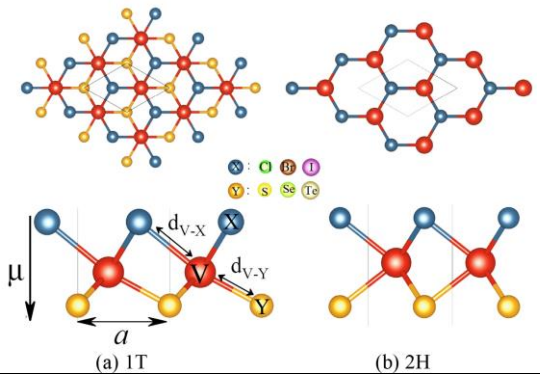

Figure 1: The top and side views of the (a) 1T and (b) 2H phases of VXY (X = Cl, Br, I; Y = S, Se, Te) monolayers.

References

[1] R. Caglayan, A. Mogulkoc, Y. Mogulkoc, M. Modarresi, and A. N. Rudenko, Phys. Rev. B 110, (2024), 094440.