Magnetic properties of two-dimensional binary and Janus Cr_2XYSe_2 (X,Y=F,Cl,Br,I) compounds

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Abstract

In this study, we explore the structural, electronic, and magnetic properties of orthorhombic two-dimensional Cr_2XYSe_2 (X, Y= F,Cl,Br,I) compounds using first-principles density functional theory (DFT+U). Our phonon calculations confirm the dynamical stability of eight distinct compositions. Notably, all stable systems exhibit ferromagnetic ground states with magnetic moments approaching 3 μB per Cr atom.
We find that the exchange parameters (J_1, J_2, J_3) are highly dependent on chemical substitution and the Hubbard parameter U, indicating a competition between localized superexchange and itinerant RKKY-type interactions in the metallic regime. Magnetic anisotropy plays a crucial role in controlling the easy-axis orientation and opens a finite magnon gap, which stabilizes long-range magnetic order.
Furthermore, our renormalized magnon spectra predict Curie temperatures of up to approximately 200 K for iodine-containing compounds, demonstrating enhanced thermal robustness. The Janus structures exhibit intrinsic out-of-plane dipole moments resulting from broken mirror symmetry, offering additional tunability through internal electric fields. This research highlights the combined influence of halogen chemistry, electron correlation, and symmetry reduction in establishing a design strategy for engineering magnetic behavior in van der Waals materials. Our findings position Cr-based chalcogenide monolayers as promising candidates for future two-dimensional spintronic applications.

References

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Figures

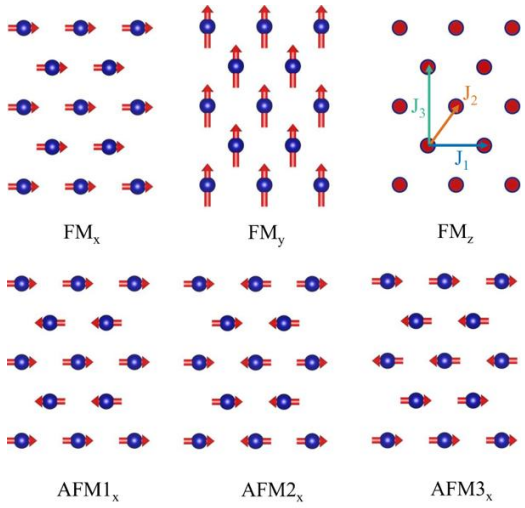

Figure 1: Spin configurations of Cr_2XYSe_2 monolayers

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).