Magnetic anisotropy and Curie temperatures of chromium chalcohalide two-dimensional Janus ferromagnets

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We revisit the magnetic properties of the recently proposed noncentrosymmetric 2D magnetic materials [1-4], chromium chalcohalide Janus monolayers (MLs), Cr*XY* (*X*=S, Se, Te; *Y*=Cl, Br, I), that have attracted significant attention due to their promising magnetic properties, e.g., large predicted Dzyaloshinskii-Moriya interaction (DMI). To date, key aspects of their magnetic behavior such as magnetic anisotropy and Curie temperatures (T_C) have not been decisively established yet. In the present study, we address these properties using ab intio calculations.

Our total-energy calculations reveal that all dynamically stable Cr*XY* MLs exhibit FM ordering. However, robust out-of-plane magnetic anisotropy is observed only in the CrSI and CrSeI compositions (for both 1T and 1H structures), which arises from a constructive interplay between single-ion and anisotropic exchange terms that overcome the dipole-dipole interaction.

We further quantify the DMI of CrSI and CrSeI and reveal a weak-to-moderate DMI strength as compared to the isotropic exchange interaction term. By estimating T_C of the 1T and 1H CrXI (X=S, Se) we find that while the 1T-CrXI exhibit T_C values in the range of 150-188 K, the 1H-CrXI reach T_C close to room temperature. All other Cr*XY* MLs display easy-plane-like behavior, preventing them from supporting magnetic ordering at elevated temperatures. Our results refine the previously published data on the magnetic anisotropy type and energy of the Cr*XY* Janus MLs as well as provide realistic estimates of their T_C.

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References

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Figures