Tuning the Magnetic Landscape of Two-Dimensional $CrCl_3$ through Ruthenium Doping: A First-Principles Investigation

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Controlling spin interactions in atomically thin magnets is a key challenge for next-generation spintronics [1,2]. Here, we investigate the magnetic energy landscape of pristine monolayer $CrCl_3$ and the prospect of tuning it through substitutional ruthenium doping. Spin-polarized density functional theory with Hubbard corrections and spin–orbit coupling is combined with Wannier-based magnetic-interaction analysis. For pristine $CrCl_3$, isotropic exchange parameters (J_{ij}) and Dzyaloshinskii–Moriya vectors ($\mathbf{D}_{ij}$) are obtained using TB2J [4], while magnetocrystalline anisotropy (K) is determined from spin-direction-dependent total energies. The calculated exchange interactions resolve the principal magnetic couplings, whereas the antisymmetric exchange is very weak, consistent with the symmetry of the pristine monolayer. These results provide a microscopic reference for separating exchange-driven effects from spin–orbit contributions. Ruthenium substitution at a chromium site is then examined as a route to perturb the local magnetic environment; exchange-parameter extraction for this doped system is ongoing. This comparative first-principles framework establishes a basis for assessing chemically controlled magnetic interactions in two-dimensional chromium trihalides and for future spin-dynamics investigations [3].

References

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