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First-principles investigation of the magnetic behavior and interlayer coupling in layered $CrCl_3$ and $CrTe_3$

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Abstract

The crystallographic, electronic and magnetic properties of layered $CrCl_3$ and $CrTe_3$ were investigated using density functional theory (DFT) employing the newly developed spin van der Waals density functional (svdW-DF). The $CrTe_3$ layers are made up of lozenge-shaped Cr_4 tetramers with nonequivalent Cr sites carrying antiparallel spins in each layers with a weak van der Waals bonding between the layers. However, in $CrCl_3$, Cr moments are aligned anti-ferromagnetically out of plane and ferromagnetic in-plane. In both materials, our results indicate that treatment of the long-range interlayer forces with the svdW-DF improves the accuracy of crystal structure predictions. The cleavage energies were estimated to be 0.29 and 0.5 J/m^2 for $CrCl_3$ and $CrTe_3$, respectively, suggesting that they are cleavable using standard mechanical exfoliation techniques. These materials produce sizeable band gaps and can be used in electronic device applications. Furthermore, our results indicate that these materials are useful for low dimensional (including monolayer) magnetism. These results were consistent with experimental findings.

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