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First-principles investigation of the interlayer coupling in chromium-trichloride-a layered magnetic insulator[1] SANTOSH KC, MICHAEL A. MCGUIRE, VALENTINO R. COOPER, Oak Ridge National Lab — The crystallographic, electronic and magnetic properties of layered $CrCl_3$ were investigated using density functional theory. We use the newly developed spin van der Waals density functional (svdW-DF) in order to explore the atomic, electronic and magnetic structure. Our results indicate that treatment of the long-range interlayer forces with the svdW-DF improves the accuracy of crystal structure predictions. The cleavage energy was estimated to be 0.29 J/m^2 suggesting that $CrCl_3$ should be cleavable using standard mechanical exfoliation techniques. The inclusion of spin in the non-local vdW-DF allows us to directly probe the coupling between the magnetic structure and lattice degrees of freedom. An understanding of the link between electronic, magnetic and structural properties can be useful for novel device applications such as magnetoelectric devices, spin transistors, and 2D magnet.

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