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First principles study of electronic, magnetic and inter-layer coupling in a layered magnetic insulator SANTOSH KC, San Jose State University, MICHAEL MCGUIRE, VALENTINO 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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