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2D magnetism of CrI3 – how density functional theory can be used to explain its magnetic properties?

2D magnetism of few-layer CrI_3 was discovered in 2017 (Nature 546, 270-273, 2017). Since then, this van der Waals material has been studied intensively. The interplay between stacking of the material of van der Waals crystal structure and its interlayer exchange interactions is especially intriguing, and may lead to very interesting physics in few-layer samples.

The nature of both intralayer and interlayer exchange interactions, the role played by local Coulomb interactions, and especially the nature of the anisotropic interactions deserve further attention. Density functional theory ((DFT) poses as a unique tool to study the enigmatic properties of this material; however, modeling interlayer exchange is challenging for DFT because it is a small quantity not much higher than the accuracy of the current DFT codes and local density functionals perform poorly to describe the tails of wave functions that control interlayer exchange. I am interested in overcoming these challenges to shed some light on the open questions regarding 2D CrI_3.

- I work at an undergraduate institution and I am looking for collaborators who share my research interests. I have experience on Monte Carlo and molecular dynamics simulations, but I am new to DFT.