

AI guided materials discovery of two-dimensional magnets

Trevor David Rhone

Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute

The discovery of van der Waals (vdW) materials with intrinsic magnetic order in 2017 has given rise to new avenues for the study of emergent phenomena in two dimensions. In particular, monolayer CrI_3 was found to be ferromagnet. Other vdW transition metal halides were later found to have different magnetic properties. How many vdW magnetic materials exist in nature? What are their properties? How do these properties change with the number of layers? A conservative estimate for the number of candidate vdW materials (including monolayers, bilayers and trilayers) exceeds $\sim 10^6$. A recent study showed that artificial intelligence (AI) can be harnessed to discover new vdW Heisenberg ferromagnets based on $\text{Cr}_2\text{Ge}_2\text{Te}_6$ [1,2]. In this talk, we will harness AI to efficiently explore the large chemical space of vdW transition metal halides and to guide the discovery of magnetic vdW materials with desirable spin properties. That is, we investigate crystal structures based on monolayer Cr_2I_6 of the form A_2X_6 , which are studied using density functional theory (DFT) calculations and AI. Magnetic properties, such as the magnetic moment, are determined. The formation energy is also calculated and used as a proxy for the chemical stability. We show that AI combined with DFT can provide a computationally efficient means to predict the thermodynamic and magnetic properties of vdW materials [3]. This study paves the way for the rapid discovery of chemically stable magnetic vdW materials with applications in spintronics and data storage.

[1] T. D. Rhone, et al., “Data-driven Studies of Magnetic Two-dimensional Materials,” *Scientific Reports* 10, 15795 (2020).

[2] Y. Xie, et al., “Data-Driven Studies of the Magnetic Anisotropy of Two-Dimensional Magnetic Materials,” *J. Phys. Chem. Lett.*, 12, 50, 12048–12054 (2021).

[3] T. D. Rhone et al., “Artificial Intelligence Guided Studies of van der Waals Magnets,” *Adv. Theory Simulations*, 6, 2300019 (2023).

This research was primarily supported by the NSF CAREER, under award number DMR-2044842.