Data-driven studies of magnetic van der Waals materials

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When the dimensionality of an electron system is reduced from three dimensions to two dimensions, new behavior emerges. This has been demonstrated in gallium arsenide quantum Hall systems since the 1980's, and more recently in van der Waals (vdW) materials, such as graphene. The discovery of vdW materials with intrinsic magnetic order in 2017 has given rise to new avenues for the study of emergent phenomena in reduced dimensions. These materials are at the forefront of condensed matter physics research. 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 ~10^6. In this talk, we will use materials informatics (machine learning combined with materials science) as a tool to efficiently explore this large materials space and attempt to discover magnetic vdW materials with desirable spin properties. We will focus on crystal structures based on monolayer $Cr_2Ge_2Te_6$ (CrI_3), of the form $A_2B_2X_6$ (A_2X_6), which are studied using density functional theory (DFT) calculations and machine learning methods. Magnetic properties, such as the magnetic moment are determined. The formation energies are also calculated and used to estimate the chemical stability. We show that machine learning methods, combined with DFT, can provide a computationally efficient means to predict properties of vdW magnetic materials. In addition, data analytics provides insights into the microscopic origins of magnetic ordering in two dimensions. We also explore how our study of magnetic monolayers [1] can be extended, with proper modification, to multilayer vdW materials. This non-traditional approach to materials research paves the way for the rapid discovery of magnetic vdW materials that are chemically stable.

[1] Trevor David Rhone, Wei Chen, Shaan Desai, Steven B. Torrisi, Daniel T. Larson, Amir Yacoby & Efthimios Kaxiras, Data-driven studies of magnetic two-dimensional materials. Sci Rep 10, 15795 (2020).