Quantum materials discovery using AI

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Quantum materials are at the forefront of materials research with a wide range of potential applications including sensing, data storage, spintronics and quantum computing. These materials have highly correlated electronic degrees of freedom, which give rise to emergent behavior. In this talk, I will describe how materials discovery can be accelerated by combining tools from condensed matter physics and artificial intelligence (AI). In particular, I will focus on materials with emergent spin degrees of freedom, such as vdW materials with intrinsic magnetic order. The discovery of these materials 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. Materials informatics (AI combined with materials science) is used 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 AI. 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 AI tools, 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, 2] can be extended, with proper modification, to vdW materials with both magnetic and topological order. This non-traditional approach to materials research paves the way for the rapid discovery of quantum materials with novel properties.

[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. *Scientific Reports* 10, 15795 (2020).

[2] Yiqi Xie, Georgios A. Tritsaris, Oscar Grånäs, and Trevor David Rhone, Data-Driven Studies of the Magnetic Anisotropy of Two-Dimensional Magnetic Materials, *The Journal of Physical Chemistry Letters 12* (50), 12048-12054 (2021).