Accelerating the discovery of van der Waals quantum materials using AI

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van der Waals (vdW) materials are exciting platforms for studying emergent quantum phenomena, ranging from long-range magnetic order to topological order. A conservative estimate for the number of candidate vdW materials exceeds ~10^6 for monolayers and ~10^{12} for heterostructures. How can we accelerate the exploration of this entire space of materials? Can we design quantum materials with desirable properties, thereby advancing innovation in science and technology? A recent study showed that artificial intelligence (AI) can be harnessed to discover new vdW Heisenberg ferromagnets based on $Cr_2Ge_2Te_6$ [1], [2] and magnetic vdW topological insulators based on $MnBi_2Te_4$ [3]. In this talk, we will harness AI to efficiently explore the large chemical space of vdW materials and to guide the discovery of vdW materials with desirable spin and charge properties (see Fig. 1). We will focus on 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 also investigate monolayers based on $MnBi_2Te_4$ of the form AB_2X_4 to identify novel topological materials. Further to this, we study heterostructures based on $MnBi_2Te_4/Sb_2Te_3$ stacks. We show that AI, combined with DFT, can provide a computationally efficient means to predict the thermodynamic and magnetic properties of vdW materials [4],[5]. This study paves the way for the rapid discovery of chemically stable vdW quantum materials with applications in spintronics, magnetic memory and novel quantum computing architectures.

References

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Figures

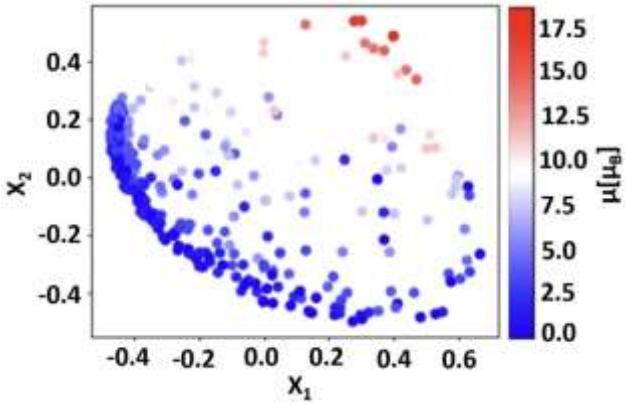

Figure 1. The 2D projection of the embedding space of the autoencoder neural network is displayed. The first and second principal components, X_1 and X_2, are on the horizontal and vertical axis, respectively. A pattern in the data emerges indicating a connection between the position in embedding space and the value of the magnetic moment.