Harnessing Artificial Intelligence for Predicting Proximity Effects in Van der Waals Heterostructures

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The emergence of van der Waals (vdW) heterostructures has revolutionized materials science by enabling the design of complex systems with tailored electronic, optical, and mechanical properties [1]. These heterostructures, constructed by stacking atomically thin layers of two-dimensional (2D) materials, exhibit proximity effects that can profoundly influence their performance in applications such as spintronics, quantum computing, optoelectronics, and energy storage. However, accurately predicting these effects, driven by subtle interlayer interactions, presents a significant challenge due to the computational expense of traditional first-principles methods like density functional theory (DFT). In contrast, artificial intelligence promises rapid exploration of vast parameter spaces, identifying optimal vdW heterostructure configurations for targeted applications.

In this work, we introduce a machine learning (ML) framework to predict proximity effects in vdW heterostructures with high fidelity and computational efficiency, based on the assumption that proximity effects are determined by the local atomistic environment. The approach leverages a dataset generated through extensive DFT calculations, encompassing diverse combinations of 2D materials with varying stacking geometries, interlayer distances, and electronic properties.

We evaluate the performance of multiple ML algorithms, including prototypical regression models, support vector machines, and neural networks, comparing the predictive accuracy across the test set. By incorporating domain knowledge, we ensure that the models capture critical physics, such as orbital hybridization and layer-resolved density of states. Feature importance analysis highlights the pivotal role of material-specific properties, providing insights into the mechanisms underpinning proximity effects.

We validate the model predictions against independent DFT simulations and (if available) experimental data, achieving remarkable agreement. As a case study, we present the results for twisted $CrGeTe_3$/Gr heterostructure (see Fig. 1). CrCeTe3 is a semiconducting 2D ferromagnet [2]. In this stacked heterostructure, magnetic moments are induced in the graphene layer. In addition, Moire patterns (specific atomistic configurations appearing periodically along the plane) occur due to the relative twisting of the layers. Characterizing these complex patterns is not feasible in DFT as it requires very large simulation cells. Thus, it offers a perfect test case for showcasing the abilities of ML-driven material science.

This study underscores the transformative potential of artificial intelligence in advanced materials research, offering a pathway to accelerate the discovery and optimization of vdW heterostructures. By integrating ML with first-principles calculations, we bridge the gap between computational efficiency and predictive accuracy, paving the way for novel material functionalities. The framework is extensible to other material classes, highlighting its versatility in addressing broader challenges in condensed matter physics and materials design.

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References

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[2] A. Noah, H. Alpern, et al. Nano Letters, 22/7 (2022) 3165-3172.

Figures

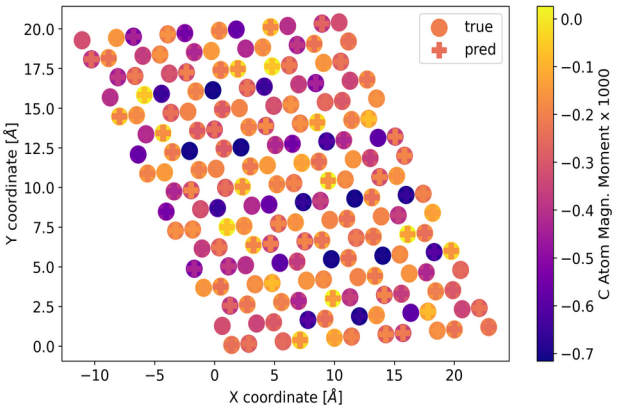

Figure 1. DFT (“true”) vs. ML-predicted values of the magnetic moments of C atoms in a graphene layer stacked on a layer of ferromagnetic $CrCeTe_3$ and twisted with respect to it. The magnetic moments are induced by proximity effects.