Learning Understandable Hamiltonian Models for 2D Materials

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The integration of first-principles techniques with machine learning holds significant potential to transform computational materials science. Recent efforts have aimed to streamline the computationally intensive self-consistent field iterations of Density Functional Theory (DFT) and enhance the efficiency of ab initio electronic-structure calculations. Notably, approaches like the atomic cluster expansion method [1] and message passing neural networks [2] have demonstrated high accuracy and broad applicability.

This presentation delves into the challenges of developing accurate yet straightforward Hamiltonians for 2D materials. The method discussed here involves quasi-atomic orbitals disentanglement [3] and multi-center tight-binding expansion [4,5], offering a relatively simple parameterization with clear physical interpretations. The presented data-driven approach opens avenues for studying complex materials systems such as twisted van der Waals structures.

References

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