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Next-Level Optoelectronic Property Predictions with Hamiltonian Learning

Short abstract:

Machine learning (ML) has revolutionized computations of molecules and materials, ranging from predicting protein structures to data-driven discoveries of new compounds, automated synthesis and more. Here, I will present ML models to predict the quantum-mechanical Hamiltonian, which is the key quantity in electronic structure theory from which many optoelectronic properties can be straightforwardly computed. Our contribution to the rapidly advancing field of Hamiltonian learning concerns optoelectronic properties of semiconductors at finite temperatures, where we aim to bypass costly explicit first-principles calculations and leverage accurate yet computationally cheap ML models instead. I will demonstrate application of such models to halide perovskite supercells containing tens of thousands of atoms and present new workflows to predict thermal behavior of defective materials.