

AI-Accelerated Discovery of Emergent Properties in 2D Materials and Moiré Superlattices

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Moiré superlattices formed in twisted and stacked 2D materials offer a powerful platform for engineering interfacial electronic and optical properties. Their vast supercells and complex reconstructions, however, challenge the limits of conventional first-principles methods. In this talk, I will present machine-learning assisted first-principles calculations that enable large-scale simulations of moiré structures, capable of handling twisted multilayer homo and heterostructures with varying composition, twist angles, stacking, and layer numbers.

Demonstrated on twisted MoTe₂, our calculations capture topology-driven band transitions and provide a scalable solution for studying correlated moiré phenomena in complex environment, predicting emergent electronic features such as flatter Chern bands. The emergent moiré potentials and band structures in turn govern the behavior of excitons with unusually large dipole moments and tunable spatial profiles. By incorporating spin-lattice descriptors, the same machine-learning assisted framework reveals pathways to coupled excitonic and magnetic responses.

Our AI-accelerated strategy extends the predictive reach of first-principles theory, providing new insights into how twist angle, stacking order, and electric control can be used to design moiré materials with tailored optical, electronic, and spin functionalities.