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Constructing realistic low-energy effective models of materials

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Abstract

Model hamiltonians are a useful tool to approach the many-body problem in materials. They often provide valuable physical insight and enable larger length-scale studies. However, since model parameters are invariably unknown, this approach often lacks predictive power, an issue that turns more significant in materials with strong electronic correlations. Being able to controllably construct accurate effective models of materials is thus highly desirable. I will present a methodology that uses highly accurate many-body simulations to inform the construction of model hamiltonians that accurately approximate a material's low-energy physics. I will show results on low-dimensional materials.