From real materials to model Hamiltonians: multiscale modelling of strongly correlated electronic systems

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Given a realistic material with all its intrinsic complications, how does one develop simple reliable models for understanding its properties? Theoretical insight has been the key driver of this process leading to simple few-band pictures. When the interactions are comparable or much stronger than the kinetic energy, it is convenient to adopt the real space lattice approach. The effective Hamiltonian involves a considerable renormalization of parameters. Estimating these values is important for several applications in physics and chemistry. Bands/states far from the Fermi level play a significant role in the screening of Coulomb interactions leading to Hubbard U's that have been traditionally hard to determine reliably. Here we discuss an approach that we have been developing which builds in several safeguards and provides a way of obtaining effective Hamiltonians which can be simulated using techniques specifically defined for small local Hilbert spaces.