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Towards prediction of correlated material properties using quantum Monte Carlo methods

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Correlated electron systems offer a richness of physics far beyond noninteracting systems. If we would like to pursue the dream of designer correlated materials, or, even to set a more modest goal, to explain in detail the properties and effective physics of known materials, then accurate simulation methods are required. Using modern computational resources, quantum Monte Carlo (QMC) techniques offer a way to directly simulate electron correlations. I will show some recent results on a few extremely challenging materials including the metal-insulator transition of VO_2, the ground state of the doped cuprates, and the pressure dependence of magnetic properties in FeSe. By using a relatively simple implementation of QMC, at least some properties of these materials can be described truly from first principles, without any adjustable parameters. Using the QMC platform, we have developed a way of systematically deriving effective lattice models from the simulation. This procedure is particularly attractive for correlated electron systems because the QMC methods treat the one-body and many-body components of the wave function and Hamiltonian on completely equal footing. I will show some examples of using this downfolding technique and the high accuracy of QMC to connect our intuitive ideas about interacting electron systems with high fidelity simulations. The work in this presentation was supported in part by NSF DMR 1206242, the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program under Award Number FG02-12ER46875, and the Center for Emergent Superconductivity, Department of Energy Frontier Research Center under Grant No. DEAC0298CH1088. Computing resources were provided by a Blue Waters Illinois grant and INCITE PhotSuper and SuperMatSim allocations.