

Electron correlation effects are particularly strong in materials containing transition metals. Historically, it has not been practical to directly calculate these effects from first principles because of the large Hilbert spaces involved. For the first time, using quantum Monte Carlo techniques, we have explicitly simulated electron correlations in several challenging materials from first principles, including the parent materials of the high temperature superconducting cuprate materials and the correlated metal vanadium dioxide. Our simulations accurately reproduce many important physical quantities about these materials, including the interaction-induced gaps and the superexchange coupling between copper spins, with no additional parameters beyond fundamental constants. We further use these high accuracy achieved here to gain insight into physical questions about these materials, elucidating the origin of the metal-insulator transition in vanadium dioxide and spin-lattice coupling in the cuprate materials. The latter may have important implications for the origin of pairing in the superconducting phase.

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