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Quantum Monte Carlo Calculations of Transition Metal Oxides[1]

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Quantum Monte Carlo is a powerful computational tool to study correlated systems, allowing us to explicitly treat many-body interactions with favorable scaling in the number of particles. It has been regarded as a benchmark tool for first and second row condensed matter systems, although its accuracy has not been thoroughly investigated in strongly correlated transition metal oxides. QMC has also historically suffered from the mixed estimator error in operators that do not commute with the Hamiltonian and from stochastic uncertainty, which make small energy differences unattainable. Using the Reptation Monte Carlo algorithm of Moroni and Baroni(along with contributions from others), we have developed a QMC framework that makes these previously unavailable quantities computationally feasible for systems of hundreds of electrons in a controlled and consistent way, and apply this framework to transition metal oxides. We compare these results with traditional mean-field results like the LDA and with experiment where available, focusing in particular on the polarization and lattice constants in a few interesting ferroelectric materials. This work was performed in collaboration with Lubos Mitas and Jeffrey Grossman.

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