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Application of Quantum Monte Carlo Methods to Describe the Properties of Manganese Oxide Polymorphs JOSHUA SCHILLER, ELIF ERTEKIN, Univ of Illinois - Urbana — First-principles descriptions of the properties of correlated materials such as transition metal oxides has been a long-standing challenge. Manganese oxide is one such example: according to both conventional and hybrid functional density functional theory, the zinc blende polymorph is predicted to be lower in energy than the rock salt polymorph that occurs in nature. While the correct energy ordering can be obtained in density functional approaches by careful selection of modeling parameters, we present here an alternative approach based on quantum Monte Carlo methods, which are a suite of stochastic tools for solution of the many-body Schrodinger equation. Due to its direct treatment of electron correlation, the QMC method offers the possibility of parameter-free, high-accuracy, systematically improvable analysis. In manganese oxide, we find that the QMC methodology is able to accurately reproduce relative phase energies, lattice constants, and band gaps without the use of adjustable parameters. Additionally, statistical analysis of the many-body wave functions from QMC provides some diagnostic assessments to reveal the physics that may be missing from other modeling approaches.

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