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***Ab initio* quantum Monte Carlo calculations of ground-state properties of manganese's oxides**[1] VINIT SHARMA, JARON T. KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, P.R.C. KENT, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, FERNANDO A. REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — One of the critical scientific challenges of contemporary research is to obtain an accurate theoretical description of the electronic properties of strongly correlated systems such as transition metal oxides and rare-earth compounds, since state-of-art ab-initio methods based on approximate density functionals are not always sufficiently accurate. Quantum Monte Carlo (QMC) methods, which use statistical sampling to evaluate many-body wave functions, have the potential to answer this challenge. Owing to the few fundamental approximations made and the direct treatment of electron correlation, QMC methods are among the most accurate electronic structure methods available to date. We assess the accuracy of the diffusion Monte Carlo method in the case of rocksalt manganese oxide (MnO). We study the electronic properties of this strongly-correlated oxide, which has been identified as a suitable candidate for many applications ranging from catalysts to electronic devices. "This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division."

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