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Quantum Monte Carlo study of the oxygen vacancy in vanadium dioxide[1] JARON KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 U.S.A., YE LUO, ANOUAR BENALI, Argonne Leadership Computing Facility, Argonne National Laboratory, Argonne, Illinois 60439 U.S.A., JANAKIRAMAN BALACHANDRAN, PANCHAPAKESAN GANESH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 U.S.A., OLLE HEINONEN, Materials Science Division, Argonne National Laboratory, Lemont, IL 60439 U.S.A., PAUL R. C. KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 U.S.A. — Transition metal oxides (TMO's) have presented fundamental challenges for accurate fully ab initio calculations. Vanadium dioxide, in particular, has remained difficult to describe in a consistent and predictive manner for leading theoretical approaches, such as density functional theory (DFT). Quantum Monte Carlo (QMC) methods present an attractive alternative to DFT as they have been shown to be accurate for a range of TMO's, including bulk phases of VO_2. In this work we expand the application of QMC to inquire into the behavior of isolated oxygen vacancies in VO_2, carefully controlling for known sources of systematic error. We compare our preliminary results with broadly used DFT approximations including hybrid functionals and Hubbard-U type approaches.

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