Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Diffusion Quantum Monte Carlo predictions for bulk $MnNiO_3$[1]

CHANDRIMA MITRA, JARON KROGEL, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — $MnNiO_3$ is a strongly correlated transition metal oxide that has recently been investigated theoretically for its potential application as an oxygen-evolution photo-catalyst. However, there is no experimental report on critical quantities like its band gap or its bulk modulus. Recent theoretical predictions with standard functionals, such as PBE+U and HSE show large discrepancies in the band-gaps (about 1.23 eV), depending on the nature of the functional used. Hence, there is clearly a need for an accurate quantitative prediction of the band-gap in order to decide its usefulness as a photo-catalyst. In this work, we present Diffusion Quantum Monte Carlo (DMC) study of the bulk properties of $MnNiO_3$. This includes the quasiparticle band gap for the two spin channels, the equilibrium lattice parameter and the bulk modulus. The DMC approach has already been shown to achieve excellent agreement with experimental results for other oxides such as ZnO NiO and Fe_2O_3. To our knowledge, $MnNiO_3$ is the first case where this theory is applied before experiments are done.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

Chandrima Mitra
Oak Ridge National Laboratory

Date submitted: 05 Nov 2015 Electronic form version 1.4