Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Defect formation energies and equations of state of Mn oxides using diffusion Monte Carlo VINIT SHARMA, JARON KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, PAUL KENT, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, FERNANDO REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Quantum Monte Carlo (QMC) methods are the most accurate methods available for *ab-initio* calculations of systems with more than 100 electrons. A family of projector methods allows the direct treatment of electron corrections by statistical sampling. Using the diffusion quantum Monte Carlo (DMC) method, as implemented in QMCPACK, we calculate the cohesive energy, formation energy and the structural parameters of MnO and MnO_2 and the ternary perovskite $LaMnO_3$. Next, we study the oxygen vacancy and cationic dopants in $(La,A)MnO_3$ (A = Ca, Sr, and Ba) which have been identified as suitable candidates for improving the electro-chemical properties of the parent material. The goals the present work are (a) to quantify the accuracy of the DMC method to study the transition metal oxides, (b) to establish the accuracy of different approximations of density functional theory as compared with DMC results, and (c) to demonstrate in another case that QMC methods are an accurate tool for the prediction of the properties of strongly correlated systems.

Vinit Sharma
Oak Ridge National Lab

Date submitted: 12 Nov 2016 Electronic form version 1.4