Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A Study of Phase Stability and Properties of TiO2 Polymorphs with Diffusion Monte Carlo YE LUO, ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories, JARON KROGEL, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory — In the past decades, many studies have focused on the fundamental properties of TiO_2 due to its important role in effectively converting solar energy such as in photovoltaic batteries and photocatalic water splitting. TiO2 presents many stable and metastable phases of which, Rutile Anatase and Brookite are the most studied. Using density functional theory (DFT), the energy ordering of these phases depends strongly on the scheme describing the electronic correlation, for instance GGA+U and Hybrid functionals, often tied to an empirical parameter for reproducibility with no guarantee of predictability. We present the first analysis of the polymorphic energy ordering and properties of three naturally existing phases Rutile, Anatase and Brookite, by performing the highly accurate ab initio calculation with fixed node diffusion Monte Carlo (DMC) implemented in QMCPACK[1]. [1] QMCPACK, http://www.qmcpack.org

Ye Luo
Argonne National Laboratory

Date submitted: 06 Nov 2015 Electronic form version 1.4