Abstract Submitted
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Structural Stability and Ionic Defects in ZnO from Quantum Monte Carlo[1] JUAN A. SANTANA, Oak Ridge Assoc Univ, JARON T. KROGEL, JEONGNIM KIM, PAUL R.C. KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — An accurate method capable of describing atomic, molecular and solid-state systems is required to take a full advantage of computer-aided materials discovery and design. We show that the many-body *ab-initio* diffusion monte carlo (DMC) method is now a practical method for such tasks. We have studied the atomic, molecular and solid-state properties of the Zn-O system with DMC. In particular, the equation of state of bulk Zn and ZnO in the rock salt, zinc blend and wurtzite phases and the properties of ionic defects in wurtzite ZnO were studied. The first ionization potential of O and Zn, and the atomization energy of O_2, ZnO dimer, and wurtzite ZnO as well as the band gap of this material were evaluated with DMC, and the results agree with experimental measurements to within 0.2 eV. The DMC atomization energy of bulk Zn, 1.00(1) eV, is also in good agreement with the experimental value, 1.35 eV, considering the complexity of this metallic system. The DMC calculated properties of Zn and ZnO under pressure, and the formation energy for the oxygen vacancy, hydrogen impurities and Zn interstitial defects in ZnO will be discussed in comparison with results from experiments and density functional theory approximations.

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