Diffusion Monte Carlo Calculations of the Equation of State, Band Gaps and Point Defect properties of Transition Metal Oxides

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It has been argued that the highly-localized partially-occupied d orbitals increase the role of exchange and correlations in transition metal oxides (TMO). Therefore key properties of TMO remain outstanding problems for methods based on the usual approximations of density functional theory (DFT). Recent advances in algorithms and computers have allowed the study of TMO with Diffusion Monte Carlo (DMC) and other many-body methods. We will discuss the DMC calculations performed by our team in this area. The equation of state of multiple oxides such us ZiO, NiO, SrO, LaO, $SrFeO_3$ and $LaFeO_3$ will be presented. Calculations were also performed with various (DFT) approximations for comparison. For all these materials DMC reproduces the measured cohesive energies within 0.25 eV of experiments or better and the structural properties within 1% of the experimental values or better. The DMC formation energies of the oxygen vacancy in ZnO, NiO, $SrFeO_3$ and $LaFeO_3$ under oxygen-rich conditions will be presented and compared with similar calculations performed with semi-local DFT approximations \. Comparison of charge densities shows that current DFT approximations tend to over delocalize impurity electrons in defected oxides as compared with DMC results.