Abstract Submitted
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Quantum Monte Carlo Applied to Binary Transition Metal-Oxides[1] JUAN A. SANTANA, Oak Ridge Assoc Univ, JARON T. KROGEL, CHANDRIMA MITRA, PAUL R.C. KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — Materials based on transition metal-oxides (TMO) play a central role in many applications and in the fundamental research of advanced materials. However, this class of materials is one of the most challenging for computation. The standard computational methods to study them are based on Density Functional Theory (DFT), which often fails to provide the required level of accuracy. A natural solution to overcome the intrinsic limitations of DFT approximations is to directly solve the many-body problem in TMO. For large systems, this can be made practical by applying quantum Monte Carlo (QMC) methods. These methods are very expensive computationally, but recent developments in algorithms and computational infrastructures have enabled their application to real materials. We will show that QMC methods, such as diffusion Monte Carlo (DMC), are now practical to study multiple properties of TMO. The application of DMC to study the structural, electronic and ionic defect properties of various binary TMO, including FeO, CoO, NiO, and ZnO will be discussed. We will also outline current limitations in hardware and algorithms.

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