Abstract Submitted
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Parameters Free Computational Characterization of Defects in Transition Metal Oxides with Diffusion Quantum Monte Carlo[1] JUAN A. SANTANA, University of Puerto Rico at Cayey, JARON T. KROGEL, PAUL R. KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — Materials based on transition metal oxides (TMO's) are among the most challenging systems for computational characterization. Reliable and practical computations are possible by directly solving the many-body problem for TMO's with quantum Monte Carlo (QMC) methods. These methods are very computationally intensive, but recent developments in algorithms and computational infrastructures have enabled their application to real materials. We will show our efforts on the application of the diffusion quantum Monte Carlo (DMC) method to study the formation of defects in binary and ternary TMO and heterostructures of TMO. We will also outline current limitations in hardware and algorithms.

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