

Abstract Submitted  
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**An effective model for LaTiO<sub>3</sub> using first principles quantum Monte Carlo** KIEL WILLIAMS, LUCAS WAGNER, Univ of Illinois - Urbana  
— The rare earth perovskites have long been of interest due in part to the interplay of their geometries and electronic properties. The perovskite LaTiO<sub>3</sub> in particular is an antiferromagnetic insulator with a small 0.2 eV band gap that displays the GdFeO<sub>3</sub> distortion at ambient pressure. We apply a new technique[1] to derive an effective model for LaTiO<sub>3</sub> as a function of the distortion. Since this technique treats one and two-body degrees of freedom on an equal footing, we use it to evaluate the evolution of effective model parameters with changes in the lattice. We will report on the progress in assessing whether the insulating nature is due to the distortion, or vice versa. [1] Changlani, Zheng, and Wagner J. Chem. Phys. 143, 102814 (2015).

Kiel Williams  
Univ of Illinois - Urbana

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