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$BaTiO_3$ and Quantum Monte Carlo: Lattice Constants LUCAS K. WAGNER, LUBOS MITAS, North Carolina State University — Transition metal oxides are well-known to be difficult to describe using standard first principles techniques like Density Functional Theory. For example, straightforward application of generalized gradient and local density approximations make errors of about 3% on the primitive cell volume of $BaTiO_3$ in the tetragonal phase, one of the simplest ferroelectrics. Since the ferroelectric properties are extremely sensitive on lattice constants and structural parameters one has to either adjust the functionals or set the lattice constant to experiment with a resulting error in phase transition temperature. We show progress on calculations using Quantum Monte Carlo (QMC) to predict the static properties of $BaTiO_3$, using correlated sampling to overcome the statistical error on these extremely small energy differences. Preliminary results indicate that QMC is able to predict the tetragonal volume to less than 1%(the error bars) without experimental input, as well as describe the band gap with a good agreement with experiment.

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