Abstract Submitted
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Electronic Structure Calculations of BiFeO3[1] DAVID SULOCK, LUCAS K. WAGNER, LUBOS MITAS, North Carolina State University — Bismuth Ferrite (BiFeO3) is a potentially useful material because it exhibits both ferroelectricity and antiferromagnetism, providing a link between magnetic and ferroelectric action in the same material. Experimentally BiFeO3 has been reported to have a spontaneous polarization ranging from .06 C/m2 to 1.50 C/m2, possibly indicating a large dependence on experimental setup. Theoretical efforts thus far within Density Functional Theory in the LDA approximation have settled on a value of around 0.95 C/m2; however, it is not clear that LDA provides a sufficient description of the material as it predicts a lattice constant in error by .2 angstroms and zero band gap for some parts of the ferroelectric distortion. To check the results provided by LDA we use Quantum Monte Carlo (QMC), which allows us to treat the system in a fully correlated way. We use the Reptation Monte Carlo algorithm of Moroni and Baroni to calculate the polarization and other properties, allowing us to then evaluate the accuracy of QMC versus LDA.

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