Auxiliary Field Quantum Monte Carlo Calculations of Ferroelectric Instability

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College of William and Mary — The perovskite structure alloys (BiScO)\textsubscript{3-x} - (PbTiO\textsubscript{3})\textsubscript{x} have strong ferroelectric instabilities. The ferroelectric double-well depths of BiScO\textsubscript{3}, calculated by density functional theory (DFT), are an order of magnitude larger than for PbTiO\textsubscript{3} and PbZrO\textsubscript{3}\textsuperscript{2}. We carry out quantum Monte Carlo (QMC) calculations on BiScO\textsubscript{3} to help assess the accuracy of DFT. We use a recently developed auxiliary field QMC method \textsuperscript{3}. The two-body electronic Coulomb interactions are decoupled using a Hubbard-Stratonovich transformation. The method iteratively projects out the ground state from an initial trial wave function by random walks in the space of Slater determinants. The trial wave function is a single Slater determinant constructed from a DFT calculation using ABINIT \textsuperscript{4}. A plane wave basis and periodic boundary conditions were used in the calculations. The ions are represented by norm-conserving Kleinman-Bylander non-local pseudopotentials. Applications of the method on simpler systems gave very encouraging results.

\textsuperscript{1}Supported by NSF, ONR
\textsuperscript{4}http://www.abinit.org

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Date submitted: 01 Dec 2004

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