Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Auxilliary Field Quantum Monte Carlo Calculations of Ferroelectric Instability[1] HENDRA KWEE, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — The perovskite structure alloys $(BiScO_3)_{1-x}$ - $(PbTiO_3)_x$ have strong ferroelectric instabilities. The ferroelectric double-well depths of $BiScO_3$, calculated by density functional theory (DFT), are an order of magnitude larger than for $PbTiO_3$ and $PbZrO_3$[2]. We carry out quantum Monte Carlo (QMC) calculations on $BiScO_3$ to help assess the accuracy of DFT. We use a recently developed auxilliary field QMC method [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 [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.

[1]Supported by NSF, ONR
[2]J. Íñiquez, D. Vanderbilt, L. Bellaiche, *Phys. Rev B* **67**, 224107 (2003)
[3]S. Zhang, and H. Krakauer, *Phys. Rev. Lett* **90**, 136401 (2003)
[4]http://www.abinit.org

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Date submitted: 01 Dec 2004 Electronic form version 1.4