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**Quantum Monte Carlo calculations of BiScO<sub>3</sub> ferroelectric well-depths**<sup>1</sup> HENDRA KWEЕ, College of William and Mary, HENRY KRAKAUER, College of William and Mary, SHIWEI ZHANG, College of William and Mary — The perovskite (1-x) BiScO<sub>3-x</sub>PbTiO<sub>3</sub> alloy has been reported as having a large piezoelectric properties.<sup>2</sup> Density functional theory (DFT) using local density approximation (LDA) predicts an extraordinarily large ferroelectric well depths (about 1.2 eV) of the end point compound BiScO<sub>3</sub>.<sup>3</sup> We perform quantum Monte Carlo calculations on BiScO<sub>3</sub> to calculate these well depths. In our QMC method,<sup>4</sup> the two-body terms coming from electron-electron interactions are decoupled using a Hubbard-Stratonovich transformation. The ground state is obtained from projection of an initial trial wave function by random walks in Slater determinant space. To control the sign/phase problem, a trial Slater determinant is used, which in our calculations is taken directly from the DFT calculations. We find in the QMC calculation large finite-size effects in the primitive cell, on the order of a few eV. We study these finite-size effects and explore several schemes to reduce them.

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<sup>2</sup>R.E. Eitel, *et al.*, *Jpn. J. Appl. Phys.*, Part 1 **40**,5999 (2001); R.E. Eitel, *et al.*, *ibid.* **41**, 1 (2002)

<sup>3</sup>J. Íñiguez, D. Vanderbilt, L. Bellaiche, *Phys. Rev B* **67**, 224107 (2003)

<sup>4</sup>S. Zhang, H. Krakauer, *Phys. Rev. Lett* **90**, 136401 (2003)

Hendra Kwee

hendra@camelot.physics.wm.edu  
College of William and Mary

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