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Quantum Monte Carlo calculations of $BiScO_3$ ferroelectric well-depths[1] HENDRA KWEE, College of William and Mary, HENRY KRAKAUER, College of William and Mary, SHIWEI ZHANG, College of William and Mary — The perovskite (1-x) $BiScO_3$-x $PbTiO_3$ alloy has been reported as having a large piezoelectric properties.[2] 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 $BiScO_3$.[3] We perform quantum Monte Carlo calculations on $BiScO_3$ to calculate these well depths. In our QMC method,[4] 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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Hendra Kwee
College of William and Mary

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