Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First principles study of the band gaps and edges of (111) epitaxially strained $SrTiO_3$ SEBASTIAN E. REYES-LILLO, Molecular Foundry, Lawrence Berkeley National Laboratory, ROBERT F. BERGER, Department of Chemistry, Western Washington University, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory; Department of Physics, University of California-Berkeley — $SrTiO_3$ is a tunable material with potential use in energy applications. Previous experimental and first principles results demonstrated controllable manipulation of the electronic band gap in (001) biaxially strain, and predicted a large room-temperature band gap reduction (0.3 eV) for (111) epitaxial growth at small and large strains. In this work, we revisit and examine the effect of (111) epitaxial strain on the structural and electronic properties of $SrTiO_3$ using density functional theory calculations at low and room temperatures. Under (111) epitaxial strain at low temperature, we find that $SrTiO_3$ has an antiferrodistortive ground state at large compressive strains ($<$ -1%) and a ferroelectric phase transition between -1% $< \eta <$ 4% biaxial strains. While structural distortions widen the band gap compared to the paraelectric phase, an effective reduction of band gap is observed for the distorted structure at large compressive strains compared to bulk. This work is supported by DOE, computational resources are provided by NERSC.

Sebastian E. Reyes-Lillo
Molecular Foundry, Lawrence Berkeley National Laboratory,
Berkeley, California 94720, USA

Date submitted: 14 Nov 2014 Electronic form version 1.4