Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Manipulating the Band Structure of $SrTiO_3$ with Strain[1] DARRELL G. SCHLOM, CHARLES M. BROOKS, Cornell University, DAGMAR CHVOSTOVA, VLADIMIR TREPAKOV, Institute of Physics ASCR, MEGAN E. HOLTZ, Cornell University, NIK J. PODRAZA, University of Toledo, ROBERT F. BERGER, Lawrence Berkeley National Laboratory, LENA F. KOURKOUTIS, TASSILO HEEG, Cornell University, MARGITTA BERNHAGEN, REINHARD UECKER, Leibniz Institute for Crystal Growth, JUERGEN SCHUBERT, Research Centre Juelich, CRAIG J. FENNIE, Cornell University, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, DAVID A. MULLER, Cornell University, ALEXANDR DEJNEKA, Institute of Physics ASCR — $SrTiO_3$, the hydrogen atom of perovskites, is a very stable photocatalyst for water splitting. In this talk we demonstrate that the bandgap of $SrTiO_3$ can be altered by ± 10% (0.3 eV) using biaxial strain in combination with phase transitions. The strain behavior is predicted and experimentally observed to be significantly different for (100) vs. (111) biaxially strained $SrTiO_3$ surfaces. In the absence of phase transitions the bandgap of biaxially strained $SrTiO_3$ decreases. In contrast, a strain-induced ferroelectric phase transition results in an increase in the bandgap. The band structure can also be morphed from indirect to direct bandgap through an antiferrodistortive phase transition. Both of these phase transitions can be manipulated using experimentally realizable biaxial strains, providing a new means to accomplish bandgap engineering of $SrTiO_3$ and related perovskites.

[1]This work was supported by DOE under Grant No. DE-SC0001086.

Darrell G. Schlom
Cornell University

Date submitted: 15 Nov 2013 Electronic form version 1.4