Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Predicting In-Situ X-ray Diffraction for the $SrTiO_3$/Liquid Interface from First Principles[1] KENDRA LETCHWORTH-WEAVER, DENIZ GUNCELER, RAVISHANKAR SUNDARARAMAN, XIN HUANG, JOEL BROCK, T. A. ARIAS, Cornell University — Recent advances in experimental techniques, such as in-situ x-ray diffraction, allow researchers to probe the solid-liquid interface in electrochemical systems under operating conditions. These advances offer an unprecedented opportunity for theory to predict properties of electrode materials in aqueous environments and inform the design of energy conversion and storage devices. To compare with experiment, these theoretical studies require microscopic details of both the liquid and the electrode surface. Joint Density Functional Theory (JDFT), a computationally efficient alternative to molecular dynamics, couples a classical density-functional, which captures molecular structure of the liquid, to a quantum-mechanical functional for the electrode surface. We present a JDFT exploration of $SrTiO_3$, which can catalyze solar-driven water splitting, in an electrochemical environment. We determine the geometry of the polar $SrTiO_3$ surface and the equilibrium structure of the contacting liquid, as well as the influence of the liquid upon the electronic structure of the surface. We then predict the effect of the fluid environment on x-ray diffraction patterns and compare our predictions to in-situ measurements performed at the Cornell High Energy Synchrotron Source (CHESS).

[1]This material is based upon work supported by the Energy Materials Center at Cornell (EMC2), an Energy Frontier Research Center funded by the U.S. Department of Energy.

Kendra Letchworth-Weaver
Cornell University

Date submitted: 09 Nov 2012 Electronic form version 1.4