Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Electronic Structure and Properties of $CePO_4$[1] NICOLE ADELSTEIN, H. RAY, L.C. DE JONGHE, Dept. Materials Science and Engineering, UC Berkeley, B.S. MUN, Dept. Applied Physics, Hanyang University, Republic of Korea, P.N. ROSS JR., Advanced Light Source, LBNL, M. ZBORAY, Dept. Chemical Engineering, UC Berkeley, J.B. NEATON, Molecular Foundry, LBNL — Structural and electronic properties of cerium orthophosphate ($CePO_4$), a mixed electronic and protonic conducting electrolyte, are calculated using density functional theory (DFT) and beyond, and compared with experiments. A Hubbard-like parameter U is employed to reduce the self-interaction for localized Ce 4f states. As U is varied from 1-5 eV, the band structure is found to undergo significant changes, with the Kohn-Sham gap varying between 0.8 and 4.3 eV. Interestingly, the lattice parameters are unchanged, indicating structural properties are far less sensitive to U. The valence band energies and the optical band gap of $CePO_4$ are measured using photoemission and optical reflectance spectroscopy. The structure was determined using XRD. The choice of U = 4 eV provides the best match between the calculated density of states and the experimental photoemission and optical reflectance spectra. The activation energy of the minimum energy path for proton transfer will be calculated and compared to that of $LaPO_4$, another proton conducting electrolyte.

[1]Supported by the Director of the U.S. Dept. of Energy and NERSC

Nicole Adelstein
Dept. Materials Science and Engineering, UC Berkeley

Date submitted: 18 Nov 2009 Electronic form version 1.4