Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles Study of CeO2/BiVO4 Interfaces[1] GUO LI, Lawrence Berkeley Natl Lab, ANIKETA SHINDE, LAN ZHOU, DAN GUEVARRA, SANTOSH SURAM, California Institute of Technology, FRANCISCA TOMA, QIMIN YAN, Lawrence Berkeley Natl Lab, JOEL HABER, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Jeffrey Neaton Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using density functional theory calculations, we investigate the structural, energetic, and electronic properties of CeO2/BiVO4 interfaces. We find that, despite a 5% mismatch, thin CeO2 layers (with thicknesses of up to three monolayers) can be epitaxially grown on BiVO4(010) substrates. At these epitaxial interfaces, all the atoms are fully coordinated. Thus, no localized interface state appears in the band gap. More importantly, the surface states of BiVO4, which serve as recombination centers for excited charges, are eliminated by the CeO2 coating layers. These findings explain the significant decrease of charge recombination observed in experiments.

[1]The work was supported as part of Joint Center for Artificial Photosynthesis, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science and supported by the Molecular Foundry of LBNL

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Date submitted: 10 Nov 2016 Electronic form version 1.4