Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Interplay between chemical and electronic properties of native oxides at photoelectrochemical interfaces[1] TUAN ANH PHAM, Lawrence Livermore National Laboratory, XUEQIANG ZHANG, University of Notre Dame, BRANDON WOOD, Lawrence Livermore National Laboratory, SYLWIA PTASINSKA, University of Notre Dame, TADASHI OGITSU, Lawrence Livermore National Laboratory — Native surface oxidation of photoelectrodes in aqueous solutions is known to play a critical role in the performance and stability of photoelectrochemical cells for solar water splitting; however, probing atomistic details of such process under operating conditions presents significant challenges. Here, we use high-level first-principles simulations of GaP/InP photoelectrodes in contact with water to accurately predict the influence of surface oxide species on the semiconductor band edges. Theoretical results were then combined with band edge measurements to predict the surface chemistry under realistic environments, suggesting that dissociated and non-dissociated adsorbed water coexist on the GaP/InP surfaces, as well as a more rigid hydrogen-bond network at the GaP-water interface. Ambient pressure X-ray photoelectron experiments validate the theoretical predictions, while providing detailed information of surface oxide species.

[1]Part of this work was performed under the auspices of the U.S. Department of Energy at LLNL under Contract DE-AC52-07A27344.

Tuan Anh Pham
Lawrence Livermore National Laboratory

Date submitted: 11 Nov 2016 Electronic form version 1.4