Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Validating First Principles Molecular Dynamics Calculations of Solid/Liquid Interfaces with X-ray Reflectivity KENDRA LETCHWORTH-WEAVER, MARIA K. Y. CHAN, PAUL FENTER, Argonne National Laboratory, ALEX GAIDUK, GIULIA GALLI, University of Chicago — The interface between a metal oxide electrode and liquid water plays a crucial role in energy conversion processes such as photo-electrochemical water splitting and CO_2 reduction to create fuel from sunlight. First principles electronic structure calculations are useful tools to obtain electronic properties relevant to catalysis, such as electron energy alignment between the electrode surface and a reacting molecule, but their ability to predict realistic structural models requires careful validation. We combine calculations of interfacial X-ray structure factors [1] from ab-initio molecular dynamics trajectories with experimental X-ray reflectivity measurements [2] to obtain a validation protocol for structural models of aqueous interfaces. Simultaneously, we provide a means to interpret X-ray reflectivity measurements without the need for model-dependent empirical fitting, offering unique insight into the influence of atomic-scale structure upon reaction mechanisms at surfaces. We will discuss in particular the case of the water/Al_2O_3 (001) interface [3]. [1] M. Plaza et al, *JACS* **138**, 4 (2016) [2] J. G. Catalano, *Geochimica et Cosmochimica Acta* **75**, 10 (2011) [3] P. Huang et al, *J Phys. Chem. C* **118**, 8 (2014).

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Date submitted: 10 Nov 2016 Electronic form version 1.4