Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Optical fingerprints of solid-liquid interfaces: a joint ATR-IR and *first principles* investigation[1] L. YANG, F. NIU, S. TECKLENBURG, M. PANDER, S. NAYAK, A. ERBE, S. WIPPERMANN, Max-Planck-Inst für Eisenforschung, F. GYGI, University of California, Davis, G. GALLI, University of Chicago — Despite the importance of understanding the structural and bonding properties of solid-liquid interfaces for a wide range of (photo-)electrochemical applications, there are presently no experimental techniques available to directly probe the microscopic structure of solid-liquid interfaces. To develop robust strategies to interpret experiments and validate theory, we carried out attenuated total internal reflection (ATR-IR) spectroscopy measurements and *ab initio* molecular dynamics (AIMD) simulations of the vibrational properties of interfaces between liquid water and well-controlled prototypical semiconductor substrates. We show the Ge(100)/H_2O interface to feature a reversible potential-dependent surface phase transition between Ge-H and Ge-OH termination. The Si(100)/H_2O interface is proposed as a model system for corrosion and oxidation processes. We performed AIMD calculations under finite electric fields, revealing different pathways for initial oxidation. These pathways are predicted to exhibit unique spectral signatures. A significant increase in surface specificity can be achieved utilizing an angle-dependent ATR-IR experiment, which allows to detect such signatures at the interfacial layer and consequently changes in the hydrogen bond network.

[1]Funding from DOE-BES Grant No. DE-SS0008939 and the Deutsche Forschungsgemeinschaft (RESOLV, EXC 1069) are gratefully acknowledged.

L. Yang
Max-Planck-Inst für Eisenforschung

Date submitted: 11 Nov 2016 Electronic form version 1.4