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A joint first principles and ATR-IR study of the vibrational properties of interfacial water at semiconductor-water solid-liquid interfaces LEI YANG, STEFANIE TECKLENBURG, FANG NIU, ANDREAS ERBE, STE-FAN WIPPERMANN, Max-Planck-Institut für Eisenforschung, FRANCOIS GYGI, University of California, Davis, GIULIA GALLI, University of Chicago — Despite the importance of understanding the structural and bonding properties of solidliquid 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. We carried out joint ATR-IR spectroscopy measurements and *ab initio* molecular dynamics simulations of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates. In particular, the  $Ge(100)/H_2O$  interface is shown to feature a reversible bias potential dependent surface phase transition. Our study highlights the key role of coupled theory-experimental investigations on well controlled and characterized interfaces, in order to develop robust strategies to interpret experiments and validate theory. The authors wish to thank T. A. Pham for helpful discussions. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SS0008939.

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