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A joint *first principles* and ATR-IR study of the vibrational properties of interfacial water at Si(100):H-H_2O solid-liquid interfaces[1] LEI YANG, STEFANIE TECKLENBURG, ANDREAS ERBE, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research, FRANCOIS GYGI, University of California, Davis, GIULIA GALLI, University of Chicago — Understanding the structural and bonding properties of solid-liquid interfaces is crucial for a wide range of (photo-)electrochemical applications, such as e. g. solar water splitting and electrolysis. However, there are no experimental techniques presently available allowing one to directly probe the microscopic structure of solid-liquid interfaces. We present a joint investigation of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates, i.e. hydrogenated silicon surfaces. We carried out attenuated total internal reflection (ATR-IR) spectroscopy measurements and *ab initio* molecular dynamics simulations. The latter allowed us to interpret the experiments and to unravel specific bonding configurations and interactions of water molecules with the solid surfaces. 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.

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