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Water at a hydrophilic solid surface probed by *ab-initio* molecular dynamics: inhomogeneous thin layers of dense fluid. GIANCARLO CICERO, JEFFREY GROSSMAN, LLNL, Livermore CA, ALESSANDRA CATELANI, CNR-IMEM, Parma Italy, GIULIA GALLI, LLNL, Livermore CA — We present a microscopic model of the interface between liquid water and a hydrophilic, solid surface, as obtained from *ab-initio* molecular dynamics simulations. In particular, we focused on the (100) surface of cubic SiC, a leading candidate semiconductor for bio-compatible devices. Our results show that, in the liquid in contact with the clean substrate, molecular dissociation occurs in a manner unexpectedly similar to that observed in the gas phase. After full hydroxylation takes place, the formation of a thin ($\sim 3 \text{ \AA}$) interfacial layer is observed, which has higher density than bulk water and forms stable hydrogen bonds with the substrate. The liquid does not uniformly ‘wet’ the surface, rather molecules preferably bind along directions parallel to the Si dimer rows. Our calculations also predict that at $\sim 1 \text{ nm}$, the structural and electronic properties of liquid water are weakly affected by one-dimensional confinement between hydrophilic, solid substrates. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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