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Water monomer interaction with H-passivated Si nanowires from density functional theory ABRAHAM HMIEL, YONGQIANG XUE, University at Albany-SUNY — A molecular-level understanding of the interaction between water and nanomaterials is essential for such important phenomena as corrosion, catalysis, electrochemistry and biology. In this talk we present density functional (DFT) study of the structure and energetics of water monomer binding to the surfaces of hydrogen terminated silicon nanowires (SiNWs), which represents the initial phase of interfacial water. We present results on the binding site and orientation of individual water molecules on the surfaces of [112] and [110] oriented SiNWs and analyze the energetics of water adsorption through potential energy surface scan along selected degrees of freedom.

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