

Abstract Submitted
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Field-effect modulation of water adsorption on the TiO₂ (110) surface from van der Waals density functional theory¹ ABRAHAM HMIEL, YONGQIANG XUE, State University of New York at Albany - College of Nanoscale Science and Engineering — The interaction of water and the titanium dioxide surface has been identified as a target problem across many possible fields of application of electrochemical devices and sensors, as the surface chemistry at the interface is not well-understood. This work applies self-consistent van der Waals density functional theory and the effective screening medium theory² to study the surface chemistry and wetting of H₂O on nanostructured TiO₂ surfaces. Water-TiO₂ substrate interactions are probed from the monomer limit up to monolayer coverage under an external electric field in a charged capacitor model. We illustrate the competitive effect between the electric field and the descriptions of the hydrogen bonding induced by the application of the van der Waals functional by analyzing the energetics, charge partitioning, and bonding at the interface.

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