Seminarankündigung

Dienstag, 1. Juni 2021
17:00 Uhr

ONLINE via ZOOM

"Aqueous interfaces with pristine and chemically-modified TiO_2 surfaces: Insights from ab-initio based simulations"

Due to its natural abundance, chemical stability, and environmental compatibility, TiO2 still is one of the most widely used photocatalysts for scientific and technological applications. Of particular relevance is the anatase phase of TiO2, which predominates at the nanoscale. Since TiO2 photocatalysis usually takes place in humid or aqueous environment, the interface of anatase TiO2 with water is of fundamental importance, e.g., for elucidating the detailed mechanisms of photochemical water splitting and UV-induced hydrophilicity, and for improving the performance of TiO2 nanomaterials in various devices. In this talk I shall discuss recent applications of ab-initio based molecular dynamics to the elucidation of anatase-water interfaces. These will include large scale neural network simulations of the water interface with the most abundant anatase (101) surface, revealing an entropy-driven dynamical equilibrium of molecular and dissociative adsorption of water at the interface. Simulations of formic and acetic acid coated anatase TiO2 in contact with water will also be presented, providing insight into the role of the competitive interactions of carboxylic acid and water on functionalized TiO2 and the observed hydrophobic behavior of TiO2 surfaces under ambient conditions.

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