

Comparison of Pure and Salty Water on Rutile Surfaces

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Titanium dioxide (TiO₂, titania) is one of the industrially most relevant materials and, consequently, a vast number of studies can be found in the literature [1-3]. Since many applications involve the presence of an aqueous environment, the solid – water interface is of particular interest [4,5]. There has been a large number of studies on the gas-phase H₂O – TiO₂ interaction, but the liquid – solid interface is more relevant for applications. Titania surfaces also frequently contain defects, which adds to the complexity. One recent study on such a complex water – titania interface used a combination of state-of-the-art experimental and theoretical methods to show the formation of an ordered hydroxyl overlayer, which has not been observed under ultra-high vacuum conditions [6]. Gaining atomic-level information of this kind is vital in understanding the processes occurring at titania-based materials and may help to optimise their performance.

Going towards even more realistic TiO₂ – liquid interfaces requires taking into account the effect of dissolved (salt) ions, which are especially important in (photo-)electrochemical applications. As a first step, the current work uses density functional theory to analyse the effect of sodium and chloride ions on the water – rutile TiO₂(110) interface. The calculations encompass structure optimisations of sodium hydroxide and hydrogen chloride co-adsorbed with small amounts of water molecules as well as ab initio molecular dynamics simulations on the solution – titania interface. This enables us to study the influence of these ions on the interface structure in a detailed and systematic way. The results provide new insight into the interaction of titania with aqueous environments.

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