Structure of hematite(0001) and water splitting mechanism from ab-initio simulations

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Hematite has recently raised considerable interest as a possible photocatalyst for water oxidation. Despite the on-going research efforts, its efficiency is still unsatisfactory. To understand the behaviour of the (0001) surface of hematite in a realistic environment, we have performed first-principles simulations based on density functional theory. By taking into account the presence of water and oxygen under illumination, we show that the thermodynamically stable termination under reaction conditions is oxygen rich. On this termination, water oxidation proceeds by nucleophilic attack with an overpotential of 0.84 V. Finally, we have considered the possible effect of surface modifications such as impurities and ultrathin films on the properties of the surface. Nitrogen doping lowers the over-potential, while detrimental surface states disappear in presence of ultrathin films of gallium oxide or aluminium oxide. I am going to compare calculations with available experiments, and to discuss open questions and future developments in this field.