

Density Functional Theory Modeling of the Metal Oxide Water Interface



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Presented by...

Professor Michiel Sprik

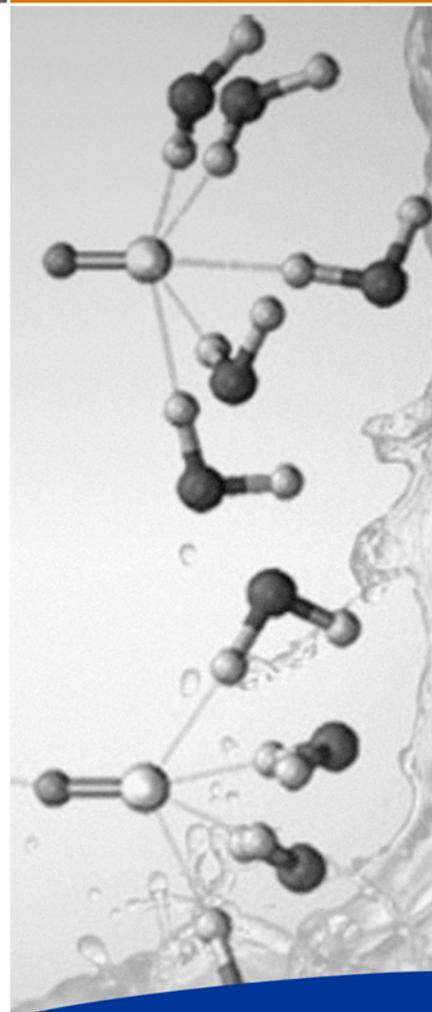
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Abstract

The interface between a metal oxide and an aqueous solution is a complex environment controlled by the exchange of charge between solid and electrolyte. Coordination with the positive metal ions increases the acidity of adsorbed water which at high pH leads to deprotonation and the buildup of negative charge. Alternatively basic oxygen sites on the surface can become protonated at low pH. Metal oxides can also exchange electronic charge with the electrolyte if the metal ions are redox active. Examples are transition metal ions. Modeling these processes is a major challenge for electronic structure calculation. In this talk, Professor Sprik will outline the DFT-based molecular dynamics methodology that was developed to meet this challenge using the calculation of the pH of zero proton charge, the potential at zero electronic charge and electric double layer capacitance of a small set of structurally related semiconductor oxides as validation. The key tool in the approach is a scheme for a molecular dynamics normal hydrogen electrode. As an application, Professor Sprik will discuss the thermochemistry of the creation of hydroxyl radicals at the TiO_2 /water interface. All these calculations have been carried out using the CP2K package. The recent implementation of efficient methods for the evaluation of exact exchange in extended systems has been in particular critical for the application to semiconductor oxides as reported in this talk.

More info?

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Date: February 27

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Auditorium

Time: 10-11 am