Interaction of water with rutile (1 1 0) – Ground and excited states

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Photochemical reactions are of great interest in modern chemistry and are hard to model theoretically. Especially photo-catalytic reactions on surfaces are a great challenge. By combining quantum chemical and quantum dynamical methods, we were able to elucidate the photodesorption of small molecules from metal oxide surface from first principles.[1]

In this contribution we present first results for the water adsorption on a rutile (1 1 0) surface. This process might become very important in the near future because of the possibility to split water into oxygen and hydrogen using the energy of sun light. Thus, this reaction can open an economical and ecological relevant route to hydrogen.

Our approach is to model the H_2O/TiO_2 system by a finite cluster embedded in a field of about 4500 point charges to include long range Coulomb interaction. The cluster is of stoichiometry $Ti_9O_{18}Mg_7^{14+}$ and has successfully been used for describing the photodesorption of CO from rutile (1 1 0).[2]

Potential energy surfaces for the electronic ground state and selected electronically excited states are calculated on the CASSCF level of theory, giving the possibility to describe the bond breaking properly. The electron correlation is included by a CASPT2 treatment.

These potential energy surfaces are used for quantum dynamical calculations based on Gadzuk's jumping wave-package approach.[3, 4] Therefore, the dynamics is treated fully quantum mechanically and can include effects like tunneling or isotope substitution.

In this contribution we present first quantum chemical results for the adsorption in the electronic ground state and some preliminary results for excited states.

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