Molecular dynamics studies on the pH-dependent mechanism of phosphonic acid adsorption on anatase (101)

Dustin Vivod[1,2], Dirk Zahn[1,2]

[1] *Computer-Chemie-Centrum and Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Nägelsbachstraße 25, 91052 Erlangen, Germany*

[2] *Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Nägelsbachstraße 25, 91052 Erlangen, Germany*

For dye-sensitized solar cells using titania nanotubes the mechanism behind the adsorption of phosphates onto a anatase surface is a vital process. By using molecular dynamics simulation the assosiation, adsorption, and desorption are investigated.

The adsorption of ethylphosphonic acid onto the anatase (101) surface under acidic conditions is investigated in a two step procedure. First the physisorption is evaluated by generating the potential of mean force, and in a second step a water exchange reaction is examined by comparing the difference in potential energy.

Multiple different configurations which may result from a deprotonation of the acid are considered. The energetics of the reactions on the surface are evaluated in comparison to the reaction in solution. It is shown that condensation reactions are energetically unfavored. Instead the configuration after a proton transfer to the solvent is the only one favored.

The desorption under neutral conditions is investigated by umbrella sampling.