

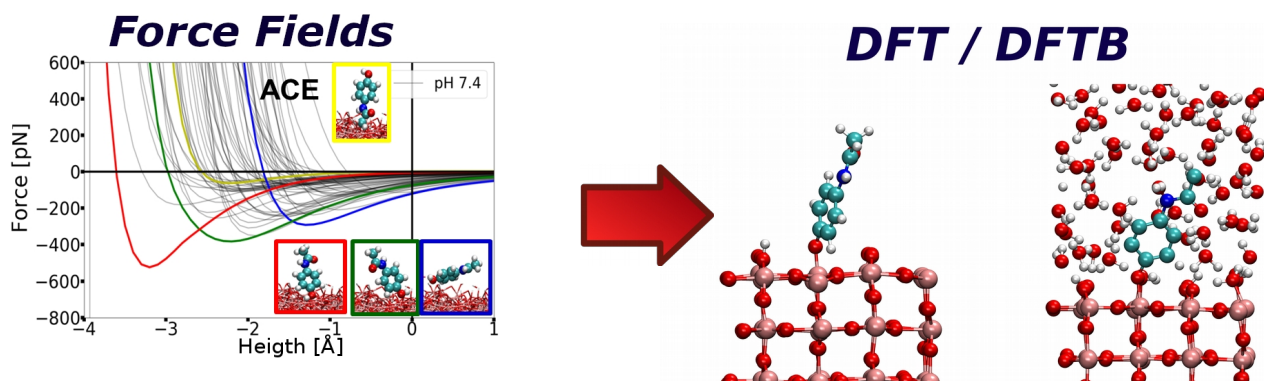
# Water contaminants on different models of rutile TiO<sub>2</sub>

## - a DFT(B) / FF approach

*F. Balzaretti, V. Gupta, M. Romero, S. Köppen*

*University of Bremen, Faculty of Production Engineering, Hybrid Materials Interfaces,  
and Bremen Center for Computational Materials Science (BCCMS)  
and Bremen Center for Materials and Processes (MAPEX)  
Bremen, Germany*

The impact of TiO<sub>2</sub> as a fundamental material for new technologies is still nowadays worldwide recognized. Independently from its two main phases, anatase and rutile, this semiconductor proved to be able of major photocatalytical activity within visible light irradiation, which turns out to be a powerful tool for relevant engineering applications such as water splitting or environmental cleaning [1, 2]. Moreover, TiO<sub>2</sub> powders with negligible rate of impurities can be synthesized at very affordable prices, enabling it to reach a primary role with respect to other materials. Optimal reaction rates at basic pH conditions have been reported for several adsorbates [3, 4, 5], showing an environmental dependence. This motivates more complex simulations of small organic pollutants taking into account surface defect states, aqueous environment with varying pH conditions as well as the presence of different pollutants at different concentrations.



Here we present extensive interaction studies of nine worldwide abundant aqueous contaminants, for which force-displacement curves were evaluated at different molecules orientations through *Force Fields (FF)* methods. Among other very reactive contaminants, the Glyphosate revealed interaction forces higher by a factor of 10. Next to this prominent herbicide, the most favorable final configurations of two other pollutants belonging to the pharmaceutical and intensive breeding sectors were taken as initial structures for both *Density Functional Theory (DFT)* and *Tight Binding (DFTB)* approaches. Independently from the class of applications, all contaminants show thermodynamically stable geometries with hydroxyl and carboxylic groups towards the surface on pristine and reconstructed surfaces of rutile [6].

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