How to survive: the power of TiO_2

Influence of environment on the adsorption properties of TiO_2

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In Short

- Titanium Dioxide can provide efficient waste water cleaning for molecules adsorbing at the surface.
- The project aims to understand on the atomistic scale how water pollutants can dissociate on TiO_2 surfaces with many different approaches.
- Different slab models for both Anatase and Rutile has been created and are now ready to be further implemented.

TiO_2 has been worldwide recognized as an important material due to its outstanding photo catalytical properties and chemical stability 1 2, which can be of major relevance for technical applications. Especially in terms of waste water purification, indeed, hybrid Titania surfaces are able to deal with some of the most common pollutants such as pesticides, insecticides or antibiotics 3 4, providing photo degradation under a constant ultraviolet irradiation but simply the huge mass of waste water all over the world offers a strong necessity for optimization of in principle well know processes.
One way is the deeper understanding of the photo catalytic degradation of such molecules on an atomistic scale. Here, the necessity of (I) high accuracy methods in terms of time depending DFT codes competes with (II) the complexity of such systems. This is far from being a trivial task, since this kind of systems not only show high complexities due to molecules-solvent competitions in adsorbing at rough surfaces, but they are also strongly affected by different pH values 5 like shown in Fig. 1.

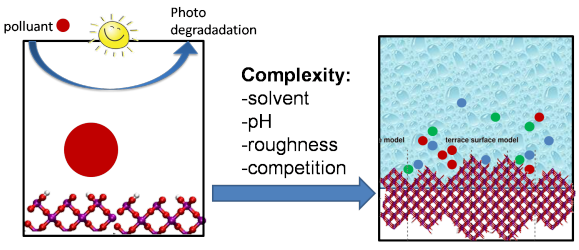

***Figure 1:** Differences between pure theoretical and realistic model.*

Although several different slab models (100 and 110 for Rutile, 101 and 001 for Anatase) have already been extensively investigated by our group 6 7 8, some efforts in surface reconstructions should help in better understanding how different rough shapes affect the molecules adsorption in water. To this purpose, the energetically higher and less literally-known Rutile (001) facet was developed with different approaches adding TiO_2 units on the top via Molecular Dynamics (MD) simulations, leading to different reconstruction motifs shown in Fig. **??**. In the present proposal, the reconstructed surface models will be used for simulations on the pollutant titania interface systems.

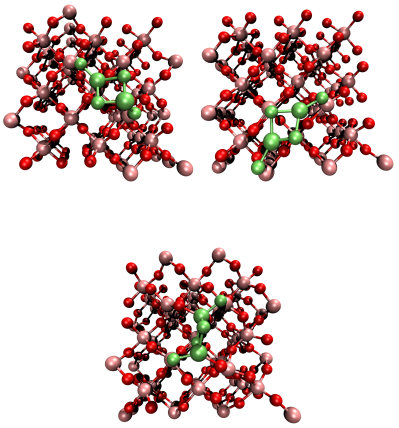

***Figure 2:** Different reconstruction motifs for Rutile (001) surface.*

The request for using High-Performance Computing resources is then provided by the next steps we would like to proceed with.

- Since adding several amounts of TiO_2 units on the Rutile (001) surface in our MDs gave basically combinations of the three stable reconstructed motifs, a series of more complex reconstructions should be established with algorithms based on Group Theory. Those different rough surfaces will be useful to afterwards parametrize a proper Force Fields, but they require DFT-MD simulations in a first place.
- Adding water to fill up the void beneath the periodic image of the system is fundamental since protonations and hydroxilations are the main mechanisms that provide mineralizations of organic compounds. Moreover, different slab models enable different H_2O configurations at the surface. A deep DFT study shall be then taken into account.
- The interactions between functional groups, typically present in the structure of the polluting

molecules, or directly between those harmful compounds and the different reconstructed surfaces of Rutile (001) shall be considered at the DFT level of theory in a water solvent.

Thanks to the above simulations, very important conclusions about molecular and atomistic mineralizations on TiO_2 for water treatments will be hopefully better understood and afterwards used to finally move considerations about the electronic excited states, namely the Titanium Dioxide photo catalytical activity.

WWW

https://www.rtg-qm3.de/research/research-projects/p6/

More Information

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