How to survive: the power of TiO_2

Adsorption of relevant water pollutants on 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 how water pollutants can be degraded on TiO_2 surfaces on the atomic scale.
- Two pollutants with significant environmental footprint are investigated through their adsorption on different titania surfaces.

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 herbicides, insecticides or antibiotics [3, 4, 5]. It provides 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 show high complexities due to molecules-solvent competitions in adsorbing at rough surfaces, like shown in Fig. 1.

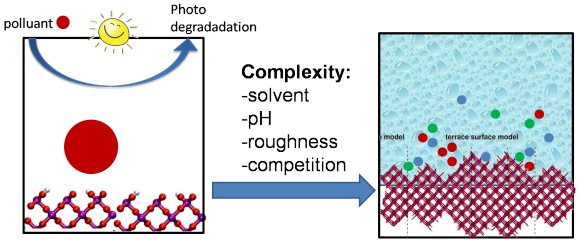

***Figure 1:** From perfect one molecules systems to complexity of the titania interface.*

In this project we focus on the approximation of pollutants to different titania surface models. Here smooth as well as reconstructed models are taken into account. One focus is the competition between water and the contaminant molecules directly on the surface. NEB simulations based on DFT will be used to understand the displacement of water in favour of contaminants.

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

- The adsorption of a number of pollutants which are estimated to have significant interaction forces through Titaniumdioxid will be simulated with VASP
- The approach through the surface will be accelerated by the use of implicit solvent models as implemented in VASP via VASPsol.
- The resulting adsorption modes will be solvated with explicit water and further molecular dynamics simulations should reveal thermodynamically stable adsorption configurations
- These results can be used as final inputs for NEB simulations through the tool VTST to reveal displacement of water with pollutant molecules.

The described simulations will deal as another piece of puzzle through the optimization of waste water cleaning and therefore a step towards the protection of the ecosystem.

WWW

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

More Information

[1] U. Diebold, *Surface Science Reports* **48**, 53-229, 2003.

[2] Y. Lan, Y. Lu and Z. Ren, *Nano Energy* **2**, 1031-1045, 2013.

[3] K. Dai, P. Tianyou, H. Chen et al., *Environ. Sci. Technol.* **42**, 1505-1510, 2008.

[4] J. Madhavan, F. Gieser and M. Ashokkumar, *Separation and Purification Technol.* **73**, 409, 2010.

[5] X. Zhu, Y. Wang, R. Sun and D. Zhou, *Chemosphere* **92**, 53-229, 2003.

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