

# Rutile Slab Models for Environmental Water Cleaning

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The importance of TiO<sub>2</sub> has been worldwide recognized due to its outstanding photocatalytical properties and chemical stability<sup>1</sup>, which can be of major relevance even for a huge problem such as wastewaters. Indeed, hybrid Titania surfaces are able to deal with some of the most common pollutants such as pesticides, insecticides or antibiotics<sup>2,3,4</sup>, providing photodegradation under a constant ultraviolet irradiation.

Using different levels of accuracy, from Density Functional Theory up to Force Fields, a satisfying study of Rutile facet behaviors, including environmental aspects, is in the focus of my work. Three different slab models (001, 100 and 110 directions) were cut out from an optimized Bulk Structure. After some comparisons with literature values<sup>5</sup>, water addition was provided to fill out the periodic box and look at its density distribution among the first layer. Meanwhile, due to its higher Surface Energy, an accurate reconstruction procedure on the 001 facet has been investigated.

On-going work is actually focusing on some of the main pollutant molecules to be put over all the different surfaces created so far, while a study of Oxygen vacancies affection is also playing an important role.

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