Structure and reactivity of oxides through a combined DFT and experimental approach

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Combining experiments and DFT calculations is a powerful method to analyze complex systems and unravel their properties at an atomistic level.

To face the global increase of energy demand while producing a cleaner energy, it is mandatory to find new means of production. Among the different investigated possibilities, harvesting solar energy to produce clean hydrogen from water appears as one of the most promising options. Among possible materials for this approach, one can mention hematite which checks several requirements but presents a too low efficiency. To solve this issue, doping has often been proposed but the exact role of the introduced dopant at the reactive interface has never been determined.

In this presentation, I will present our recent work using combined NAP-XPS experiments and DFT calculations to investigate the modification of the water/hematite interface induced by Ti dopant. Both the thermodynamic and kinetic modifications induced by titanium will be discussed. In particular we will focus on the key role of surface Ti to modify water adsorption and reactivity.