M2 Sciences des Matériaux et Nano-Objets (SMNO)

Sorbonne Université, ENS Ulm, Chimie ParisTech, ESPCI, l'École Polytechnique

Proposition de stage 2018-2019

Laboratoire : INSP

Adresse : 4, place Jussieu

Directeur du laboratoire : Christophe TESTELIN

Responsable(s) du stage : Slavica Stankic et Fabio Finocchi
Téléphone : 01.44.27.46.50 et 01.44.27.51.16
e-mail : stankic@insp.upmc.fr et fabio.finocchi@insp.upmc.fr

Water on TiO_2-anatase : Combining experiments and DFT calculations

In ambient conditions, the surfaces of metal oxides are generally covered with water. Therefore, understanding the interaction with H_2O is crucial for determining properties of metal oxides as well as for their potential applications in ambient conditions. Among others, the surfaces of wet TiO_2 have been the object of several studies, which mostly focused on the (110) surface of TiO_2 rutile. However, another TiO_2 polymorph, the anatase, is active in photo-catalysis while its interaction with water is much less known. Many issues are still open or debated, such as the relative proportion of dissociated water molecules, the atomic-level structure and the relevance of defects on the surface reactivity towards water.
The goal of this M2-internship is to study water adsorption and dissociation on TiO_2 nanopowders of a very high surface-to-volume ratio, which makes them especially suitable to study the interaction with molecular species. We aim at combining transmission electron microscopy(TEM), transmission infrared spectroscopy (FTIR) and calculations based on density functional theory (DFT), in order to characterize the water adsorption mechanisms on TiO_2 surfaces as a function of the temperature T and the water partial pressure P_{H2O}. The morphology of nano-structured TiO_2 nano-powders, which would likely contain a variable proportion of rutile and anatase, will be firstly characterized by TEM. The FTIR measurements will be conducted by controlling two key parameters: i) the water partial pressure P_{H2O}, spanning ultra-high vacuum to atmospheric conditions; ii) the temperature, from ambient T (300K) down to very low ones (15K). We will pay special attention to the low-T, low-P_{H2O} measurements, trying to solve the contributions of anharmonic vibrations and adsorption kinetics for almost isolated molecules, which will also be computed in parallel on the perfect and, possibly, defective TiO_2 anatase surfaces. The combination of IR and DFT calculations could provide a thorough understanding of the atomic-scale processes beneath water adsorption and dissociation.

Techniques utilisées : Infrared spectroscopy, Transmission Electron Microscopy, DFT calculations (experimental + theoretical)

Qualités du candidat requises : ……..

Rémunération éventuelle du stage : oui
Possibilité de poursuivre en thèse ?
Si oui, mode de financement envisagé :