

Molecular Dynamics of TiO₂ Anatase (001) Surface Co-doped by Ruthenium and Platinum Ions

Yuchi Zhang and Dmitri S. Kilinota

University of South Dakota

Abstract

Understanding the charge transfer on TiO₂ surface is critical for solar device design and optimization. The charged wet TiO₂ anatase (001) surface functionalized by ruthenium and platinum ions is studied by computational modeling, since Pt and Ru were both demonstrated for improvement on electron transfer on TiO₂ surface in our previous study.^{1,2} The calculations are based on DFT and PBE and optimize the co-doped nanostructure by using VASP software. All simulated properties of this model are in equilibrium geometry and at ambient temperatures. Through their density of states, we can analyze the possibility of charge transfer at the crystal surface and compare the co-doping elements affect the charge transfer direction. A comparison the computer absorption spectra and the charge density of the co-doped nanostructures indicate the possibility of the bandgap tuning and molecular dynamics variation in photocatalytic energy nanomaterials.

(1) Zhang, Y.; Kilin, D. S. *Int J Quantum Chem* 2012, 112, 3867.

(2) Zhang, Y.; Qiu, C.; Kilin, D. *Mol. Phys.* 2013, in print, DOI: 10.1080/00268976.2013.836609