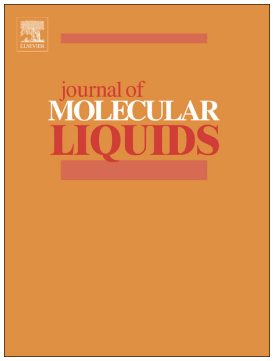

Water distribution in layers of an aqueous film on the titanium dioxide surface: A molecular dynamic simulation approach

K. Hamideh Babazadeh, Masumeh Foroutan

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Water distribution in layers of an aqueous film on the titanium dioxide surface: A molecular dynamic simulation approach

Hamideh Babazadeh K., Masumeh Foroutan*

Department of Physical Chemistry, School of Chemistry, College of Science, University of Tehran, Tehran, Iran

Abstract

Water adsorption and wetting of titanium dioxide surface along with its structure and dynamics of liquid water molecules has recently been studied as an important subject. In the current work, the interface of water and (110) surface of titanium dioxide is analyzed based on the formation and distribution of water molecules in the first and second layer from a molecular dynamics perspective. The simulation results illustrate that the water molecules form a linear chain in the interfacial layer, also known as the first layer. As the number of water molecules increases a second layer forms while the TiO_2 surface remains partially dry. Further increase results in the exchange of water molecules between first and second layers which facilitates the filling of the first layer. These results are extracted from density profiles, lifetime and number of hydrogen bonds in different layers, order parameter, mean squared displacement and, the orientation of water molecules at different distances from the surface all of which are in line with the reported quantum calculations and experimental data.

Keywords: Nanocrystal Titanium Dioxide; Interfacial layer; Nano droplet; Water distribution; Molecular dynamics simulation.

* Corresponding author, foroutan@ut.ac.ir (M. Foroutan), Telefax: +982166495291