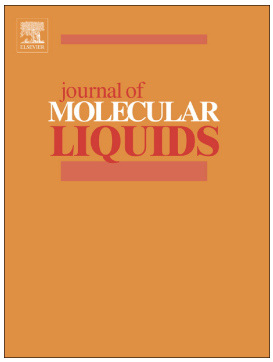

Water chain formation on rutile TiO2 (110) nanocrystal: A molecular dynamics simulation approach

Masumeh Foroutan, Mehdi Darvishi, S. Mahmood Fatemi, K. Hamideh Babazadeh

PII: S0167-7322(17)34759-1
DOI: doi:10.1016/j.molliq.2017.12.021
Reference: MOLLIQ 8317

To appear in: *Journal of Molecular Liquids*

Received date: 8 October 2017
Revised date: 2 December 2017
Accepted date: 5 December 2017

Please cite this article as: Masumeh Foroutan, Mehdi Darvishi, S. Mahmood Fatemi, K. Hamideh Babazadeh , Water chain formation on rutile TiO2 (110) nanocrystal: A molecular dynamics simulation approach. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2017.12.021

Water Chain Formation on Rutile TiO_2 (110) Nanocrystal: A Molecular Dynamics Simulation Approach

Masumeh Foroutan[*], Mehdi Darvishi[‡], S. Mahmood Fatemi[‡], Hamideh Babazadeh K.[‡]

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

Abstract

Understanding the properties of the interface of water nano-droplet and rutile TiO_2 (110) nanocrystal has attracted the attention of many surface scientists. In this research the interface of water nano-droplet and (110) plane of Rutile titanium dioxide nanocrystal along with the formation of water chains was studied based on a molecular dynamics approach. Density profiles of oxygen and hydrogen atoms of the water molecules show less movement in hydrogen atoms that reside closer to the TiO_2 surface than the ones that are further away. The calculated results indicate that the average interlayer hydrogen bonds per water molecule is about 0.51 at the interface where water molecules form two different water-water hydrogen bonds with 28.55 and 670.24 ps lifetimes. The simulation data reveal the formation of one-dimensional chain structures of water on the TiO_2 substrate. Certain values for the estimated angles among every three water molecules that participate in the formation of the chain structures is observed. The electrostatic energy contour map and the orientation of water molecules at the interface suggests that these molecules form ordered and periodic pair structures around the regions with high negative charge on titanium dioxide. The dynamical analysis of the water molecules indicates a dynamical

[*]Corresponding author: Tel +98 21 61112896; Fax: +98 21 66495291, foroutan@khayam.ut.ac.ir
[‡] Contributed equally to this work.