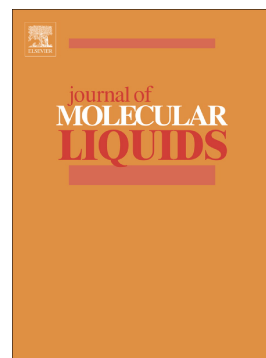


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## Water Chain Formation on Rutile TiO<sub>2</sub> (110) Nanocrystal: A Molecular Dynamics Simulation Approach

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### Abstract

Understanding the properties of the interface of water nano-droplet and rutile TiO<sub>2</sub> (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<sub>2</sub> 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<sub>2</sub> 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

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