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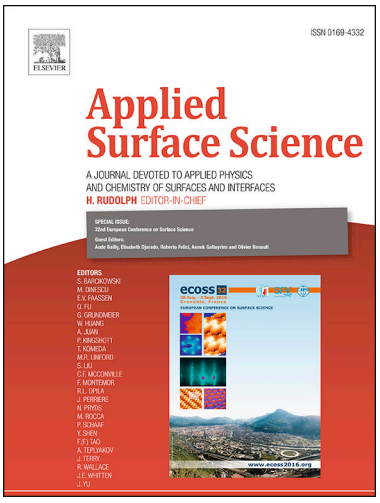

Full Length Article

Molecular dynamics simulation of a water nano-droplet on graphene oxide surface at high temperature: evaporation or spreading?

Hojat Zahedi, Masumeh Foroutan

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Molecular dynamics simulation of a water nano-droplet on graphene oxide surface at high temperature: evaporation or spreading?

Hojat Zahedi and Masumeh Foroutan*,

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

Abstract

In this work, the behavior of a water nano-droplet on hydrophilic graphene oxide (GO) is studied at high temperatures using molecular dynamics simulation. The results showed that, with increasing temperature, spreading would overcome the evaporation of water molecules on the surface of GO. At high temperatures, the regime changes from partial to total wetting. After the spreading is complete and the surface is completely covered by water, evaporation of water occurs more rapidly. Simulation results revealed that as the system temperature rises, the number of hydrogen bonds between water molecules decreases. The water molecules reorient to the GO surface as the temperature increases and the number of possible H-bonds inside the bulk of the droplet decreases. However, the formation of H-bonds between water molecules and GO increases with temperature. The results obtained in terms of the contact angle and the density of the water molecules on the surface of the GO revealed that at different temperatures more water molecules spread on the surface of GO during simulation time. Increasing the temperature leads to increase in the number of evaporated water molecules from the surface of GO. Investigations of the dipolar momentum of water molecules in different layers of GO surface showed that water molecules in the initial layers tend to approach the surface with hydrogen atoms.

KEYWORDS: Graphene Oxide, Water Nano-droplet, Contact Angle, Evaporation, Spreading, Molecular Dynamics Simulation.

* Corresponding author: Tel +98 21 61112896; Fax: +98 21 66495291, foroutan@khayam.ut.ac.ir.