Structural and transport properties of confined water in nano geometries

Alberto Zaragoza[1,3], Miguel Ángel González[2], Ana Laura Benavides[1], and Chantal Valeriani[3]
[1]División de Ciencias e Ingenierías, Universidad de Guanajuato, Lomas del Campestre, 37150 León, Mexico
[2]Facultad de Ciencias Químicas, Universidad Complutense de Madrid, av. Complutense s/n, 28040 Madrid, Spain
[3]Facultad de Ciencias Físicas, Universidad Complutense de Madrid, av. Complutense s/n, 28040 Madrid, Spain

Water is undoubtedly the most relevant molecule for living organisms both at a macroscopic scale —the human body consists of 65-70 % of water and a tree of 20-70 %— and at a microscopic scale —a human cell consists of 70-80 % of water and a plant one of 60-70 %. At the latter scale, the features of confined water, that differ with respect of bulk water, play a vital role and understanding them could be of interest in the development of nanomaterials such as nanochannels. In particular, under confinement, water has a different behaviour than in bulk showing a different phase diagram [1] that is still under study. It is important to study water at nanoscale to understand biological/industrial processes such us ions exchange in cells or water desalination [5, 6], respectively.

Computer simulations based on molecular dynamics have shown to be a reliable and powerful tool to study the features, from a molecular approach, of nanoconfined water. At these small scales, experimentalists may find issues to measure some properties or even to work at some conditions of temperature. That is the reason why molecular simulation is a very useful technique to find out how confinement changes the water properties.

In the last decade, works focused on understanding transport properties of confined water have not shown conclusive results [7, 8, 9, 10]. Our goal is to set up numerical simulations that could be considered as a benchmark for future works of confined water.

In this work, by means of molecular dynamics simulations, we study TIP4P/2005 [4] water confined inside nanomaterials (both hydrophobic and super-hydrophobic) such as two parallel sheets and single wall carbon nanotubes (SWCNTs) with a wide diameter range. Structural an dynamical properties, such as diffusion, density, viscosity and the number of formed/broken hydrogen bonds were computed and analysed at several temperatures taking into account the finite size corrections proposed by theoretical studies [3, 2].

Our preliminary results shown that key factors such as hydrogen bonds or viscosity allow water to diffuse faster when confined down to a "limit" diameter ($\approx$ 2 nm). If water is confined under this "limit" size, it trends to adopt chain-like structures that make its dynamic slows-down.

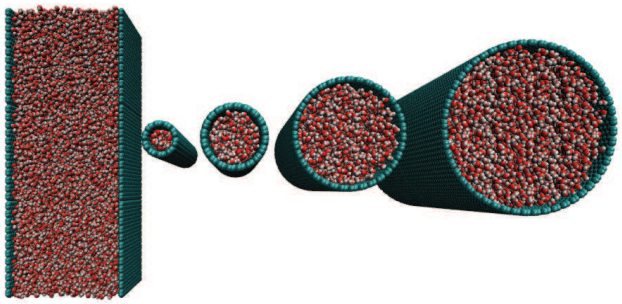

Fig. 1. From left to right: Two parallel graphene sheets having confined water inside, four SWCNTs confining water and with diameter from 1.3 to 7 nm. Carbon atoms are represented by cyan spheres and thewater molecules by red (oxygen) and white (hydrogen) spheres.

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