

Liquid water confined in graphene nanochannels at supercritical conditions

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The microscopic behavior of liquid water near surfaces has been a topic of great interest for the last decades,¹ basically because of the enormous influence of the surface on the properties of the water molecules close to it.

In this communication we report the results of a series of molecular dynamics simulations of water inside a narrow graphite channel at supercritical conditions. We considered N water molecules embedded into two parallel graphite plates with no defects to model two sheets of highly oriented pyrolytic graphite (HOPG). We set up a simulation box in the x , y , and z directions of 34.4, 34.1 and 31 Å, respectively. These values correspond to the geometry of HOPG in the real system. We assumed the z coordinate to be perpendicular to the graphite layers, and the usual periodic boundary conditions were considered only in the x and y directions. The temperature of the system was kept at $T=673\text{K}$. Different number of molecules were assumed ranging from $N=100$ to $N=800$ to cover a range of densities from $\rho=0.08$ to $\rho=0.66$ gcm^{-3} .

Water-water inter- and intramolecular interactions were modeled with a flexible simple-point-charge (SPC) potential which was specifically reparametrized to reproduce the main trends of the infrared spectrum of water at ambient conditions². This flexible SPC potential has a critical point ($T_c = 643$ K, $\rho_c = 0.32$ gcm^{-3}) which is very close to the experimental one ($T_c = 647$ K, $\rho_c = 0.322$ gcm^{-3}).³ Water-carbon forces were assumed to be of the Lennard-Jones type with the same parametrization employed in previous studies of water near graphite (see for instance Ref. 4.)

During the simulations, we separately analyzed the properties of two different groups of water molecules directly related by their locations with respect to the graphite walls: *adsorbed* for water in the closest layer and *bulk* for water far from the graphite. The exact definition of these regions in each case comes from the corresponding oxygen density profiles (see FIG. 1). The residence times of water molecules in both the adsorbed and bulk regions were determined. A thorough analysis of the structure, hydrogen bonding, dielectric and dynamic properties of the systems was performed. Finally, our present results were compared with previous stud-

ies of liquid water confined in graphene nanochannels at ambient^{5,6} and high temperature⁷ conditions.

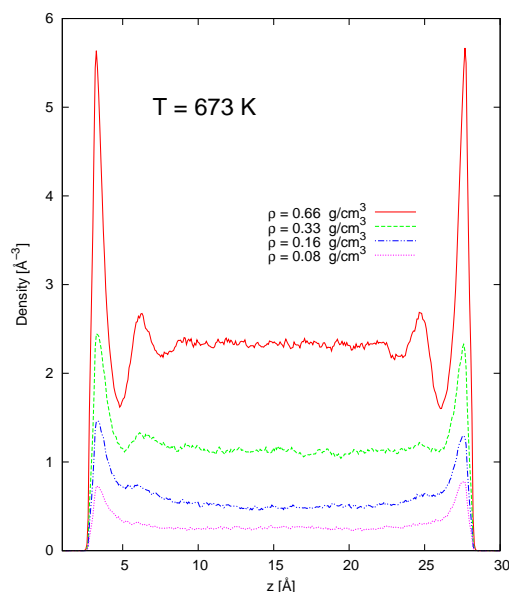


Figura 1. Oxygen density profiles of water molecules.

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