

6. Dynamic properties of water confined with hydrophobic plane walls

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Near a hydrophobic wall, the structure as well as dynamics of water molecules change as compared to bulk water. The scope of the perturbation introduced by the presence of hydrophobic wall has been subject of some controversy in recent publications. To study this problem we simulate a system of water confined by two parallel hydrophobic amorphous walls by Molecular Dynamics. The hydrophobic wall was built using a binary mixture of Lennard-Jones particles, defining the parameters of interaction of this mixture so that the diffusion coefficient of the mixture is much less than that corresponding to the water in the temperature range chosen (near ambient temperature). For water we used the SPC/e model. We studied the hydrogen-bond network, density and density time correlations as a function of the distance from the wall at five reference temperatures: 270K, 285K, 300K, 315K and 330K. The results show both for structural analysis or dynamics that the presence of the wall produced one perturbation of several orders of magnitude higher than what was believed in recent decades, showing one strong coincidence with some recent experimental results.