14. Water confined in model hydrophobic cavities and tunnelsand carbon nanotubes

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Through molecular dynamics simulations we analyze the behavior of water in contact with model hydrophobic cavities and tunnels. We study the hydration and filling propensity of cavities and tunnels carved in monolayers of alkanes and single-wall carbon nanotubes of similar size. Our results determine the dependence of the filling propensity according to the size of the cavity, showing the dynamic nature of the process. We compare the minimum diameter of solvation in the tunnels carved into monolayers with the diameter of carbon nanotubes and found that the diameter of the first ones is approximately twice compared with the minimun solvatation diameter of the carbon nanotubes, showing a more hydrophobic behavior. It also discusses the existence of water-water hydrogen bonds inside the hydrophobic cavities, which is a necessary condition for penetration into them.