The hydrophobic effect: Molecular dynamics simulations of water confined between extended hydrophobic and hydrophilic surfaces

Structural and dynamic properties of water confined between two parallel, extended, either hydrophobic or hydrophilic crystalline surfaces of n-alkane C36H74 or n-alcohol C35H71OH, are studied by molecular dynamics simulations. Electron density profiles, directly compared with corresponding experimental data from x-ray reflectivity measurements, reveal a uniform weak de-wetting characteristic for the extended hydrophobic surface, while the hydrophilic surface is weakly wetted. These microscopic data are consistent with macroscopic contact angle measurements. Specific water orientation is present at both surfaces. The ordering is characteristically different between the surfaces and of longer range at the hydrophilic surface. Furthermore, the dynamic properties of water are different at the two surfaces and different from the bulk behavior. In particular, at the hydrophobic surface, time-correlation functions reveal that water molecules have characteristic diffusive behavior and orientational ordering due to the lack of hydrogen bonding interactions with the surface. These observations suggest that the altered dynamical properties of water in contact with extended hydrophobic surfaces together with a partial drying of the surfaces are more indicative of the hydrophobic effect than structural ordering, which we suggest to be independent of surface topology. (C) 2004 American Institute of Physics.