

73g Water Condensation in Hydrophobic Nanopores

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Adsorption of water in hydrophobic materials has been the subject of numerous studies in the past decade, owing to the possible use of such materials as efficient shock absorbers. In this paper we report some new experimental data as well as a Grand Canonical Monte Carlo study of water adsorption-intrusion in nanoporous zeolite Silicalite-1. Several standard (and less standard) water forcefields are tested in the simulations. We find that most of these effective potentials are capable of reproducing the essential experimental features of reversible water intrusion-extrusion in Silicalite-1, as long as enough care is taken in deriving the right balance between the guest-host and the guest-guest interactions. The second part of the work is devoted to the description of the gas-liquid transition mechanism at the molecular level. An interesting heterogeneous filling of the pore volume is observed in the simulations and discussed in terms of water clusters formation, hydrogen bonding and available pore volume. The picture of water confined to hydrophobic spaces of nanoscopic dimensions that emerges from this work is a strongly depleted and highly inhomogeneous fluid.