

Structure and Dynamics of Water in Carbon Nanotube Confinement

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Abstract. The incorporation of water into carbon nanotubes provides a simple analogue of biologically important trans-membrane channels and so is of large interdisciplinary scientific interest. Recently quasi-one-dimensional water encapsulated inside carbon nanotubes (*nanotube-water*) at different temperatures (4-300 K) and pressures (1-3700 atm) were studied by means of neutron diffraction, quasielastic, inelastic and deep inelastic neutron scattering and observed extremely soft dynamics of nanotube-water at low temperatures were explained by molecular dynamics (MD) simulations. Application of a 'parallel tempering' MD algorithm allowed to calculate the structural and dynamical properties of nanotube-water simultaneously for different temperatures and revealed the phase transitions in temperature - pressure nanotube-water phase diagram, which were really observed in neutron scattering experiments.

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