INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE
2A&B, Raja S.C. Mullick Road, Jadavpur, Kolkata-700032, India

Seminar

Org. by

Solid State Physics

Speaker: Prof. Chandan Dasgupta

Affiliation: Department of Physics, IISc, Bangalore

Date & time: Thursday, February 1, 2018; 4:00 pm

Venue: Theoretical Physics Seminar Room # 406

Title: Equilibrium and Dynamic Properties of Water Molecules Confined in Narrow Carbon Nanotubes

Abstract: Large-scale molecular dynamics (MD) simulations are used to study the thermodynamic and dynamic properties of water molecules inside narrow (6,6) carbon nanotubes that allow the entry of only a single file of water molecules. Nanotubes immersed in a bath of water at room temperature get spontaneously filled with water. The water molecules inside a nanotube form a "chain" that exhibits solid-like ordering even at room temperature, due to strong hydrogen bonding. The mode of diffusion of the water molecules inside short nanotubes is found to be Fickian, due to their strong positional ordering. The orientational relaxation of these water molecules exhibits strong anisotropy: the dipole moment relaxes
with a time scale of several nanoseconds, whereas the relaxation time of the vector joining the two hydrogen atoms of a water molecule is found to be about 150 femtoseconds. These water molecules also exhibit "bistability" in their orientational relaxation which proceeds via angular jumps between two locally stable states. The presence of these angular jumps makes the orientational relaxation non-diffusive. We also show that the dipole moments of water molecules inside a nanotube immersed in a bath of water get partially aligned when the water flows in a direction parallel to the axis of the nanotube. Simple models that reproduce and explain the simulation results are discussed.

This work was done in collaboration with Biswaroop Mukherjee, Hemant Kumar, Prabal K. Maiti and A. K. Sood.

All are cordially invited to attend the Seminar