



PONDICHERY UNIVERSITY

DEPARTMENT OF PHYSICS

Invited Lecture

on

**"Structure, dynamics and thermodynamics of water
under nano-confinement"**

by

Dr Prabal K Maiti

Associate Professor, Center for Condensed Matter Theory, Department of Physics,
Indian Institute of Science, Bangalore, India.

Date: 28th March, 2016 (Monday)

Time: 2:30 p.m

Venue: Raman Seminar Hall, Department of Physics

Abstract

We study the various translational and orientational dynamics of water molecules confined inside carbon nanotube using atomistic Molecular dynamics simulation (MD). The water molecules inside the nanotube show solid-like ordering at room temperature and surprisingly exhibit Fickian diffusion instead of single-file even if the particles can not cross one another. We propose model systems where single-file diffusion can be observed and test the prediction doing simulation in a nanoring. The confinement leads to strong anisotropy in the reorientational relaxation of the confined water molecules. The time scale of the relaxation of the dipolar correlations become ultra-slow. In contrast, the relaxation of the vector that joins the two hydrogens in a molecule becomes much faster. We also give the thermodynamics of water entry inside hydrophobic nanotube by calculating the Helmholtz free energy of water using two-phase thermodynamic (2PT) method.

All are Welcome

Alok Sharan

Dr Alok Sharan
(Seminar Coordinator)

A handwritten signature in blue ink, appearing to read 'R Murugan'.

Prof Ramaswamy Murugan
Professor & Head of the Department
Department of Physics
Pondicherry University