

Service des Photons, Atomes et Molécules
SÉMINAIRE

Jeudi 5 mai 11h00

CEA-Saclay ;b; ;font color = 'red';SPAM;/font;/b; Bât 522, p 138

Structure and dynamics of nanoconfined water

Branka M. LADANYI

Department of Chemistry, Colorado State University, USA

Understanding the behavior of water in confining geometries is of interest in many fields of science and technology. Examples include geology (for example, water in clays and porous minerals), microfluidic devices, and biological systems such as ion channels, membrane pores and protein cavities. In my group we are using molecular theory and simulation to study water confined in reverse micelles and in silica nanopores. In the first set of systems, water is present as surfactant-coated nanodrops formed in water/surfactant/oil systems with a continuous oil phase. The droplets are approximately spherical with diameters proportional to the molar ratio $w_0 = [\text{water}]/[\text{surfactant}]$. The silica pores are designed to be models for Vycor glass, which has approximately cylindrical pores with diameters in the several nanometer range. In both cases we are studying the effects of confinement on the interfacial structure and on the translational and rotational mobility of the water molecules. The results of molecular dynamics simulation are compared to experimental data from time-resolved infrared and quasi-elastic neutron scattering experiments.

Contact : caroline.lebe@cea.fr - Tel : +33 1 69 08 30 95
http://iramis.cea.fr/Phocea/Vie_des_labos/Seminaires/index.php