

Séminaire Physico-chimie & Biologie

Vendredi, 21 Septembre 2012

11:00

Bât. 563 - salle 15

Crystallization of water: from bulk to the nanoscale

Valeria Molinero

Department of Chemistry, University of Utah

valeria.molinero@utah.edu

One of water's puzzles is what determines the lowest temperature at which liquid water and aqueous solutions can be cooled before freezing to ice. The increase of ice nucleation rates as water is supercooled correlates with a dramatic increase in the heat capacity and compressibility of supercooled water, raising the question of whether a structural transformation occurring within the liquid phase controls the rate of nucleation of ice. We used molecular simulations to elucidate the mechanism of water freezing and its relation to the thermodynamics and structure of supercooled water. A main finding of our study is that the kinetics of water freezing is controlled by a structural transformation in supercooled liquid water that blurs the boundary between the liquid and crystal states. I will discuss whether this implies an end to the metastable liquid state, what confinement of water in nanopores can teach us about the nature of that transformation and –if time allows– what is the effect of solutes on the structural transformation and crystallization of supercooled water.

Télécopieur 33 (0) 1.69.08.82.61