**INSTITUT DE MINERALOGIE, DE PHYSIQUE DES MATERIAUX ET DE COSMOCHIMIE**

Unité Mixte de Recherche 7590
Code 115, 4 Place Jussieu F-75252 Paris CEDEX 05

# SÉMINAIRE
# Mardi 10 juin, 10 h 30

*Salle de Conférence, 4e étage, Tour 22-23, Salle 1*
*IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris*


# Valeria MOLINERO

*The University of Utah*


# LOW-DENSITY WATER IS THE MOTHER OF ICE


**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 investigate the crystallization of ice 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 steeply increases the fraction of four-coordinated water molecules in the liquid, blurring the boundary between the liquid and crystal states. Our results provide a microscopic foundation to the known correlation between nonequilibrium freezing temperatures and the thermodynamics of supercooled liquid water. We will discuss the effect of confinement of water in nanopores and as nanodroplets, and the addition of salts on the mechanisms and temperatures of crystallization of ice as well as on the structure of the ice formed at temperature close to the limit of supercooling.**



Tel**: 33-(0)1 44 27 42 20 --**Fax**: 33-(0)1 44 27 44 69 –**
Courriel**: catherine.dreyfus@impmc.jussieu.fr**