

**Laboratoire de Biochimie Théorique**  
**Institut de Biologie Physico-Chimique**  
13, rue Pierre et Marie Curie  
75005 PARIS

## **S E M I N A I R E**

Andrei Neamtu

\*Suprachem Lab, “Petru Poni” Institute of Macromolecular Chemistry,  
Romania

### **« Molecular simulation of water and ion transport through membrane channels »**

Artificial water channels show promising perspectives for applications in water desalinization as cheap, low-power substitutes for aquaporin synthetic films. Over the last decade many attempts have been made in designing nanoscale membrane structures imitating aquaporin filtration capabilities. Here we present several results of an ongoing effort made to describe artificial self-assembling scaffolds for selective water transport in membranes, using molecular simulation. Theoretical modelling was mainly concerned with the study of the self-assembly process of the candidate molecules in phospholipid bilayers and water transport evaluation, suggesting models of the permeation mechanism at atomic level. Understanding ion permeation mechanisms through natural ion channels is essential not only from a physiological or medical perspective, but also for designing artificial nanostructures displaying conductive properties similar to the natural ones. The selectivity and permeation of divalent cation channels are much less understood at present compared with monovalent cations. Here we present molecular dynamics simulations and quantum calculations performed in order to get a deeper mechanistic insight into the selectivity and activation determinants of MgtE  $Mg^{2+}$  channels, complementing thus the static structural view provided by X-ray crystallography experiments. The simulation results successfully provided explanations at atomic level on the discrimination mechanism between  $Mg^{2+}$  and  $Ca^{2+}$  together with identification of permeation pathway along the channel's pore.

Mardi 31 octobre 2017  
14h30

[Salle de conférence](#)