

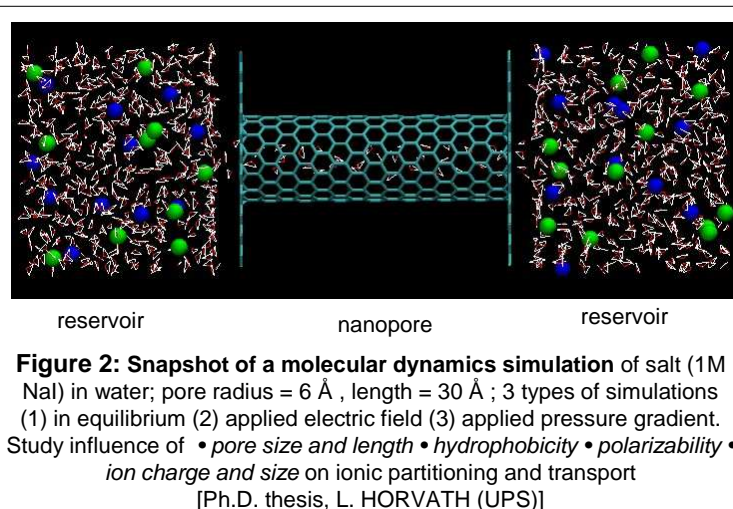
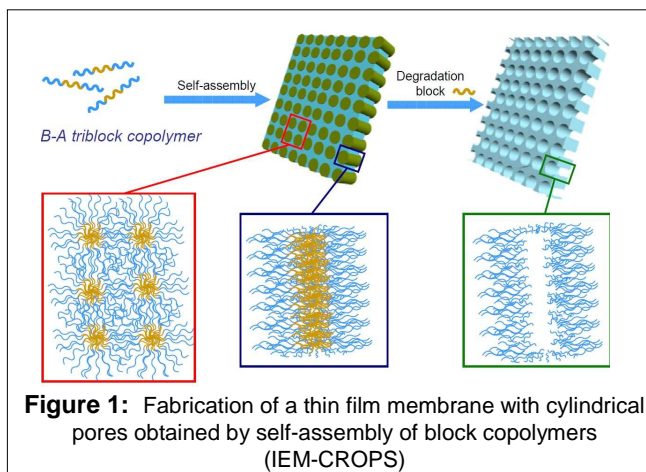
Simulation and MOdeling of transport across polymeric NANOporous MEMbranes prepared by self-assembly of block copolymers [SIMONANOMEM]

Coordinator: John PALMERI (LPT-Toulouse)
[ANR-07-NANO-055] February 2008 – January 2011

Project Objective: to explain and predict the nanoscale liquid phase transport properties of small neutral solutes and ions in nanoporous membranes as a function of material structure: *synergetic three-pronged approach*

- 1. Experimental membrane preparation and characterization** of model membranes by self-assembly techniques to obtain block copolymer nano-materials with tailor-made structures (Figure 1).
- 2. Molecular level simulations** of interfaces, surfaces, and nanopores [Molecular Dynamics, Monte Carlo]: role of inter-molecular forces and specific ion effects (*charge, size, and polarizability*). (Figure 2)
- 3. Theory and modeling:** Statistical Field Theory that goes beyond Mean Field continuum methods.

Long term goal: computer aided development of new nanofiltration membranes with controlled structure and transport properties in the liquid phase via theory, modeling, and molecular simulations \Rightarrow *industrial applications: seawater desalination, biotechnology (ion channels),..*



Partners:

- 1. Laboratoire de Physique Théorique (LPT),** Université Paul Sabatier-CNRS UMR 5152, Toulouse 3; J. PALMERI (CNRS) john.palmeri@irsamc.ups-tlse.fr (tél: 05.61.55.65.82), D. DEAN, M. MANGHI (UPS). *Theory, modeling, and molecular simulations.* S. BUYUKDAGLI (Postdoc ANR), L. HORVATH (doctorant)
- 2. Institut Européen des Membranes (IEM),** CNRS–ENSCM–Université Montpellier 2, UMR 5635, A. DERATANI (CNRS) andre.deratani@iemm.univ-montp2.fr (tél: 04.67.14.91.20), D. QUEMENER (UM2). *Experimental membrane preparation and characterization.* Guilhem BONNIOL (Ass. Ing. ANR)
- 3. Laboratoire Chimie Provence,** Equipe CROPS, Université de Provence-CNRS UMR 6264, D. GIGMES didier.gigmes@up.univ-mrs.fr (tél: 04.91.28.80.83), T. PHAN, D. BERTIN. *Experimental membrane preparation and characterization.* Q. N. TRAN (Postdoc ANR)
- 4. Institut Charles Gerhardt (ICGM),** CNRS–ENSCM–Université Montpellier 2, UMR 5253, Montpellier; B. COASNE (CNRS) benoit.coasne@univ-montp2.fr (tél: 04.67.14.33.78), F. HENN (UM2). *Modeling and molecular simulations.* P-A CAZADE (Postdoc ANR)