

## **POST-DOCTORAL OFFER**

### **TITLE**

# **Molecular simulation of the barrier properties of polymeric materials for small organic molecules – Application to reverse osmosis membrane.**

**Location :** Orsay and Massy, 25 km in the south of Paris (France)

### **PRESENTATION OF THE INSTITUTE AND THE LABORATORY**

AgroParisTech is the Paris Institute for Life, Food and Environmental Sciences. It is a member of the Paris Institute of Technology, a consortium of 10 of the foremost French graduate institutes in science and engineering. It was founded on January 1<sup>st</sup> 2007 by three graduate institutes :

INA P-G - Institut National Agronomique Paris-Grignon

ENGREF – Ecole Nationale du Génie Rural, des Eaux et des Forêts

ENSIA – Ecole Nationale Supérieure des Industries Agricoles et Alimentaires

Belonging to AgroParisTech, UMR 1145 "Génie Industriel Alimentaire" is a joint research unit in the field of food engineering. Its main purpose is a better understanding of the mechanisms involved in food processing in order to improve current processes and design innovative ones. Separation and purification processes using membranes and ion-exchange are especially focused because they play a major role for safer and cleaner production.

### **DESCRIPTION OF THE PROJECT**

Reverse osmosis and nanofiltration are widely used processes for purification of industrial effluents and recycling of water. Although mechanisms are well understood for the separation of salt solutions, no general methodology exists to predict a priori the efficiency of the separation process of effluents with organic small pollutants. The post-doctoral position is dedicated to the study of permeation of aqueous solutions through aromatic polyamide membranes. The general objective is to understand the molecular mechanisms which control the selectivity of the polymer. The work will be focused on the prediction of solubility for typical pollutants, which are poorly retained by the membrane.

Molecular simulations will be used to obtain a microscopic description of the permeation process:

- The first steps will consist in generating the amorphous cross-linked polymer structure and in equilibrating it subsequently with water. The initial structure will be prepared using an Amorphous cell method. The equilibration with water will be performed either in the osmotic ensemble or in the Gibbs ensemble. The properties of the final structures will be compared with structures determined using X-ray photoelectron and neutron-scattering.
- Solubilities of small organic compounds (e.g. furfural and acetic acid) will be estimated in the osmotic ensemble. To estimate the possible interactions between solutes, the calculations will consider either a single solute or mixture of solutes. The results will be compared with experimental partition coefficients between water and the membrane.

This project is carried out in close collaboration with the Laboratoire de Chimie Physique (UMR CNRS -Paris XI University).

**GRANT** : Grant of the Region Ile de France (**2100** euros net/month)

**DURATION** : **18 months** (starting between April and September 2008)

**CANDIDATE PROFILE**: The candidate is a young researcher (Doctorate thesis or PhD obtained after 2004) with a background in materials science and experience in molecular modeling. Knowledge in commercial software (e.g. Materials Studio, Accelrys, USA) or in open source software (e.g. LAMMPS, DL-POLY, AMBER, GROMACS...) is required.

**CONTACTS AND APPLICATION** (CV and motivation letter) **before January 15<sup>th</sup> 2008**:

<p><u>Pr. Marie-Laure Lameloise</u> AgroParisTech Equipe Techniques Séparatives UMR 1145 Génie Industriel Alimentaire AgroParisTech - site de Massy 1 av des Olympiades 91744 Massy cedex</p> <p>Tel : +33 (0)1 69 93 50 76 e-mail: <a href="mailto:marie-laure.lameloise@agroparistech.fr">marie-laure.lameloise@agroparistech.fr</a></p>	<p><u>Dr. Bernard Rousseau</u> Senior researcher at CNRS Laboratoire de Chimie Physique UMR 8000 CNRS/ Univ. Paris-Sud 11 Université Paris-Sud 11, Bât 349 F 91405 Orsay</p> <p>Tel : +33 (0)1 69 15 30 30 e-mail: <a href="mailto:bernard.rousseau@lcp.u-psud.fr">bernard.rousseau@lcp.u-psud.fr</a></p>
--	---