The SUpface of Organosilicate Membranes (SUMO) - Ph.D. project (3 years).


Organosilicate membranes are promising materials for the detection, purification or separation of liquids and gases. The sorption of species at the surface of the membranes, as well as their diffusion within the membrane bulk are the two main mechanisms that condition performances. Nevertheless, the extreme surface is seldom known and very few models have been developed in order to describe sorption. In the present project, we propose to address this issue with an original methodology that combines experiments and atomistic calculations, and that aims at designing models for the surface of organosilicate membranes and for the sorption of the different interacting species.

The Ph.D. student will split his time between the CIRIMAT, in Toulouse (Supervisor: Thomas DUGUET) and the IEM, in Montpellier (Supervisor: Vincent Rouessac). Missions are described below.

- **At IEM:** Plasma enhanced chemical vapour deposition (PECVD) of organosilicate membranes with varying structures from PDMS-like to amorphous silica and intermediate hybrids, starting from different precursors to build several “model” materials dedicated to simulation studies at CIRIMAT. Characterization of the films morphology by scanning electron microscopy (SEM), of the surface energy by the sessile drop method, of the films density by X-ray reflectometry, and of their bulk composition by infrared spectrometry (FTIR). Experimental characterization of sorption properties and microporosity by quartz crystal microbalance/adsorption (QCM/ads) and ellipsometry-porosimetry studies.

- **At CIRIMAT:** chemical composition of the surface of the membranes by X-ray photoelectron spectroscopy (XPS), and micro-/nano- structure of the surface by atomic force microscopy (AFM). We aim at characterizing the surface composition in functional groups and reactive bounds, as well as the roughness and the surface defects density; 3 important features for the understanding of sorption. In addition, the student will conduct classical molecular dynamics calculations to simulate molecules/membranes interactions.

At the end of the Ph.D thesis, the atomistic models of the membranes will be used as templates for simulated experiments of membranes reactivity towards several gases actually treated in the industry. The overall objective is the virtual optimization of the membranes surface for given functionalities, rendering possible the improvement of the state-of-the-art.

**Prerequisites:**
Master in Material Science
The student should have qualities of thoroughness and care, in order to carry out the experimental work of synthesis and characterization of the membranes.
He (She) should also have strong basics in material science for the link between experimental and simulation.
Knowledge in numerical simulation will be an advantage.

Please send your CV and cover letter to thomas.duguet@ensiacet.fr and vincent.rouessac@umontpellier.fr