Institut de Physique de Rennes – Université Rennes, CNRS

PhD Position Available

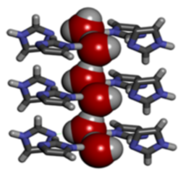
Institut de Physique de Rennes (IPR)/Institut Charles Gerhardt (ICG)

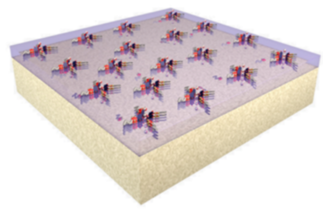
Available Oct. 2023

Molecular modelling of biomimetic composite nanofiltration membranes

Clean water is ubiquitous from drinking to agriculture and from energy supply to industrial manufacturing. Since the conventional water sources are becoming increasingly rare, the development of new technologies for water supply is crucial to address the world's clean water needs in the 21st century. Desalination is in many regards the most promising approach to long-term water supply since it potentially delivers an unlimited source of fresh water. Seawater desalination using reverse osmosis (RO) membranes has become over the past decade a standard approach to produce fresh water. While this technology has proven to be efficient, it remains however relatively costly in terms of energy input due to the use of high-pressure pumps resulting of the low water permeation through polymeric RO membranes. Recently, water channels incorporated in lipidic and polymeric membranes were demonstrated to provide a selective water translocation that enables to break permeability-selectivity trade-off.

Biomimetic Artificial Water channels (AWCs) are becoming highly attractive systems to achieve a selective transport of water. The first developed AWCs formed from imidazole quartet (I-quartet) embedded in lipidic membranes exhibited an ion selectivity higher than AQPs however associated with a lower water flow performance. We conducted very recently pioneer work in this field with the fabrication of the first AWC@Polyamide (PA) composite membrane with outstanding desalination performance. However, **the microscopic desalination mechanism** in play **is still unknown** and its understanding represents the shortest way for a long-term conception and design of AWC@PA composite membranes with better performance. **We aim to gain an unprecedented fundamental understanding and rationalization of the nanostructuration of the AWC@PA membranes and the microscopic mechanism at the origin of their water transport and ion rejection performance.**





In this quest, during the internship will begin to explore how to optimize the AWC/PA interfaces to ensure an optimal integration of AWC in the PA matrix. The main objective will be to understand the key factors controlling the spatial organization of the AWCs in the PA membrane. More broadly, we will want to determine how to tune the structural and chemical features of the AWC and PA in a rationale way to fabricate AWC@PA membranes with improved performances?

Atomistic models of AWC@PA composites will be constructed in silico by force field molecular dynamics simulations recently validated by collaborators on similar systems [7]. This simulation effort will be validated by a combination of advanced experimental characterization tools deployed on a first set of AWC@PA systems prepared by another group of collaborators. This simulation work will be then systematically applied to a large variety of AWCs and PAs with different chemical and structural features to unravel the interfacial interactions in the AWC@PA membranes and their resulting nanostructuration.

Candidates. Applicants should have a master in physics, chemistry or materials science with strong background in physics, physical chemistry, chemical physics.

Practical aspects. The position is available starting Oct. 2023 and lasts for 36 months. The net take home salary is about ~1500 euros/month. Applicants should provide a CV, a letter of motivation, and the names and e-mail addresses of 2 or 3 references to: **Aziz Ghoufi**, aziz.ghoufi@univ-rennes.fr, **Guillaume Maurin**, guillaume.maurin1@umontpellier.fr