Title	**Computational and experimental study of innovative membranes for separation and/or conversion processes**
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Project description:

The research project will be concerned with the preparation and characterization of novel dense and porous polymeric membranes, with fillers including solid and liquid crystalline phases. The experimental part of the project will be conducted by the Ph.D. student at the main ITM headquarter in Rende (CS). Modeling and computational studies, both DFT and MD simulations, using several QM and MD software (ADF, Gaussian, Gromacs, LAMMPS) will be run by the Ph.D. student at the ITM Padova Unit. The candidate will develop suitable Force Fields, if needed, and run the simulation of the systems investigated experimentally. Among these, as an example, we mention Artificial Water Channels (AWC), where a self-assembled oligomeric structure is embedded in a dense/porous polymeric membrane: AWC have recently attracted the attention of the scientific community as systems able to perform a selective transport of water with complete ion rejection, therefore having a huge potential for water desalination. Nevertheless, the performance is still significantly lower than the corresponding natural channels counterparts found in lipid membranes, that is aquaporins. A second system worth of investigation is inorganic/mixed matrix membranes with regular cylindrical pores filled with (ionic) liquid crystalline phases. Data reported in the literature have shown an increase in the ionic conductivity of the LC phase compared to the bulk LC and dependent on the LC orientation within the cylindrical pore. However, no clear mechanism has been proposed and the MD simulations will be used to shed light on this behavior and address further experimental work.

Publications:

a) J. Ariai, G. Saielli; *ChemPhysChem* **2019**, 20, 108-115. b) G. Saielli; *Adv. Theory Simul.* **2018**, 1, 1800084. c) G. Saielli, T. Margola, K. Satoh; *Soft Matter* **2017**, 13, 5207-5213; d) T. Marino, F. Galiano, A. Molino, A. Figoli, New frontiers in sustainable membrane preparation: Cyrene™ as green bioderived solvent; *J. Mem. Sci* **2019**, 580, 224-234; e) F. Galiano. I. Friha, S. A. Deowan, J. Hoinkis, Y. Xiaoyun, D. Johnson, R. Mancuso, N. Hilal, B. Gabriele, S. Sayadi, A. Figoli, Novel low-fouling membranes from lab to pilot application in textile wastewater treatment, *J. Colloid and Interface Sci*. **2018**, 515, 208-220.

Collaborations/Network:

Prof. Yanting Wang, CAS-Institute of Theoretical Physics, Beijing.

Research funding:

CNR-CAS bilateral project 2017-2019