Title	**Computational studies of polymeric membranes for separation and/or conversion processes**
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Project description:

The research project is concerned with the characterization of the structural and dynamic properties of porous polymeric membranes, with fillers including solid and liquid crystalline phases. 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, Department of Chemical Sciences. The project will benefit from a strong collaboration with the experimental group of dr. A. Figoli at ITM-CNR headquarter in Rende (CS). The candidate will develop suitable Force Fields 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 recently studied experimentally is made of innovative membranes for water desalination based on polymerized discotic ionic liquid crystals having a rejection rate of NaCl close to that one of commercial products available today on the market. 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. Finally, computational xenon NMR, that is the prediction by relativistic DFT methods of the chemical shift of Xe-129 in various polymeric environments, including hybrid membranes and zeolites, will be used as a tool for structural elucidation by comparison of the computed results with experimental data.

Publications:
a) G. Saielli, *ChemPhysChem* **2024**, 25, e202300963. b) G. Saielli, *Comprehensive Computational Chemistry* **2024**, 3, 723; c) T. Marino, F. Galiano, A. Molino, A. Figoli, *J. Mem. Sci* **2019**, 580, 224-234.

Collaborations/Network:
Dr. Alberto Figoli, ITM-CNR, Headquarter in Rende (CS); Prof. Yanting Wang, CAS-Institute of Theoretical Physics, Beijing; Prof. Katsuhiko Satoh, Osaka Sangyo University, Japan; Prof. F. Castiglione, Politecnico di Milano.

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