Aromatic Ionomers with Controlled Architectures: the challenge of PEMFC (AICA)

The present project is oriented towards the improvement of the performances of PEMFC system through original macromolecular architecture for membrane and catalyst active layer (electrodes). The project aims, through symbiotic academic/finalized research approaches, at developing new nano-structured materials based on aromatic ionomers and at their thorough and multidisciplinary characterization. The project will be developed in the frame of an international collaboration between LEPMI and Simon Fraser University (SFU), Prof. Steven Holdcroft through two PhD subjects (co-supervised by LEPMI and SFU), one in France (funded by CEMAM), and the other in Canada, funded by Automotive Partnerships Canada (APC) and Natural Sciences and Engineering Research Council of Canada (NSERC). The former will be dedicated to the synthesis and fundamental understanding of the structure-transport-functional properties interplay in a selection of new ionomers targeting membrane and/or electrode elaboration, while the latter will more specifically address the functional optimization, electrode formulation and MEA elaboration process and testing in real devices. Both studies will be tightly related through *a regular back-forth process* between formulation, characterization and device integration, and will benefit from cross-fertilized analysis and diagnosis.

PhD at LEPMI

Taking in consideration the very promising preliminary results on aromatic ionomers bearing perfluoroalkyl sulfonic functions we propose in this project to push on this research area and design ionomers with improved structure in order to (i) enhance the ionic conductivity at low RH and high temperature, (ii) to permit a unique tuning of the targeted properties to meet both membrane and electrodes functionality/fabrication requirements. Moreover, in line with its core competence, SFU will develop for the first time with this kind of ionomers the electrodes and the membrane electrode assemblies (MEAs) and will also proceed to the in-situ electrochemical characterization in PEMFC.

Understanding the role of the polymer architecture on the transport and mechanical properties is one of the key factors of many materials implied in electrochemistry (*Structure/transport interplay/functional properties*). The ionic conduction mechanism in polymer electrolytes is intimately associated with the local segmental motions of the polymer, the proton-anion interactions, the local confinement and connectivity, and the state and properties of water molecules. AICA ionomers will be characterized by a combination of experimental techniques used for both structural and dynamical studies, from molecular to macroscopic scales. Ionic conductivity, mechanical measurements, permeability and water sorption will be systematically backed up by the coupled investigation of:
- long-range ordering by AFM (LMOPS); TEM, DRX; Small Angle X-ray and Neutron Scattering (SAXS/SANS) (collaboration SPrAm, experiments performed at the ILL, LLB and ESRF large scale facilities).
- proton conduction mechanism through molecular dynamics and charge transport processes (Quasi-elastic Neutron Scattering (collaboration SPrAM), impedance spectroscopy, measurements of water diffusion coefficient o by pulsed NMR spectroscopy,

The functional properties of membranes; gas permeability, dynamical water vapor sorption and dynamic mechanical analyses under controlled varying conditions of both relative humidity and temperature will be deeply analyzed.

The work will be done in the CEMAM Labex (http://cemam.grenoble-inp.fr/cemam/) framework at LEPMI..

The candidate should have strong knowledge in polymer science, chemistry and physical and electrochemical characterisation techniques.

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