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Polymeric And Composite Electrolyte Membranes: Insights From Multiscale Computational Modeling

James A. Elliott
Department of Materials Science and Metallurgy
University of Cambridge, Pembroke Street, Cambridge, CB2 3QZ, UK.

Perfluorosulfonic acid (PFSA) electrolyte membranes, such as Nafion, are widely employed in fuel cells due to their high proton conductivity combined with excellent chemical and thermal stability. However, the very high degree of disorder in these materials makes it difficult, if not impossible, to deduce their bulk morphology unambiguously from experiments alone without the aid of computational modeling over multiple time and length scales, from the molecular [1] to mesoscale [2].

A further complication in the composite membrane-electrode assemblies (MEAs) is the presence of complex multiphase interfaces between the polymer, catalyst and carbon electrode. In this presentation, I will describe a recent combination of a model-independent procedure for obtaining structural information from small angle scattering based on a Maximum Entropy (MaxEnt) approach coupled with mesoscale simulations using Dissipative Particle Dynamics (DPD) of the morphology of Nafion parameterized with atomistic calculations and density functional theory [3].

These two methods show that the nanoscale ionic clustering in PFSAs is composed of a bicontinuous network of ionic clusters embedded in a matrix of fluorocarbon chains. I will also present results from composite systems in which the distribution of water and ionic groups at the interface in nanoscopic channels are compared with those in bulk membrane. The results show that the structure of thin (5-10 nm) layers of PFSA membranes is quite different to that in bulk, and may play a key role in controlling performance of MEAs.

[1] J.A. Elliott and S.J. Paddison *Phys. Chem. Chem. Phys.*, **9**, 2602-2618 (2007).
[2] D.S. Wu, S.J. Paddison and J.A. Elliott *Macromolecules*, 42, 3358-3367 (2009).
[3] J.A. Elliott, D. Wu, S.J. Paddison and R.B. Moore, *Soft Matter*, **7**, 6820-6827 (2011).