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Structure calculations for hydrated ionomer membranes[1] PHILIP TAYLOR, MEHDI HAMANEH, Case Western Reserve University — The structure of the perfluorinated ionomer Nafion is determined by a process of partial phase separation in which the ionic components form clusters within a matrix of hydrophobic material. The dipoles associated with the ionic groups tend to order in such a way as to form head-to-tail sequences. In this study we are investigating the effects of hydration on the structure and formation of the ionic clusters and their associated internal electric fields by a combination of atomistic molecular-dynamics simulations and analytical theory. We find that a useful concept is the vorticity of the electric dipole moments and its dependence on hydration. Various procedures have been used in order to develop realistic pictures of the nature of the ionic clusters and their interconnectedness, as the presence of continuous pathways through a Nafion membrane is a determining factor in the transport of protons in polymer-electrolyte membrane fuel cells.

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