Modeling of Ion Uptake to Understand Molecular Level Interactions of Pyrrole/Nafion and Aniline/Nafion Bipolar Membranes for Fuel Cell Use

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Last year's research focused on synthesizing novel bipolar membranes (BPM) for fuel cells. The results showed that Pyrrole/Nafion™ BPM performance was at par or exceeded that of traditional proton exchange membranes. Interestingly, BPM prepared with aniline, an ion similar to pyrrole, performed poorly. Understanding why could lead to further refinement of the BPM synthesis concept. This year's research focused on understanding the molecular-level phenomena occurring during the BPM synthesis. A published model was used to investigate aniline and pyrrole ion interactions within Nafion™ prior to polymerization. A close examination of the predictions shows two major energies at play inside the membrane. First, an attractive electrostatic energy associated with the membranes negative fixed charges draws aniline and pyrrole ions into the pores. This attractive energy is countered by a repulsive energy associated with the change in the solvent dielectric properties. This repulsive energy tries to keep the aniline and pyrrole ions away from the pore wall region where the electrical field strength significantly impacts the solvent. The balance between these two forces determines how much of each ion enters the membrane pores and where in the pores these ions aggregate. The results support the hypothesis that pyrrole molecules aggregate and polymerize closer to the Nafion™ pore center while the aniline molecules aggregate and polymerize at the pore wall. Segregation of pyrrole towards the pore center creates the desired bipolar structure; this is crucial for water-spitting. Lastly, this model can be used to evaluate other polymerizable cations for better bipolar membrane synthesis.

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