Molecular Modeling of Novel Fuel Cell Membranes
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Introduction
Fuel cells are clean and efficient energy conversion devices. The fuel cells of interest contain polymer electrolyte membranes (PEMs) that inhibit the conduction of electrons and facilitate the transport of protons. Nafion® is the most widely used membrane for fuel cell applications. However, alternatives are desired because Nafion® is expensive, allows significant amounts of methanol crossover, and functions poorly at low humidity or high temperature. An acid-base blend membrane composed of both acidic sulfonated poly(ether ether ketone) (Ph-SPEEKK) and basic polysulfone tethered with 5-amino-benzotriazole (PSf-BTraz) has been shown to perform better than traditional acidic PEMs such as Nafion and Ph-SPEEKK. We used molecular dynamics to study the PEM morphology and the transport of water, hydronium, and methanol in Ph-SPEEKK/PSf-BTraz blend membranes. Our aim is to understand the fundamental science behind the enhanced properties of the blend membrane.

SPEEK/PSf-BTraz Blend Membrane

- Experiment shows that this acid-base blend membrane has higher proton conductivity and lower methanol crossover vs. Ph-SPEEKK (Li et al., 2010).

References

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