

Molecular Modeling of Novel Fuel Cell Membranes

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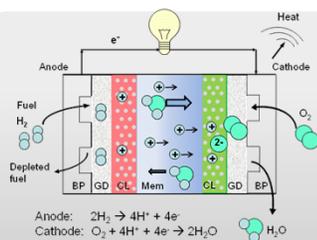


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Introduction

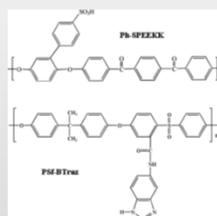
Fuel cells are clean and efficient energy conversion devices. The fuel cells of interest contain polymer electrolyte membranes (PEMs) that inhibit the conduction of electrons and facilitate the transport of protons. Nafion® is the most widely used membrane for fuel cell applications. However, alternatives 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-



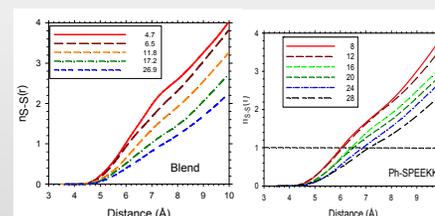
BTraz) has been shown to perform better than traditional acidic PEMs such as Nafion and Ph-SPEEKK. We used molecular dynamics to study the PEM morphology and the transport of water, hydronium, and methanol in Ph-SPEEKK/PSf-BTraz blend membranes. Our aim is to understand the fundamental science behind the enhanced properties of the blend membrane.

SPEEK/PSf-BTraz Blend Membrane

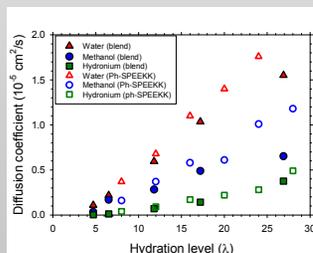
- Experiment shows that this acid-base blend membrane has higher proton conductivity and lower methanol crossover vs. Ph-SPEEKK (Li et al., 2010).



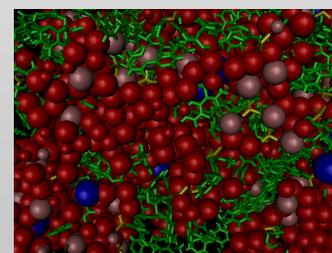
Chemical structure



Sulfur (S₂) coordination number (MD) in Blend vs. Ph-SPEEKK



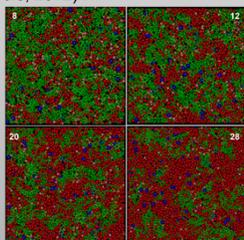
Diffusion coefficient at various hydration levels



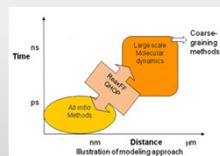
Projection of SPEEK/PSf-BTraz with lambda=11

Previous Research

- There is no membrane that meets the performance, durability, and cost requirements for widespread adoption of fuel cell technology.
- Nafion®, the most widely used PEM, sets the standard for comparative analysis.
- Aromatic membranes based on the poly(ether ether ketone) (PEEK) family show promise (Devanathan, Idupulapati, & Dupuis, 2012).



Multiscale Modeling



- Experimental studies cannot adequately describe nonoscale morphology and transport mechanisms (Devanathan, 2008).
- Multiscale modeling helps us understand the interplay between microscopic and macroscopic phenomena.
- Multiscale modeling reduces research and development costs, increases product quality, and leads to the development of new materials (Horstemeyer, 2009).
- Present work used ab initio molecular dynamics (AIMD) and molecular dynamics (MD). MD results are presented here.

References

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Acknowledgment

RD was supported by the US Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division.

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The Pacific Northwest National Laboratory, located in southeastern Washington State, is a U.S. Department of Energy Office of Science laboratory that solves complex problems in energy, national security and the environment, and advances scientific frontiers in the chemical, biological, materials, environmental and computational sciences. The Laboratory employs 4,000 staff members, has a \$760 million annual budget, and has been managed by Ohio-based Battelle since 1965.

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Image credit: Horstemeyer, 2009



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