Water Diffusion Follows Fractal Dimension in Cationic Polymers

Scientific Achievement

The diffusivity of water in nanoscale water channels formed in cationic polymers is strongly correlated with the fractal dimension of the water channels.

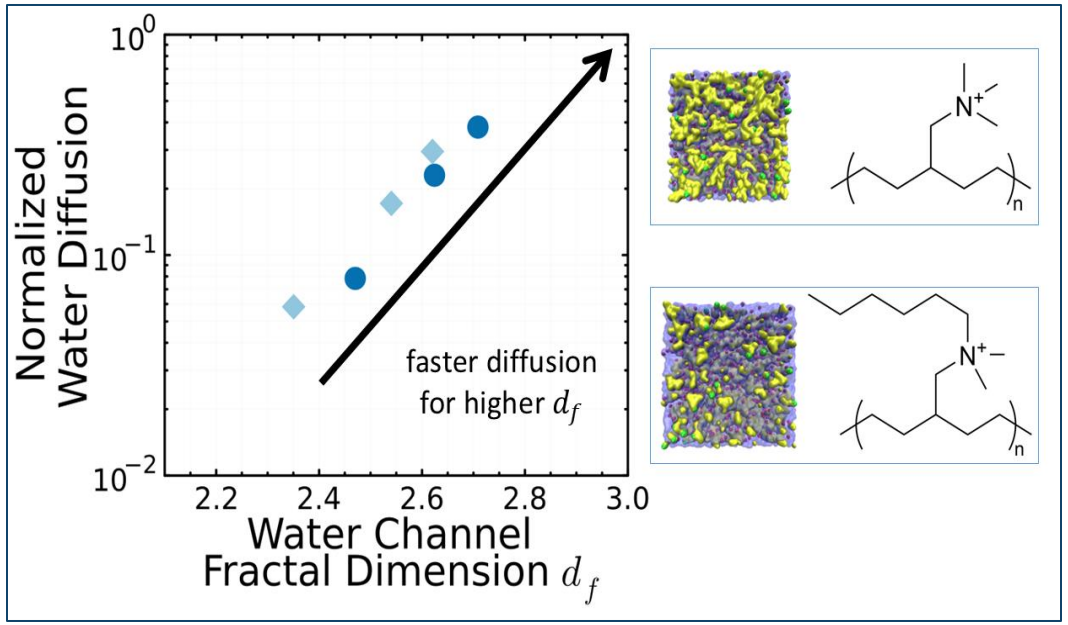

Figure: Water diffusion constants for two different quaternary-ammonium functionalized polymers (right) as a function of fractal dimension, showing good correlation for both polymers. Higher fractal dimensions leads to faster diffusion. The right boxes show snapshots from the MD simulations and the polymer structures.

Significance and Impact

The fractal dimension was found to be a useful measure for the relation between nanoscale morphology and water transport in anion-exchange polymer membranes.

Research Details

- Atomistic molecular dynamics simulations were performed on two quaternary-ammonium functionalized polymers at varying water content.
- Results agreed with previous simulations of sulfonated polymers.

Work was performed, in part, at the Center for Integrated Nanotechnologies.

Drayer, W. F., Duan, E. M., Johnson, J. C., Winey, K. I. & Frischknecht, A. L. Investigating Morphology and Diffusion in Simulations of Precise Anion-Conducting Polymers. *Macromolecules.* 2025.