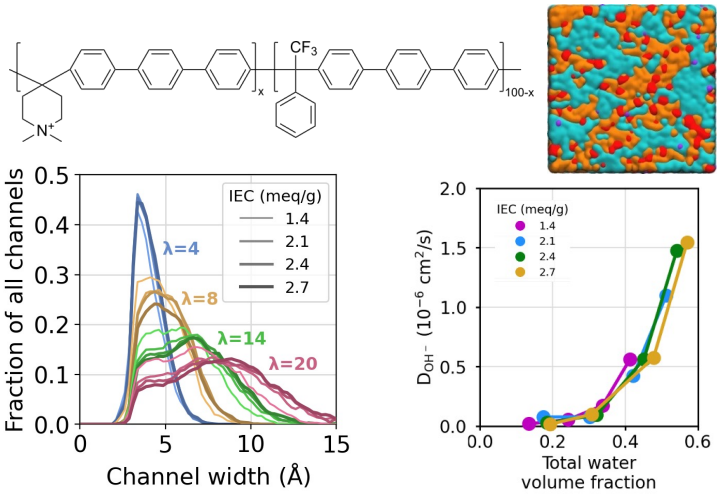
# Simulations Reveal Nanoscale Morphology in Cationic Polymer

## Scientific Achievement

The morphology of nanoscale water channels and the transport of ions in the polymer are found to be determined mostly by water content and are only weakly dependent on polymer ionic content.




Simulations of a piperidinium-functionalized polymer (upper left) nanophase-separate into water (blue) and polymeric channels (orange) (upper right). The size of the water channels depends on water content λ but less on the IEC (lower left). The hydroxide ion diffusion constant depends on water volume fraction (lower right).

## Significance and Impact

This work demonstrates that high hydroxide ion transport can be independent of cationic content, enabling more flexibility in the design of polymers for applications such as electrolyzers.

## Research Details

- Atomistic molecular dynamics simulations were performed as a function of ion content (IEC) and water content (λ)
- Simulations were in good agreement with experiment

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

Clary, J. M.; Wang, L.; Yan, Y.; Frischknecht, A. L.; Vigil-Fowler, D. Effect of Stoichiometry and Hydration Level on Water Domain Size and Transport in Poly(aryl piperidinium) Alkaline Anion-exchange Membranes. *Journal of Membrane Science* **2025**