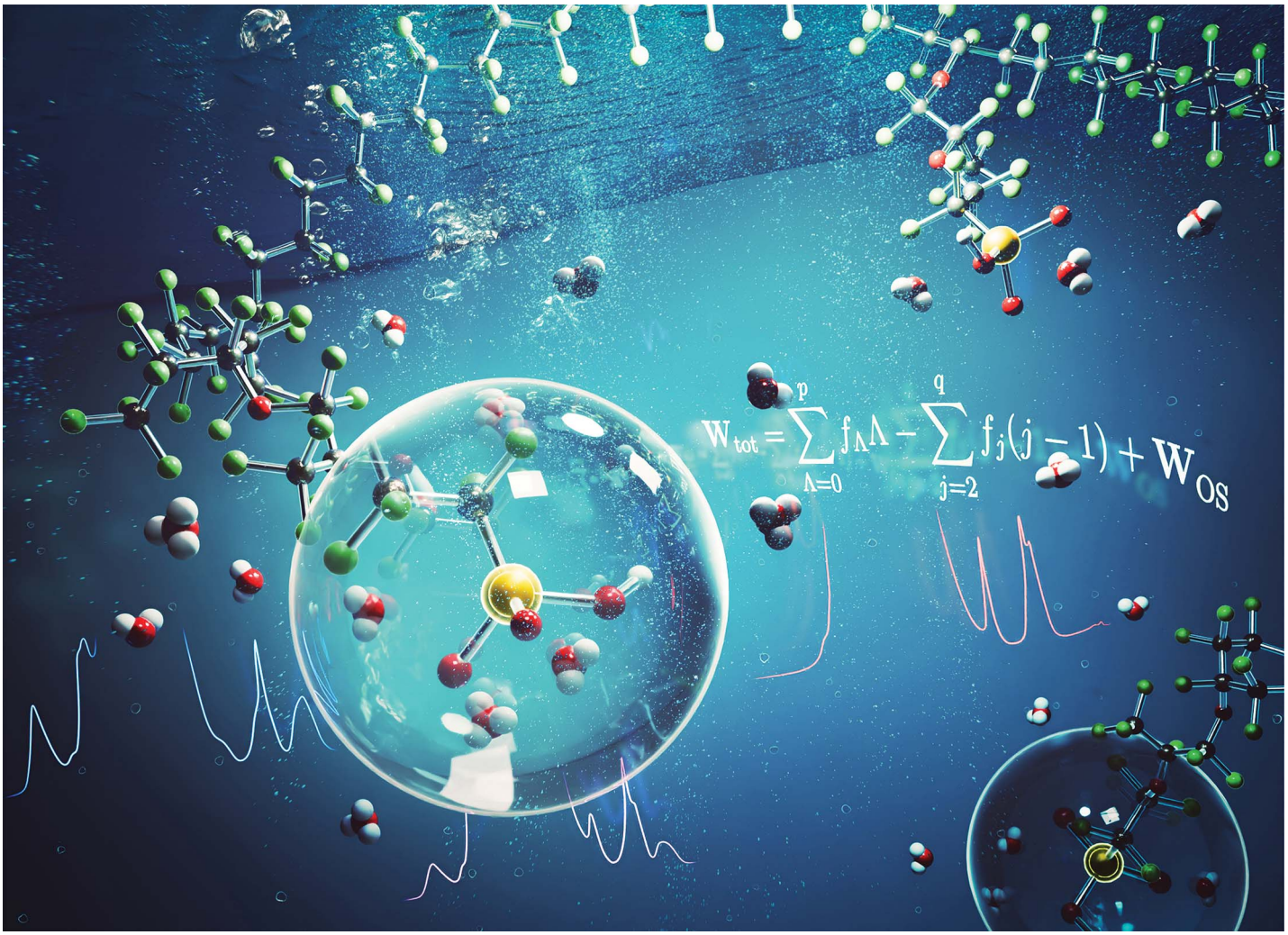

This collaborative study explores hydration effects in Nafion using simulations and spectroscopy, conducted by the labs of Dimakis (UTRGV), Jang (Georgia Tech), Goddard III (Caltech), and Smotkin (Northeastern).

Atomistic characterization of hydration-dependent fuel cell ionomer nanostructure: validation by vibrational spectroscopy

We use ReaxFF molecular dynamics and vibrational spectroscopy to study proton exchange in Nafion across nine hydration levels (λ). Simulations reveal that protonated exchange sites persist at high λ, challenging assumptions of complete ionization. By modeling realistic sites, we capture λ-dependent distributions of protonation states and local water content. These structures align with IR spectra and clarify ionomer hydration response.

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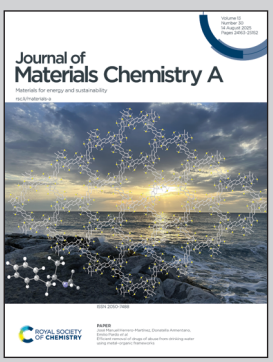

See Nicholas Dimakis, William A. Goddard, Eugene S. Smotkin *et al.*, *J. Mater. Chem. A*, 2025, **13**, 24495.

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