VIBRATIONAL SPECTROSCOPY OF ANIONIC PAH-WATER CLUSTERS

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The intermolecular forces that govern water-hydrocarbon interactions have profound effects in interfacial phenomena, like wetting, and large-scale applications to issues like water security through water desalination with two-dimensional membranes[b]. I will discuss our work on building dynamical methods and water models to describe and interpret the vibrational spectroscopy of anionic water-polycyclic aromatic hydrocarbon (PAH) clusters which act as a minimal model for aqueous-carbon interfaces. Even in a small system of one water with a charged PAH, there is significant complexity, including non-Gaussian fluctuations and ergodicity-breaking at low temperatures. Systematically accounting for these effects leads to semi-quantitative agreement between theoretical predictions and experimental measurements for the IR spectrum in the OH stretching region.

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[b]S. Strong; J.D. Eaves. The dynamics of water in porous two-dimensional crystals. *J. Phys. Chem. B* 2017, 121, 189-207