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Decoupling the Effects of Hydrophobicity and Confinement Within Nanoporous Materials Used for Water-Alcohol Separation CHUN-HUNG WANG, AURORA CLARK, Washington State University — The separation of water and alcohol within biofuel refinement has been studied extensively using nanoporous materials that include zeolites and metal-organic-frameworks (MOFs). The emerging theory for high selectivity of a material for alcohol over water is based upon the combined effects of hydrophobicity of the interior and the response of the water vs. alcohol to confinement inside the porous structure. However, to date, there has been little fundamental research that attempts to decouple the effects of these two very different properties (one chemical and one structural) upon the selectivity value. Toward this end, the solvent organization within zeolitic-imidazolate frameworks (ZIFs) will be discussed as a function of hydrophobicity/hydrophilicity of the interior, pore size/structure, and accessible volume/surface area. Using grand-canonical Monte Carlo (GCMC) and classical molecular dynamics (MD) simulations, the hydrogen-bond (H-bond) networks of water and alcohols adsorbed inside the material from the bulk liquid is investigated using network analysis algorithms. The topology of the H-bond networks has been quantified by use of the geodesic distribution (the shortest intermolecular interaction pathways between molecular vertices), and the adsorbate-adsorbate and adsorbate-adsorbent distributions of intermolecular interactions. The GCMC configurations have been used as starting points for subsequent MD simulations where the hydrophobicity is quantified based upon H-bond lifetimes and mechanisms of orientational dynamics of adsorbates.

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