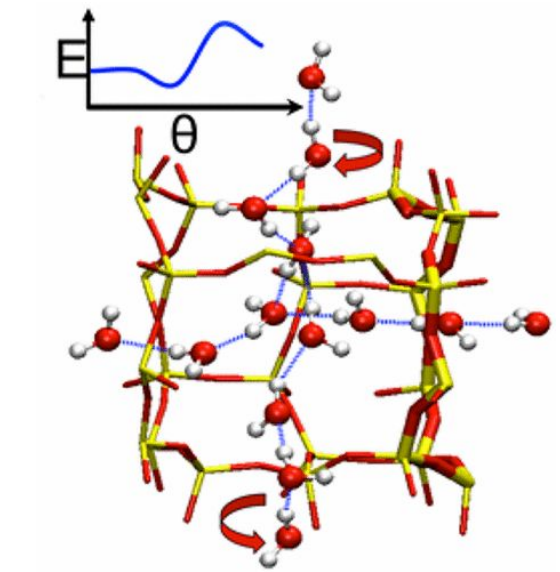
Deconstructing the Confinement Effect upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials



The confinement of water in hydrophobic adsorbents has an effect on the hydrogen bond dynamics via both pure geometric restriction and the rugged potential energy landscape for water interacting with the atomistic pore surface.

Scientific Achievement

The properties of water molecules confined in two hydrophobic all-silica zeolites were studied computationally via hydrogen bond dynamics. Geometric restriction of the water molecules in the adsorbent accounted for the majority of interaction; however, water-surface interactions played a role as well.

Significance and Impact

This work asserts that the weak water-surface interactions in hydrophobic adsorbents cannot be ignored; these findings are applicable to chemical, biological, and geological phenomena in which water is highly confined, such as carbon nanotubes.

Research Details

The structure and the dynamics of confined water in the hydrophobic all-silica zeolites FAU and MFI were studied using MD simulations and INT.

- The in-house MC simulation software package MCCCS-MN was used to calculate water adsorption isotherms and obtain equilibrium configurations at saturation loadings.
- Intermolecular network theory (INT) analyses were performed using the ChemNetworks software.

T. Zhou, P. Bai, **J. I. Siepmann**, and **A. E. Clark**, "Deconstructing the Confinement Effect Upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials: Lessons Learned from Zeolites," *J. Phys. Chem. C* **121**, 22015-22024 (2017)

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Work was performed at University of Minnesota and Washington State University.

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