Nebraska Center for Materials and Nanoscience

2019 Spring Seminar Series

Accurate modeling of liquid water and proton transfer in water

Proton transfer via hydronium and hydroxide ions in water is ubiquitous. It underlies acid-base chemistry, certain enzyme reactions, and even infection by the flu. Despite two-centuries of investigation, the mechanism underlying why hydronium diffuses faster than hydroxide in water is still not well understood. Herein, we employ state of the art Density Functional Theory based molecular dynamics, with corrections for nonlocal van der Waals interactions, and self-interaction in the electronic ground state, to model water and the hydrated water ions.

At this level of theory, structural diffusion of hydronium preserves the previously recognized concerted behavior. However, by contrast, proton transfer via hydroxide is dominated by stepwise events, arising from a stabilized hyper-coordination solvation structure that discourages proton transfer. Specifically, the latter exhibits non-planar geometry, which agrees with neutron scattering results. Asymmetry in the temporal correlation of proton transfer enables hydronium to diffuse faster than hydroxide.

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May 1, 2019 | 4 p.m. | 136 Jorgensen Hall

Refreshments in 1st floor vending area at 3:45

Host: Xiaoshan Xu

Department of Physics & Astronomy