Physical Chemistry Seminar

Prof. Carlos Baiz

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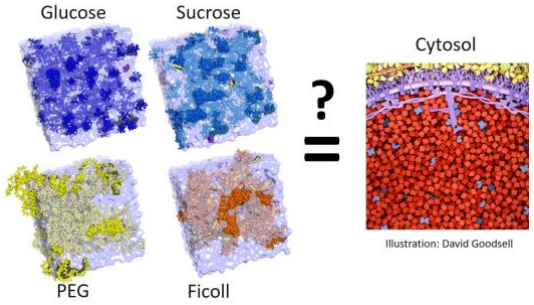
"Ultrafast studies of hydrogen-bond dynamics in complex environments"

Abstract

Cells are heterogeneous on every length scale. The cytoplasm contains thousands of proteins, lipids, and small organic molecules. Compared to pure liquid water, intracellular water is strongly confined by biomolecules. Excluded volume effects and electrostatic interactions disrupt the extended H-bond networks that support fast (sub-picosecond) H-bond dynamics in liquid water. The effects of crowding and heterogeneity in complex, multi-component systems remain difficult to characterize experimentally.



In the seminar, I will discuss our recent work combining ultrafast IR spectroscopy and molecular dynamics (MD) simulations to characterize H-bond dynamics in solutions containing crowding agents which are commonly used to mimic environments representative of the cytosol in biochemical studies (**Figure 1**).[1] The studies show that different crowders produce different dynamics despite the similar excluded volumes. Molecular dynamics simulations of the same systems revealed distance-dependent effects on the tetrahedral H-bond networks. Surprisingly at longer distances >1nm, water tetrahedral structures become more "ice-like" even compared to bulk water, as the tetrahedral ordering of water increases. This structural analysis is consistent with the dynamics observed in experiments and predicted by MD simulations. These studies have implications for understanding the non-specific effects of crowders on biomolecules.

1. You, X., Shirley, J. C., Lee, E., & Baiz, C. R. (2021). Short-and long-range crowding effects on water's hydrogen-bond networks. *Cell Reports Physical Science*, 100419.

Bio

Carlos Baiz is an Associate Professor at the University of Texas at Austin. His lab studies the biophysics of complex systems, including crowded environments, and heterogeneous lipid membranes, membrane proteins, and surfactants, using ultrafast two-dimensional infrared (2D IR) spectroscopy and molecular dynamics simulations.

DATE: TUESDAY, OCTOBER 12 **TIME: 11:00 AM**

LOCATION: 140 BARDEEN MED LAB **HOST: PROF. EDWIN SIBERT**

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