Joint

Center for Soft Matter and Biological Science

and Condensed Matter Seminar

Dr. Katie Mitchell-Koch

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How do bio molecular surfaces influence small molecule dynamics?

Monday, March 27, 2017

4:00 pm—5:00 pm

304 Robeson Hall

Our group has been using molecular dynamics simulations to study the interactions and dynamics of small molecules—solvent and substrate—at the surfaces of biomolecules. Simulations of aldehyde and alcohol substrates in the presence of the aldehyde reductase YqhD have revealed a substrate access channel that is not evident in the crystal structure. Collaborative work with Prof. Vinh Nguyen (Virginia Tech) has investigated the hydration layer dynamics around DPC micelles. Simulations coupled with GHz-to-THz measurements have shown that the slowest waters are hydrogen-bonded to the anionic phosphatidyl oxygen's, while only a modest slowdown in hydration dynamics is observed around the cationic trimethylamine groups of the zwitterionic lipids. Hydration dynamics around the enzyme *Candida Antarctica* lipase B (CALB) have been simulated, indicating heterogeneity in protein-water hydrogen bond lifetimes at the surface. CALB is an enzyme that is also used in organic solvents for the production of fine chemicals such as flavoring agents. Work is underway to characterize the solvation layer of CALB in organic solvents, connecting solvent dynamics to protein structure and dynamics.