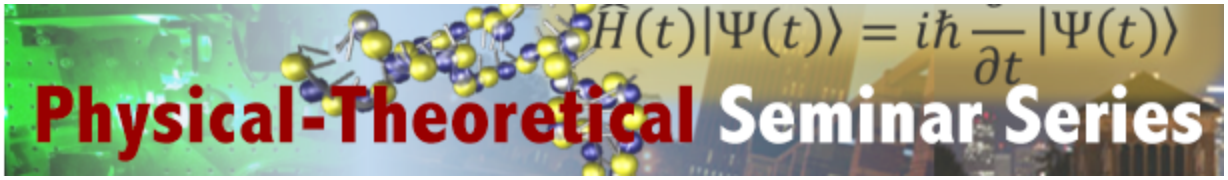

Monday, November 12, 2018, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Professor Adam Willard

Department of Chemistry
Massachusetts Institute of Technology

The statistical mechanics of hydrogen bonding at the liquid water interface

The dielectric properties of liquid water are determined in large part by the orientational fluctuations of dipolar water molecules. Near a liquid water-vapor interface these orientational fluctuations are anisotropic, leading to dielectric properties that differ significantly from their bulk values. These differences are fundamental to interface-selective chemical and physical processes, but they are generally difficult to predict. We attempt to understand these differences by considering the statistical mechanics of hydrogen bonding at the liquid water-vapor interface. Using a mean-field model, we demonstrate that the primary features of water's interfacial molecular structure are determined by the molecular orientations that best facilitate tetrahedral hydrogen bonding within the constraints imposed by the anisotropic interfacial density field. We utilize this mean field model to study the properties of hydrophilic interfaces and then adapt this perspective to the development of an order parameter that can be used to mapping the dynamic hydration properties of proteins.

Hosted by Professor Alex Benderskii

The scientific community is invited