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"From Water Structure and Fluctuations to Hydrophobicity of Proteins and Interfaces"

Water-mediated interactions (e.g., hydrophobic interactions) govern a host of biological and colloidal self-assembly phenomena from protein folding, and micelle and membrane formation, to molecular recognition. Macroscopically, hydrophobicity is often characterized by measuring droplet contact angles. Such measurements are not feasible for nanoscale surfaces of proteins or nanoparticles. How does one then characterize hydrophobicity/philicity of such interfaces? We present results from theory and simulations of hydration of a variety of surfaces to connect the behavior of water at the nanoscale interfaces and their hydrophobicity. Specifically, we show that water density fluctuations (and not the average local density) provide a quantitative characterization of the interface hydrophobicity. Density fluctuations are enhanced at hydrophobic interfaces and suppressed near hydrophobic ones. Simulations also show how properties of water at interfaces influence solute binding, folding, and dynamics of flexible molecules at interfaces. I will demonstrate that this new perspective on hydrophobicity provides a tool for characterization of hydrophobicity patterns on protein surfaces, which are relevant for binding, recognition, and aggregation. Time permitting, I will tell a story of how simulations and science have merged with arts and entertainment to develop an upcoming 3D-IMAX movie, Molecules to the MAX.