"Understanding and Characterizing How Nanostructured Surfaces Perturb Water Structure: Applications to the Prediction of Protein Interactions and the Design of Soft Materials"

**Wednesday
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3:00 pm
Wu and Chen Auditorium
Levine Hall**

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Abstract

By uncovering how water structure is perturbed by nanostructured surfaces, i.e., surfaces with chemical patterns and/or texture at the nanoscale, my group strives to understand, predict, and eventually control biomolecular interactions and assembly, as well as to inform the design of the next generation of functional soft materials. In this presentation, I will share examples of our recent successes in both of these areas.

I will first highlight our efforts in uncovering the role that water plays in mediating the interactions and self-assembly of complex molecules, including proteins, peptides, and surfactants. The extent to which the inherent structure of water is perturbed by these complex molecules, determines the thermodynamics and the kinetics of their assembly. However, accurately characterizing this perturbation is challenging, because the manner in which proteins disrupt the inherent structure of water depends not only on the chemistry of the underlying protein surface, but also on the precise topographical and chemical pattern displayed by the protein. I will discuss our recent successes in quantitatively characterizing the disruption of water structure in the hydration shell of proteins, and in using this information to predict the interfaces through which proteins interact with one another and self-assemble. Our approach also informs strategies for optimally modulating protein interactions, and facilitates the design of ligands that will bind to proteins of interest with high affinity and specificity. We hope that these advances will pave the way for the discovery of novel therapeutics that specifically target proteins of interest, and the rational design chromatographic ligands for challenging protein separations.

I will then describe our efforts in designing rough or textured hydrophobic surfaces, which are dubbed "superhydrophobic" due to their numerous desirable properties, such as water repellency and interfacial slip. Superhydrophobicity stems from an aversion of water for the hydrophobic surface texture, so that a water droplet in the superhydrophobic "Cassie state" contacts only the tips of the rough surface. However, superhydrophobicity is remarkably fragile and can break down due to the wetting of the surface texture to yield the "Wenzel state" under various conditions, such as elevated pressures or droplet impact. Moreover, due to large energetic barriers that impede the reverse transition (dewetting of the texture), this breakdown in superhydrophobicity is widely believed to be irreversible. Using molecular simulations and enhanced sampling techniques, we challenge this conventional wisdom. In particular, we show that water density fluctuations play an important role in dewetting the surface texture; by circumventing the classical dewetting pathways, fluctuations lead to a reduction in the free energetic barriers to dewetting. Importantly, an understanding of the mechanistic pathways to dewetting and their dependence on pressure allows us to augment the surface texture design, so that the barriers to dewetting are eliminated altogether and the Wenzel state becomes unstable at ambient conditions. Such robust surfaces, which defy classical expectations and can spontaneously recover their superhydrophobicity could have widespread importance, from underwater operation to phase-change heat transfer applications.

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