Title: “Discovering Molecular Scale Driving Forces at the Nano/Bio Interface”

Rational design of unique solvents and surfaces holds great potential for providing new ways to use biomolecules in engineering applications, which range from biocatalysis in ionic liquids (ILs) to surface-driven self-assembly of nano/bio materials that mimic nature. Computational models such as molecular dynamics (MD) can connect the atomic scale to the mesoscale for a wide range of problems but many challenges still limit wide-ranging use of these tools to their full potential. The theme of this talk will be to share recent advances in fundamental science and engineering of interfacial phenomena of proteins and enzymes in the context of our group’s efforts to address fundamental challenges preventing wider use of MD-based methods.

The first part of this talk will highlight how we are using simulations to understand the dominant driving forces that lead to unique orientation and conformation of peptides at the bio/nano interface. Examples range from the formation of biosilica in the simple leucine-lysine (LK) peptide systems self assembly of peptide structures at gold interfaces. The second part of the talk will discuss recent work from our group exploring how ionic liquids changes the equilibrium behavior of enzymes and proteins. I will discuss progress toward an automated computational screening procedure to evaluate enzyme/IL pairs for their suitability in biocatalysis. I will also discuss how we are applying stochastic analysis approaches to study the rates of protein unfolding in response to novel IL solvents