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 biomolecules in the context of our group’s efforts to address fundamental challenges preventing wider use of MD-based methods (e.g. timescale limitations in MD).

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 with an illustration of how the surface/peptide interface strongly dictates the dominant contributions to binding energetics. I will also discuss the challenge of accurately predicting biomolecule structure at interfaces and how a marriage of simulation and sparse experimental data can provide deep insight. Following this I will share several examples related to the formation of biosilica in two systems: peptides based on marine diatoms, and diatom mimics that use simple leucine-lysine (LK) repeat peptides.