Simulation insights into self-assembly in designer bio- and nano-materials

We discuss the development and application of novel molecular simulation methods to understand bio-inspired self-assembly principles in nanostructured materials. In the first part of the talk, we consider newly engineered peptides that hold promise as controllable, environmentally benign alternatives for nanoscale materials and scaffolds. Despite experimental advances in this area, it remains an immense challenge to predict even basic self-assembly properties from a theoretical perspective. We show how novel multiscale simulation techniques can elucidate the delicate balance of assembly driving forces and modulate novel emergent phase behavior in these systems.

In the second part of the talk, we examine self-assembly as route to chiral materials made from achiral molecules. We show that a surprisingly simple mechanism, based only on excluded volume interactions, can drive achiral particles into chiral assemblies. The mechanism quantitatively explains recent experimental results reporting emergent chirality in the two-dimensional hard triangle system, and it predicts other shapes that might exhibit similar behavior. Such results suggest a potentially powerful new knob for designing materials with unique chiral responsive behavior, and may also suggest a way that chiral structures might emerge in nature.

Biography

Prof. M. Scott Shell is an Associate Professor in the Chemical Engineering Department at UC Santa Barbara. His group develops novel molecular simulation, multiscale modeling, and statistical thermodynamic approaches to address several problems in contemporary biophysics and soft condensed matter. Prof. Shell earned his B.S. in Chemical Engineering at Carnegie Mellon in 2000 and his Ph.D. in Chemical Engineering from Princeton in 2005, followed by postdoctoral work at UC San Francisco in the Department of Pharmaceutical Chemistry. He is the recipient of a Dreyfus Foundation New Faculty Award (2007), an NSF CAREER Award (2009), a Hellman Family Faculty Fellowship (2010), a Northrop-Grumman Teaching Award (2011), and a Sloan Research Fellowship (2012).