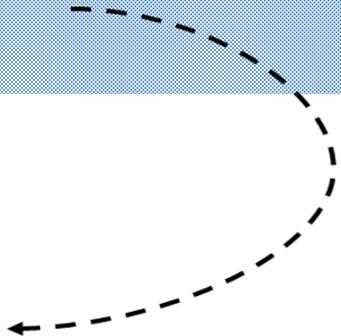


# Seminar



Wednesday, April 18, 2018

11:00 AM – 206 Furnas Hall

**M. Scott Shell**

Professor

Department of Chemical Engineering

University of California– Santa Barbara

## **Simulation design of interfaces through shape and chemistry**

The patterning of interfaces, both chemical and structural, directs an enormous range of thermodynamic and dynamic properties of the fluids that meet them. Here, we present two examples where molecular simulations allow systematic charting of the effects of different interfacial configurations, which in turn offers design principles for engineering desired structures and behaviors. In the first, we examine a route to chiral surfaces through the self-assembly of achiral, quasi-2D colloidal particles of tunable shapes. We show that a surprisingly simple mechanism, based only on excluded volume interactions, can drive achiral particles into chiral materials. The mechanism quantitatively explains recent experimental results, predicts new chiral-prone shapes, and suggests a way that chiral structures might emerge in nature. In the second part, we show that precise hydrophobic/hydrophilic chemical patterning on a variety of solid surfaces provides an important way to control the dynamic behavior of adjacent water. We develop a novel genetic optimization algorithm, coupled to iterative molecular dynamic simulations, that designs the arrangement of surface groups so as to minimize or maximize the diffusion nearby water. Surprisingly, the algorithm uncovers novel surface designs that produce a wide range of dynamics for a given constant average surface hydrophobicity fraction. We provide a molecular-thermodynamic interpretation of these results using water structural order parameters.

Refreshments at 10:45



University at Buffalo

Department of Chemical  
and Biological Engineering

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