The Graduate Simulation Seminar Series Presents

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Modeling the complex with the simple: case studies in soft matter

Abstract: Most materials are complicated systems composed of a myriad of details- multiple components, competing interactions, and physics spanning scales from quantum to macro. However, we can gain basic insights into these systems using simplistic models coupled with simulations to provide fundamental understanding of the nature of such systems. Here, I will consider a diverse set of case studies: molecular dynamics of coacervate core micelles, continuum models of crystallization in isotactic polypropylene, and Monte Carlo simulations of patchy particles as mimics for solutions of small globular proteins. In each example, I will emphasize the importance of choosing the appropriate simulation method and connecting to experimental results.

Bio: Debra Audus is a chemical engineer at NIST. She received her B.S. In Chemical Engineering from Cornell University in 2007 and her Ph.D. in Chemical Engineering from the University of California, Santa Barbara in 2013. She was a National Research Council postdoctoral fellow from 2013-2015.

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11:30 AM, Elings 1605

Career Q&A: 2:30 PM, ESB 2001

Special thanks to:
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