

ME 600 Seminar

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Georgia Tech

February 22nd at 11:00 am in 2004 Black

Title:

A Systems Engineering Approach to Molecular Organization

Simulation-based design and model-predictive control are well-established approaches for the engineering of macroscopic systems, in applications ranging from bridges to aircraft to petrochemical plants. However, the design and control of collections of molecules are often approached from an empirical perspective, especially when an explicit consideration of discrete molecular interactions is required. A key challenge in model-based design is that the time scales of molecular simulation are often much shorter than the processing time scales of interest. The crystallization of small molecules has been studied from both top-down and bottom-up perspectives and provides guidance toward a systems engineering approach to molecular organization. In this presentation, case studies in polymer organic electronics and prebiotic chemistry will be presented, which exhibit polymerization as well as the formation of paracrystalline assemblies.

Biography

Martha Grover is a Professor in the School of Chemical & Biomolecular Engineering at Georgia Tech, and Associate Chair for Graduate Studies. She earned her BS in Mechanical Engineering from the University of Illinois, Urbana-Champaign, and her MS and PhD in Mechanical Engineering from Caltech. She joined Georgia Tech as an Assistant Professor in 2003. In 2011 she received the Outstanding Young Researcher Award from the Computing and Systems Technology Division of AIChE, and in 2019 the Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education. Her research program is dedicated to understanding, modeling, and engineering the self-assembly of atoms and small molecules to create larger scale structures and complex functionality. Her approach draws on process systems engineering, combining modeling and experiments in applications dominated by kinetics, including surface deposition, crystal growth, polymer reaction engineering, and colloidal assembly. She is a member of the NSF/NASA Center for Chemical Evolution, and Georgia Tech's Decision and Control Laboratory.



This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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