“A Systems Engineering Approach to Molecular Organization”

Prof. Martha Grover

School of Chemical & Biomolecular Engineering, Georgia Tech

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.

“Systems analysis for peptide systems chemistry,” M. A. Grover, M.-C. Hsieh, D. G. Lynn, *Life*, 9(3), 55 (2019). https://www.mdpi.com/2075-1729/9/3/55