Design and Control of Molecular Self-Assembly

Martha Grover
Chemical & Biomolecular Engineering
Georgia Institute of Technology

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Abstract:
Atoms and molecules assemble to form larger structures with more complex function. By designing the molecular components and then controlling the process by which they assemble, structure and function can be engineered. Understanding of the assembly process is also critical to understanding biological design principles and the emergence of living systems on the early Earth.

Two application areas will be presented in this talk. The first is feedback control of colloidal assembly. A model-based optimal feedback policy is designed for this stochastic assembly process using dynamic programming. Voltage is manipulated to control the assembly of a large collection of particles into an ordered crystal, which is needed for optoelectronic devices. The experiments confirm that defects can be detected and healed early, before they are locked into the crystalline lattice.

The second research area is the assembly of functional biopolymers under early Earth conditions. Without enzymes available to catalyze polymerization reactions, different chemistries and environments are needed. The ester bond forms more readily than the amide bond, and thus polyesters could have been a predecessor to proteins. Modeling and experiments demonstrate the ability to synthesize proteopeptides using periodic (e.g. day/night) environmental cycles.