Seminar/Talk

Mix, match, and assemble: an inverse design approach to tailor materials

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Self-assembly is the spontaneous organization of components into defined structures without external guidance. This phenomenon underpins many natural processes, and its underlying mechanisms are increasingly being harnessed in materials science to construct complex structures with tailored functionalities. Inverse self-assembly seeks to design building blocks that guide the system toward a target structure, while avoiding kinetic traps and competing assemblies. Despite efforts involving the tuning of interactions and the use of complex shapes in single-component colloidal systems, experimental realizations remain elusive and often system-specific. We propose a different strategy: designing mixtures. To address the combinatorial complexity this entails, we recast the design challenge as a coloring task, which we then map onto a boolean satisfiability problem. This framework enables the automated generation of design options for mixtures of patchy particles targeting any desired assembly. By testing these candidates through numerical simulations, we gain insights into the self-assembly process of multi-component systems. Beyond targeting structural properties, our approach can integrate selected thermodynamic requirements directly into the design, enabling the programming of complex phase behaviors and the selection of the most effective self-assembly pathway in multi-component systems.

Thursday, September 11, 2025 11:00am - 12:00pm
Ballroom / Central Bldg

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