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Field-Theoretic Simulations: An Emerging Tool for Soft Material Design

Field-theoretic representations of many-body problems in classical and quantum statistical mechanics have been known for more than 70 years, but have largely enabled approximate analytical calculations. Over the past decade, my group has shown that the complex-valued statistical field theory models of classical fluids can be directly tackled by numerical simulation. Such "field-theoretic simulations" (FTS) are advantaged over conventional particle-based computer simulations in a variety of situations, especially dense melts of high molecular weight polymers and systems with long-ranged interactions, such as polyelectrolytes. They are also well-suited for multi-scale simulations spanning nanometers to microns.

This talk will introduce the construction of field theory models of polymeric fluids and the FTS framework. Two application examples will be provided: the design of uniquely hard-tough-elastic thermoplastics, and the complexation behavior of oppositely charged polyelectrolytes.