

INVERSE DESIGN OF INTERACTIONS FOR ASSEMBLY

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Nanometer-scale, colloidally-stable particles suspended in a fluid can be driven to assemble into a wide variety of different structures depending on the control parameters of the system and the nature of the effective interparticle interactions. In many cases, the relevant interactions are tunable via external fields, physical or chemical modification of the particle surfaces or changes in the composition of the suspending solvent. In this talk, we discuss some of the theoretical challenges associated with using inverse methods to guide the design of such interactions for assembly of colloidal mesophases with targeted structure [1-3] and the opportunities that new machine-learning based simulation approaches [4,5] may provide for addressing them.

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