Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A6] Symposium A-6

Chair: Emma Griffiths(University of Cape Town, South Africa)
2018年10月31日(水) 11:15 ～ 12:30 Room6

[SY-A6]Design of patchy nanoparticles via the self-assembly of triblock terpolymers in selective solvents

Invited

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The hierarchical self-assembly of triblock terpolymers in solution is a successful bottom-up methodology for constructing functional patchy nanoparticles with prescribed topology and shape. Currently, the design of such nanoparticles requires an iterative process to identify the experimental phase parameters needed to produce any target pattern. The broad use of this technology is therefore cumbersome and limited by an incomplete understanding of the mechanisms underlying patch transition. A detailed understanding of how thermodynamics and kinetics influence the topology of the assemblies is also missing. In this work, we present a set of rules for programming desired shapes of the nanoparticles and predicting the pathways by which they assemble. We investigate systematically the interplay between entropic and enthalpic parameters governing the self-assembly of ABC triblock copolymers in a selective solvent for the C block. We use a computational modeling at the mesoscale and thereby encompass the length and time scales associated with the motion and assembly of the polymer coils, while accurately approximating the chemically driven interactions. The phase diagram predicted by our model is consistent with experimentally identified characteristic nanoparticle shapes. We find that the effective volume fraction of the soluble block determines the size of a particle and the distribution of its patches via steric interactions. Moreover, we find that the relative fraction of the patch-forming block and its affinity with the core of a articles dictates the number and shape of its patches. As a major outcome, we construct a morphologically-based library of nanoparticles. That library can be used to hierarchically design mesoscale aggregates with specific morphologies. Our results provide insight regarding the mechanisms that determine nanometer scale objects in synthetic and naturally occurring systems.