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Predictive Modeling and Design of Corona Driven Self-Assembly

THI VO, Columbia University, OLEG GANG, Brookhaven National Lab, SANAT KUMAR, Columbia University — Nanoparticle (NP) self-assembly that result in ordered arrangements can produce materials with interesting emergent properties. However, control of the assemblies is challenging as NPs can easily phase separate out of solution. Efforts to control dispersion have focused on surface modifications to program additional interactions to NPs. While these approaches have resulted in increased miscibility and morphological control, the emphasis has predominantly focused on spherical NPs, which have a limited range of accessible morphologies. One method to search for new morphologies is to utilize differently shaped cores. Here, we propose a theory that predicts corona conformation for polymers grafted to an anisotropic core. Our results indicate a preferential partitioning of chains of differing lengths to positions of maximum curvature, giving rise to NPs with different coronal conformations. By taking advantage of corona complementarity, we can optimize NPs to pack into "lock-and-key" configurations as well as design crystal motifs that can produce morphologies with long range ordering. These results strongly suggest that corona-amplified shape complementarity is a powerful handle for precise control of self-assembly.

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