Hierarchical self-assembly of associating soft patchy particles

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We consider star-shaped block copolymers (SBC's) with a sopvophilic core and a solvophobic tail on each arm as novel, model particles which self-assemble into soft patchy colloids of tunable patchiness at the single-molecule level and then into a variety of disordered and ordered structures at finite concentrations. In particular, we use the arm number (functionality), f, as well as the fraction of attractive end-monomers, α , as control parameters of the the macromolecules, which give rise to various scenarios of self-assembly. By employing a variety of computational and theoretical tools, ranging from the microscopic to the mesoscopic, coarse-grained level in a systematic fashion, we investigate the crossover between the formation of microstructure vs. macroscopic phase separation, as well as the formation of gels and networks in the system. We finally show that SBC's can be used as building blocks for the fabrication of open crystal structures, such as the diamond or the simple-cubic lattice, taking advantage of the strong correlation between single-particle patchiness and lattice coordination at finite densities.

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