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Effect of competing monomer-monomer and monomer-particle interactions on the assembly of copolymer grafted nanoparticles[1] TYLER MARTIN, ARTHI JAYARAMAN, University of Colorado at Boulder — Functionalizing nanoparticles with copolymer ligands is an attractive method to tailor the assembly of the nanoparticles. In this talk we present simulation results that show the effect of competing monomer-monomer and monomer-particle interactions on assembly of nanoparticles grafted with AB copolymers with diblock or alternating sequence. We vary strengths of like-monomer (A-A and/or B-B) attractive interactions in the presence of strong or negligible monomer A- particle (A-P) attraction or monomer B- particle (B-P) interaction. At a constant particle size and graft length, the competing interactions and copolymer sequence dictate the amount of inter-grafted particle monomer aggregation, inter- and intra-graft monomer aggregation within the same grafted particle. The resulting monomer aggregation on/near the particle surface imparts an effective patchiness to the particle. For e.g., in case of particles grafted with AB diblock copolymer (with A block closer to the surface) the presence of strong B-P and B-B attractions leads to smaller attractive patches that extend from the surface, and in turn lead to anistropic assembly, while presence of strong A-P and A-A attractions lead to larger attractive patches closer to the particle surface and in turn isotropic assembly.

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