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**Self-assembly of Polyelectrolyte-coated Nanoparticles** CHENGYUAN WEN, SHENGFENG CHENG, Department of Physics, Center for Soft Matter and Biological Physics, and Macromolecules Innovation Institute, Virginia Tech — Polyelectrolyte adsorption and the resulting electrostatic repulsion have been widely used in the stabilization of colloids. In recent years, electrostatic self-assembly has attracted significant attention as a viable route towards novel nanostructures. We use molecular dynamics simulations to study the interactions and self-assembly of polyanion and polycation-coated nanoparticles. The nanoparticle is modeled as a layer of sites uniformly distributed on a spherical surface with a certain fraction of sites serving as the tether points of the grafted polymer brush. The polymer is modeled as bead-spring chains with a certain fraction of beads carrying charges. The solvent is treated as a uniform dielectric background but counterions are included explicitly as mobile beads. We vary the grafting density of the polyelectrolyte chains on the nanoparticles, the chain length, and the charge fraction and study their effects on the mutual interaction and the resulting assembly of nanoparticles. Our preliminary results have revealed possible routes towards supracrystals with NaCl or CsCl structure and other novel structures.

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