Electrostatic driven ridge formation on nanoparticles coated with charged end group ligands

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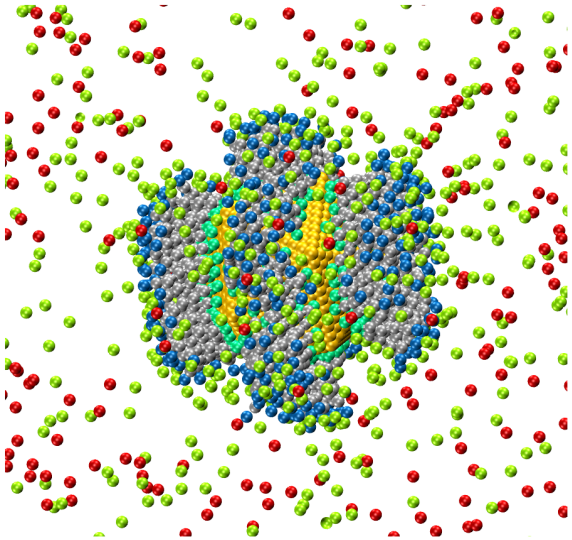
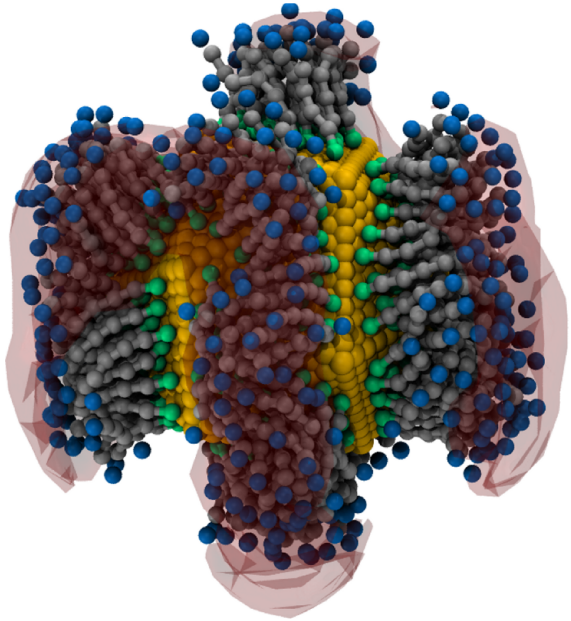
The ever-growing need for fast, compact, and inexpensive electronic devices drives active research in the field of composite materials. The main goals are to increase component density and reduce power consumption. An essential ingredient in the successful control of material properties at the nanoscale requires a robust technique for designing the material-building blocks. Using a generic coarse-grained model, we investigate the surface patterns of charged end-group ligands attached to faceted nanoparticles. A competition between electrostatic repulsion and hydrophobic ligand−ligand attraction leads to the formation of a number of different conformations of the ligand coatings. The most prominent conformation in icosahedral nanoparticles is a ridge-like structure that makes their surfaces highly anisotropic. Meanwhile, bundles seem more prominent than ridges for tetrahedral, cubic, octahedral, and dodecahedral nanoparticles of diameters comparable to the chain length. We argue that a tunable ligand-coating pattern can be used as a simple and robust tool for achieving direction-dependent interactions between nanoparticles and provide control of their assembly into composite materials with a desired symmetry.





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