

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Ridge formation of charged end group ligands grafted on faceted nanoparticle PEIJUN GUO, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — We have investigated the conformations of charged end group ligands grafted on icosahedral nanoparticles, using a coarse-grained molecular dynamics approach. Due to a competition between the electrostatic repulsion and the hydrophobic ligand-ligand attraction, the ligand coatings form a variety of different conformations. These conformations have been compared with the case of non-charged grafted ligands. We have found that the electrostatic interaction between the charged ends drives the formation of a ridge-like structure of the ligands, which makes the nanoparticle surface highly anisotropic. We argue that the ridge-like ligand structure induces controllable directional interaction between the nanoparticles, and can drive the self-assembly of the nanoparticles into crystalline structures.

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Date submitted: 18 Nov 2010

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