

98c Structure and Surface Energy of Ligands-Protected Nanoparticles in Polymeric Solutions by Density Functional Theory

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Colloidal stability is critically important in a variety of biomedical and materials applications of nanoparticles. A conventional approach is to tether nanoparticles with a layer of highly soluble ligands, thereby introducing nanoparticle functionality and preventing nanoparticle aggregation by steric repulsion. However, the microscopic structure and surface energy of ligands coated nanoparticles are not completely understood. This is particularly true if one considers the variation of interfacial properties with the particle size, the chemistry of ligands, their chain length and flexibility, and grafting density. In this work, we have investigated the solvation energy and interfacial microscopic structure of isolated ligands-protected nanoparticles in polymer solutions through density functional theory. At low surface coverage of end-grafted ligands, the insertion of large nanoparticle is energetically unfavorable and the surface energy rises monotonically with the particle size. In this case, the increase of the ligands chain length alters the thickness of the protection layer but has only minor effect on the interfacial energy. At sufficiently high surface coverage, however, the surface energy of a large nanoparticle or longer ligand chains is much more negative than that of a small particle or short ligand chains, suggesting an increase in solubility with the particle size. In both cases, longer polymer chains and lower polymer concentration lead to improved stability of nanoparticles.