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Conjugated Polymer Nanoparticle Hybrids: Structure, Dynamics and Forces[1]

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While nanoparticles (NPs) have unique tunable elctro-optical properties and exceptional mechanical strength, it remains a challenge to integrate them into devices while retaining the advantages of the nanoscale. Tethering polymeric materials to the NPs surfaces has the potential to stabilize single NPs and direct their assembly. The polymers may serve in several capacities from a simple tether to a matrix to directed assembly tool taking advantage of the inherent structure of the polymers and as an active component in a complex material. However confining a large molecule to a highly curved surface affects the inherent configuration of the polymer. These effects are of particular interests in conjugated polymer-nanoparticle hybrids, where the conformation of the polymers affects not only the assembly of the nanoparticles but also the optical and electronic communication between the NPs. Using molecular dynamic simulations we have studied the structure of a single hybrid of *para* dialkyl phenylene ethynelyne (PPE) grafted nanoparticles. PPEs are polymers whose conformation determines their degree of conjugation and therefore their electro-optical response. Using simulations coupled with neutron scattering studies we have shown that PPE is a rigid polymer that is fully extended in dilute solutions in good and theta solvents but can be forced into a collapsed configuration in a poor a solvent. When confined to a nanoparticle surface, the PPE chains are fully extended but cluster as the solvent quality is reduced. Results for the conformation of grafted PPE molecules on a single nanoparticle and the forces between two nanoparticles as a function of chain length and solvent quality will be presented. These simulations provide insight to the interactions that result in formation of tunable hybrids.

[1]This work has been done in collaboration with Gary S. Grest.