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Conformational Study of Rigid Polymers Grafted on Silica Nanoparticle SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY S. GREEST, Sandia National Laboratories — Atomistic molecular dynamics simulations have been used to study the structure and conformation of dialkyl poly *para* phenyleneethynylenes (PPEs), an electro-optically active polymer, confined to silica nanoparticles (NP), with the goal to define the factors that control the assembly of polymer-nanoparticle complexes. The conformation of PPEs determines the conjugation length and their assembly mode which in turn affects the electro-optical properties of the NP-polymer complexes. The current work investigates the structure of diethylhexyl PPE confined to silica nanoparticles as a function of solvent quality. In comparison with grafted flexible hydrocarbon chains, the PPE backbones remain stretched out away from the surface of the NP. The nature of solvents affects the distribution of the chains around the NP. In good solvent, the radial distribution of the polymer is isotropic whereas in a poor solvent distinct clustering is observed. Further studies are on their way to investigate the effects of molecular parameters including the length of the polymer and nature of the side chains coupled with molecular interactions, on the structure and the conformation of the confined PPE and extends the single particle study to an ensemble of NPs.

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