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Study of Rigid Polymers Grafted on Silica Nanoparticle as a Function of Coverage using Molecular Dynamics Simulations SABINA MASKEY, Clemson University, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories, DVORA PERAHIA, Clemson University — Nanoparticles (NPs) hybrids consisting of para dialkyl phenyleneethynylenes (PPEs) grafted to a silica NPs were studied in solution using molecular dynamic simulations. PPEs are rigid polymers whose conformation determines their degree of conjugation and assembly which in turn affects the electro-optical response of the NPs-polymer hybrids. Here we report the effect of coverage of PPE chains on their conformation, correlated with their interaction with the solvent. We have previously shown that at low coverage in good solvent, a star like hybrid is formed with the PPEs chained assuming a fully extended configuration in the corona, and associated with each other to form clusters with reduced solvent quality. Here we show that similar to the low concentration regime, increasing the coverage of PPEs in good solvents results in a homogenous corona with starched out PPE molecules. However, at higher coverage, clustering of chains becomes distinctive and their number increases with increase in the coverage of PPEs. We find that the clusters are temperature responsive and dissociate with increasing temperature. This control over clustering of the corona chains offers a mechanism to tune the electro-optical behavior of the hybrid as well as direct their assembly.

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