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Forces between nanoparticles grafted with rigid polymers: a pathway for tunable hybrids¹ SABINA MASKEY, DVORA PERAHIA, Clemson University, J. MATTHEW D. LANE, GARY S. GREST, Sandia National Laboratories — The forces between the nanoparticles hybrids that consist of para dialkyl phenyleneethynylenes (PPEs) grafted to a silica nanoparticle have been studied using molecular dynamic simulations. PPEs are rigid polymers whose conformation determines their degree of conjugation and their assembly mode which in turn affects the electro-optical response of the nanoparticle-polymer complexes. When confined to a nanoparticle surface, the PPE chains are fully extended but cluster as the quality of the solvents is reduced. Tuning the degree of clustering by tuning the solvent-polymer interaction is expected to direct the assembly of the particles. Results for the forces between two nanoparticles functionalized with rigid polymers as a function of solvent quality, velocities and distances will be presented. These simulations will provide for the first time insight to the interactions of the nanoparticles grafted with rigid polymer, which in turn, results in formation of tunable hybrids.

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