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Confinement of conjugated polymers into soft nanoparticles: molecular dynamics simulations[1] SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The structure and dynamics of conjugated polymers confined into soft nanoparticles (SNPs) have been studies by molecular dynamic simulations. This new class of tunable luminescent SNPs exhibits an immense potential as bio-markers as well as targeted drug delivery agents where tethering specific groups to the surface particles offers a means to target specific applications. Of particular interest are SNPs that consist of non- crosslinked polymers, decorated with polar groups. These SNPs are potentially tunable through the dynamics of the polymer chains, whereas the polar entity serves as internal stabilizer and surface encore. Confinement of a polymer whose inherent conformation is extended impacts not only their dynamics and as a result their optical properties. Here we will present insight into the structure and dynamics of dialkyl poly *para* phenylene ethynylene (PPE), decorated by a carboxylate groups, confined into a soft particle. The conformation and dynamics of polymer within SNP will be discussed and compared with that of the linear chain in solution.

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