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Molecular Dynamics Study of Single Conjugated Polymers Confined to Nanoparticles SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREEST, Sandia National Lab — Optically active polymers confined into nanoparticles are highly fluorescent and have potential applications in intracellular fluorescence imaging, bio-sensors and other optoelectronic devices. Internal conformation and dynamics of the polymers determines their optical properties. Using molecular dynamics (MD) simulations, we have explored the structure and dynamics of nanoparticles formed by conjugated polymers in a collapsed conformation, which is not the most stable conformation of the polymer. Nanoparticles were formed in a collapsed conformation and followed as the function of time in both poor and good solvents. We found that these nanoparticles are stable and remain collapsed in a poor solvent but rapidly expands and unraveled in a good solvent. The lengths of the side chains affect the internal packing of the side chains which in turn affect the size of the nanoparticles. $S(q,t)$ was measured to characterize the internal dynamics of the collapsed nanoparticles.

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