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Polymer Architecture Effects in Confined Geometry: Molecular Dynamics Simulation Study[1] SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Laboratories — Luminescent rigid polymers confined into nanoparticles, or polydots, are emerging as a promising tool for nano medicine. The constrained architecture of a rigid backbone trapped in nano-dimensions results in photophysics that differs from that of spontaneously assembled rigid polymers. Incorporating ionizable functionalities in the polymers, often required for therapeutics, impacts the polymer conformation in solution. Here we report fully atomistic molecular dynamics simulations on the structure of dialkyl *p*-phenylene ethynylene confined into polydots. We find that the structure and thermal stability of polydots are sensitive to both the molecular weight n and the carboxylation fraction f. At room temperature, polydots remain confined regardless of n and f. However, as temperature is increased, polydots with lower n or f rearrange whereas polydots with higher n or $f$remain confined, though no direct clustering of the ionic groups was observed.

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