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Temperature Effects on Soft Polymeric Nanoparticles: Molecular Dynamics Study[1] SABINA MASKEY, Clemson University, GARY S. GREST, Sandia National Laboratory, DVORA PERAHIA, Clemson University — Luminescent polymers collapsed into soft nanoparticles or polydots have emerged as the potential candidates for biomedical applications such as drug delivery and biosensing. Here, using fully atomistic molecular dynamics simulation, the temperatures effects on the stability, internal structure and dynamics of polydots formed by substituted and bare dialkyl *para* phenylene ethynylenes (PPEs) will be discussed. We find that with increasing temperature from 300 K to 600K both substituted and bare PPE polydots expand but do not fully unfold and remain in their confined state. As observed visually and by measurement of structure factor S(q), the overall shape of the both type of polydots changes from spherical to elongated with the increase in temperature. These effects are more pronounced for bare PPE polydots which show that interdigitation of side chains in substituted PPE polydots enhances stability. In addition, the side chains are more dynamic than the backbone..

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