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Assembly of polymeric nanoparticles: Molecular dynamics study[1]
SABINA MASKEY, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — The assembly of polymeric nanoparticles or polydots has been studied using molecular dynamics simulations. These polydots are highly fluorescent and have potential applications in intracellular imaging, biosensors and other optoelectronic devices. Therefore their assembly is the key to their utilization. Here we probe the assembly of polydots made by para dialkyl phenyleneethynylenes (PPEs) whose conformation determines their degree of conjugation and enhance their electro-optical response. As in our previous study, PPE polydots were prepared by collapsing polymer by the procedure developed. The polydots were brought together two ways. Allowing the particles to approach each other at a constant velocity of 50m/s resulted in the particles bouncing off each other which is consistent with the dense object which we have previously reported. Then polydots were brought together at constant force and interface between them has been followed. Our results show that polydots under high velocity and forces remain stable. Closer look at the interface reveals that backbones of the polymer do not inter-penetrate and side chains dominate the interface. This interfacial structure suggests that one could retain the structure of polydots upon assembly.

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