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Conformation of Ionic Conjugated Polymers: Molecular Dynamic Simulations SIDATH WIJESINGHE, DVORA PERAHIA, Clemson University Clemson SC 29634, GARY GREST, Sandia National Laboratories, Albuquerque, NM — The structure and dynamics of poly para phenylene ethynylene (PPE) with substituted carboxylate side groups have been studied using molecular dynamics simulations. These polymers consist of two highly interacting segments, conjugated groups with are luminescent and ionic groups that add functionality either for tethering bio compatible groups or ionic transport ones. Here we investigate the conformation of these polymers which is a delicate balance between the conjugation length, and electrostatic interactions. Specifically we resolved the structure of carboxylate substituted PPE chains in three different solvents, toluene, water, and vacuum. Toluene acts as a good solvent for the backbones of PPEs, water which is a good solvent for the side groups and vacuum which is a poor solvent for the entire molecule. We found out that conformation of the backbone depends on both the presence of ionic groups and the specific interactions with the solvent. As the number of ionic groups along the backbone increases the conformation of the polymer is strongly impacted by formation of ionic clusters. The study shows that proper tuning the degree of ionic substitution PPEs we can either maintain long extended chains or folded.

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