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Conformational Study of Di-Substituted *para-polyphenyleneethylene* (PPE) in Dilute Solutions SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Lab — Molecular dynamics (MD) simulations have been used to study the conformation of highly rigid di-substituted *para-polyphenyleneethylenes* (PPEs) polymers, electro-active polymers, in dilute toluene solutions. The conformation of PPEs determines the conjugation of the polymer and their assembly mode which in-turn affect the electro-optical properties. In solution, the conformation is determined by molecular parameters including the length of the polymer and the nature of the side chain, coupled with the interaction of the molecules. The present study investigates the effects of molecular weight and the nature of the side chain in toluene solutions. Toluene is a good solvent for the backbone and a poor solvent for the substituting side chains. Small angle neutron studies have shown that short alkyl PPEs are fully stretched out. With increasing molecular weights they assume a worm like configuration. The current study provides further insight into the factors that determines the conformation of the PPEs.

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