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**Molecular Dynamics Simulation of Highly Rigid Polymers in Dilute Solutions** SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREEST, Sandia National Lab — The dynamics of highly rigid polymers control their degree of conjugation and hence their electro-optical characteristics. Molecular dynamics (MD) simulations have been used to study the conformation of a dilute solution of dinonyl *para*-polyphenyleneethylene (PPE) in toluene, which is a good solvent for the backbone of the polymer. The goal of this study is to identify the factors that affect the conformation of a single chain. PPEs in solutions and at interfaces form a rich variety of optically active structures from micelles to gels, whereas the conformation of a single chain controls their optical response. Experimental studies have shown that the conformation of PPE has been affected by the nature of the solvent, the degree of polymerization as well as the nature of the side chains. The degree of cooperativity of the solvent with the polymer as well as the relative conformation of the aromatic groups within the backbone, as obtained from MD studies will be discussed, together with effects of varying the molecular weight and the nature of the side chains.

Dvora Perahia  
Clemson University

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