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Conformational studies of conjugated polymers substituted with different side chains YUNFEI JIANG, Department of Chemistry, Clemson University, Clemson, South Carolina, 29634, UWE H. F. BUNZ, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA 30313, DVORA PERAHIA — The conformation of conjugated poly(*para*phenylene ethylene) (PPE), in different complex fluids states including molecular solutions, aggregates and gels, has been studied by Nuclear Magnetic Resonance and Molecular Mechanics simulations. PPEs are inherently semiconductors. Their electro-optical response depends on their degree of conjugation, determined by the degree of torque applied on the backbone by the substituents and the association mode of the polymer. Two types of substituents were compared: a nine carbons linear chain nonyl group and a space occupying tri-*iso*propylsilyloxy (TIPS). In molecular solution the side chains are fully flexible assuming random conformations while in any aggregation mode a well-ordered stretched out conformation due to the dense packing between polymeric molecules, is detected. TIPS substituted PPEs results in a non correlated configuration in all of the association modes. These findings are consistent with our independent fluorescence studies of this system.

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