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Theoretical prediction of chain morphologies in polyfluorenes from Raman spectra calculations

Organic semiconductors, such as short-chain oligomers and long-chain polymers, are now a core constituent in numerous organic and organic-inorganic hybrid technologies. Polyfluorenes (PF) have emerged as attractive alternatives to other polymers due to their strong blue emission and high charge carrier mobilities. Almost all PF derivatives utilize side-chain substitution that improves solution processing and confers new functionality. There are many ambiguities regarding structure-property relationships in various side-chain substituted PFs. Di-octyl substituted PF (PF8) is known for its mesomorphic behavior, multitude of crystalline phases, and several conformational isomers that depend on the torsional angles between monomer units. In particular, the beta phase that represents a more planar backbone conformation dominates the optical emission although it appears as a minority constituent. The exact nature of this phase is still controversial. In this work we present first-principles Raman spectra calculations of fluorene oligomers with varying torsional angles and side-chain ordering, using Density Functional Theory in Gaussian03 program. Our calculations show that the presence of the beta conformational phase is possible only for a trans-gauche-gauche ordering of the alkyl side chains.