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Conformations in di-octyl substituted polyfluorene: a combined theoretical and experimental Raman scattering study[1] C. VOLZ, M. ARIF, S. GUHA, Dept. of Physics, University of Missouri-Columbia — The structural properties of polyfluorenes (PF) are extremely sensitive to the choice of functionalizing side chains. Di- octyl substituted PF (PF8) adopts metastable structures that depend upon the thermal history and choice of solvents used in film forming conditions. We present a detailed study of the changes in the backbone and side chain morphology in PF8, induced by the various crystallographic phases, using Raman scattering techniques. The vibrational frequencies and intensities of fluorene oligomers are calculated using hybrid density-functional theory with a 3-21G* basis set. The alkyl side chains are modeled as limiting conformations: all *anti*, *anti-gauche-gauche*, and end *gauche* representations. The calculated vibrational spectra of single chain oligomers in conjunction with our experimental results demonstrate the β phase, which is known to originate in regions of enhanced chain planarity, as a direct consequence of the alkyl side chain conformation.

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Suchismita Guha
University of Missouri

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