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Stiffness evaluation of the oligofluorene chains

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Abstract – Oligomer of fluorene (FO) and phenyl-fluorene (pFO) with several lengths have been studied by Quantum Chemistry Methods. We analyzed the relationship between the phenyl group insertion in the fluorene and the stiffness in the backbone with the growth of the chains. Our results indicated that the phenyl groups acts in the sense to harden the chain.

Organic molecular systems are of current interest for a wide range of potential applications, in particular for optoelectronic devices. In this context, fluorene and derivatives are promising compounds to be used as active molecule for OLEDs. They exhibit efficient luminescence properties, excellent thermal stability, and easy processing. They also can emit in a wide band of the visible spectrum by the incorporation of groups of narrow band gap [1-2]. Morphologies related to the planarity of the molecules as well as the crystallinity of thin films play an important role on the electronic and optoelectronic properties of such materials. Fluorene systems exhibit three complex phases: α, β and γ [3]. In this work we present a theoretical study related to the conformation of fluorene oligomer (FO) and phenyl-fluorene oligomers (pFO), obtaining electronic properties in function of chain lengths. *Ab initio* Hartree-Fock method associated to the Pople's 6-31G (d, p) basis set was used to calculate the preferential conformation of the oligomers as the chain length increases. Electronic absorption spectra were obtained by ZINDO/S-CI, a semiempirical configuration Interaction method parameterized by Zerner with spectroscopic data, which were correlated with the conformational structure. Our results showed that fluorene oligomer (FO) exhibits a helical conformation with dihedral angles distributed by $\pm$ 45°. However, stiff chains were found for phenyl-fluorene oligomers (pFO) already for trimers, indicating that the phenyl groups acts in the sense to harden the chain.

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