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Conjugated Polymers for Organic Electronics: Structural and Electronic Characteristics

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The use of organic materials to design electronic devices has actually presented a broad interest for because they constitute an ecological and suitable resource for our current "electronic world". These materials provide several advantages (low cost, light weight, good flexibility and solubility to be easily printed) that cannot be afforded with silicium. They can also potentially interact with biological systems, something impossible with inorganic devices. Between these materials we can include small molecules, polymers, fullerenes, nanotubes, graphene, other carbon-based molecular structures and hybrid materials. Actually these materials are being used to build electronic structures into electronic devices, like organic light-emitting diodes (OLEDs), organic solar cells (OSCs), and organic field-effect transistors (OFETs), constituting and already commercial reality. Some of them are used on a widespread basis¹, and are the focus of some recent researches in molecules^{2,3} and polymers⁴⁻⁶ suitable for these purposes.

In this study we analyze the electronic and molecular characteristics of some different π -conjugated structures in order to evaluate their potential as semiconducting materials for organic electronics. For this purpose we focus on the study of conjugated polymers with different backbones configurations: (i) donoracceptor configuration, (ii) 1D lineal or 2D branched conjugated backbones, and (iii) encapsulated polymers. To achieve this goal, we use a combined experimental and theoretical approach that includes electronic spectroscopies (i.e., absorption, emission and microsecond transient absorption), vibrational Raman spectroscopy and DFT calculations. These structural modifications are found to provoke a strong impact on the HOMO and LUMO levels and the molecular morphology, and, consequently, on their suitability as semiconductors in organic electronic applications.

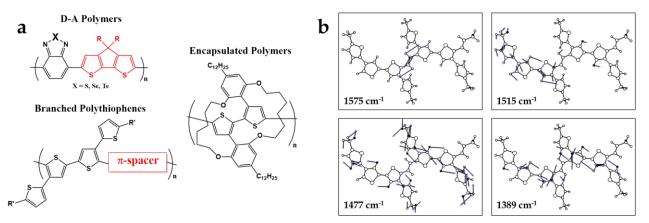


Figure 1. a) Chemical structures of different types of π -conjugated polymers under study and b) Eigenvectors analysis of a π -conjugated branched polythiophene.

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