

## Type of Contribution (Select One)

Oral  Poster

## Raman Spectroscopy and DFT calculations for the Electronic Structure Characterization of Conjugated Polymers

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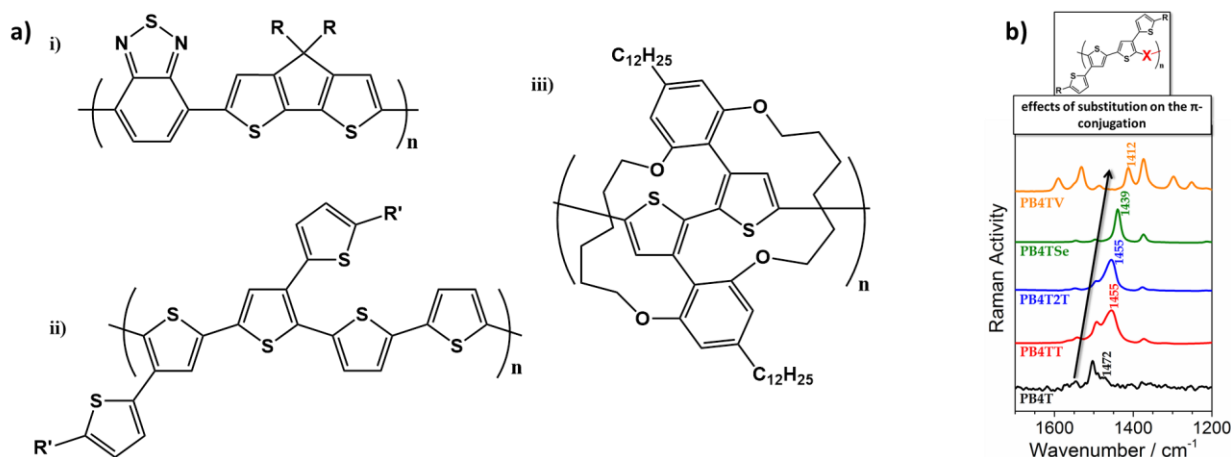
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In the last three decades, there has been a broad academic and industrial interest in conjugated polymers as semiconducting materials for organic electronics. Their applications in polymer light-emitting diodes (PLEDs), polymer solar cells (PSCs), and organic field-effect transistors (OFETs) offer opportunities for the resolution of energy issues as well as the development of display and information technologies<sup>1</sup>. Conjugated polymers provide several advantages including low cost, light weight, good flexibility, as well as solubility which make them readily processed and easily printed, removing the conventional photolithography for patterning<sup>2</sup>. A large library of polymer semiconductors have been synthesized and investigated with different building blocks, such as acenes or thiophene and derivatives, which have been employed to design new materials according to individual demands for specific applications. To design ideal conjugated polymers for specific applications, some general principles should be taken into account, including (i) side chains (ii) molecular weights, (iii) band gap and HOMO and LUMO energy levels, and (iv) suited morphology.<sup>3-6</sup>

The aim of this study is to elucidate the impact that substitution exerts on the molecular and electronic structure of  $\pi$ -conjugated polymers with outstanding performances in organic electronic devices. Different configurations of the  $\pi$ -conjugated backbones are analyzed: (i) donor-acceptor configuration, (ii) 1D lineal or 2D branched conjugated backbones, and (iii) encapsulated polymers (see Figure 1). Our combined vibrational spectroscopy and DFT study shows that small changes in the substitution pattern and in the molecular configuration have a strong impact on the electronic characteristics of these polymers. We hope this study can advance useful structure-property relationships of conjugated polymers and guide the design of new materials for organic electronic applications.



**Figure 1.** a) Chemical structures of different types of  $\pi$ -conjugated polymers under study and b) Raman analysis of the effect of chain elongation on the  $\pi$ -conjugational properties of branched polythiophenes.

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