Área: TEO **Nº de Inscrição:** _____

A theoretical study of poly(*p*-phenylenes) and their cyclodextrin-based insaluted molecular wires

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Highlights

*HOMO-LUMO gaps were obtained before and after the encapsulation process of the PPP oligomers into the β-CD tubes.
*The conductive properties of PPPs are maintained when they are covered by CDs.

Resumo/Abstract

The π-electron conjugated polymers (CPs) have been recognized as alternative and promising candidates in the electronic device fabrication. However, a fundamental requirement for adequate development, processing, and application of CPs as a molecular electronic device is the solubility. In this sense, an efficient strategy to improve the solubility of CPs is the formation of inclusion complexes with cyclodextrins (CDs), also known as CD-based insulated molecular wires (MWs) (**Fig.1**). In this work, we have performed a theoretical investigation via Semiempirical and Density Functional Theory (DFT) calculations in order to evaluate structural and electronic properties related to pristine poly(*p*-phenylene) oligomers (PPPs) and *push-pull* derivatives and their respective β-cyclodextrin (β-CD) based insulated molecular wires (MWs). As the main result, we have concluded the PPP oligomer substituted by the NH_2/NO_2 *push-pull* group (**Fig.2**) presented the lowest HOMO-LUMO gap (E_g) among all studied. After the encapsulation process of two selected structures (pristine $(PPP)_4$ and $[NH_2\text{-}(PPP)_4\text{-}NO_2]$ derivative) into β-CD dimeric tube (**Fig. 2**), it was possible to observe the PPPs conductive properties have been maintained when the "protective cylindrical coating" was used. Finally, we strongly believe that the use of PPPs in the form of insulated molecular wires is a promising and feasible approach to explore in future experimental investigations.

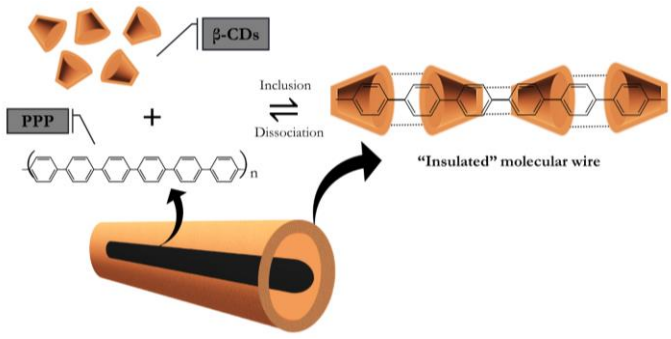

Figure 1: Schematic representation of the CD-based insulated molecular wires formation process.

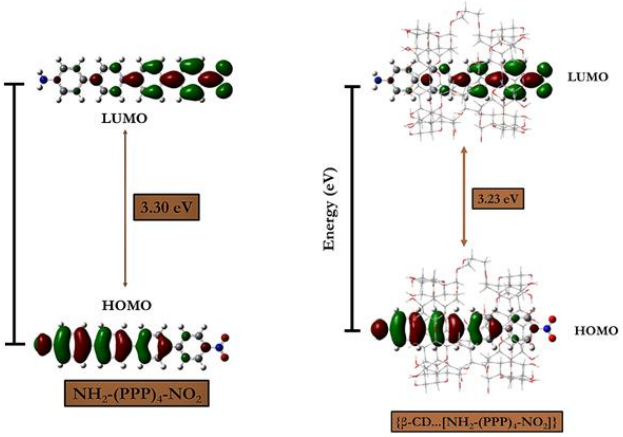

Figure 2: HOMO-LUMO gaps diagrams and contour plots for $NH_2\text{-}(PPP)_4\text{-}NO_2$ oligomer and $\{\beta\text{-CD}...[NH_2\text{-}(PPP)_4\text{-}NO_2]\}$ molecular wire.

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