PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

COMPUTATIONAL DESIGN OF NOVEL NON-FULLERENE ACCEPTORS FOR ORGANIC SOLAR CELLS

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Organic solar cells based on bulk heterojunction (BHJSC) structures represent a promising renewable energy technology, offering advantages such as flexibility and low cost1. Traditionally, fullerene-based electron acceptors have been widely used; however, their efficiency is limited by low light absorption. Non-fullerene acceptors (NFAs) with an acceptor-donor-acceptor (A-D-A) architecture have emerged as an alternative, offering enhanced absorption in the visible/infrared spectrum and superior electron mobility. These systems have demonstrated significant potential, however, their planar structure and the presence of specific side groups suggest the possibility of optimization through intermolecular interactions with tailored donor systems, paving the way for a wide range of derivatives2. In this context, computational studies serve as a viable approach for proposing new systems and understanding their operating mechanisms. In particular, our group has been investigating the potential of NFA derivatives based on dihydroxy-quinone structures, which are characteristic of melanin-related compounds, due to their intriguing semiconductor properties. In the present study, molecular modeling techniques based on density functional theory using the hybrid B3LYP functional and the 6-311G(d,p) basis set, we first fully optimized four different oxidation states for the melanin-based end-groups.

Subsequently, these structures were incorporated into the termini of the Y6 molecule and fully re-optimized with the same theoretical rigor. All calculations were performed in a vacuum, and analyses of local reactivity, electrostatic potential map, structure, and FMO (Frontier Molecular Orbital) energy levels were conducted to investigate the optoelectronic properties of all different composed structures. The results highlight the potential of these groups for new NFA design, demonstrating that some main performance parameters depend on the redox state of the investigated systems.

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Palavras-chave: non-fullerene acceptors; melanin-inspired materials; density functional theory; optoelectronic properties; redox state; organic photovoltaics.