PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

REACTIVITY AND ELECTRONIC MODULATION IN SURFACE-FUNCTIONALIZED CARBON DOTS: A DFT STUDY TOWARD NITRIC OXIDE RELEASE

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Carbon Dots (CDs) are carbon-based nanomaterials that have attracted considerable attention due to their tunable electronic structure, chemical versatility, high water solubility, and promising performance in biomedical applications [1]. Among their potential uses, functionalized CDs have been explored as platforms for nitric oxide (NO) release, a reactive radical species capable of inducing tumor cell apoptosis through oxidative and nitrosative stress pathways [2]. The efficiency of NO delivery systems is closely related to the intrinsic reactivity of the nanostructure, surface termination, and environmental conditions such as pH, which directly influence protonation states and interaction mechanisms [3]. In this work, Density Functional Theory (DFT)-based calculations were performed to investigate CD model systems bearing distinct surface terminations and functionalized with triphenylphosphonium (TPP) and cysteine-based ligands. The study comprises a comprehensive analysis of local and global reactivity descriptors, frontier molecular orbitals (HOMO–LUMO), protonation-dependent reactivity behavior, and NO-adduct

formation propensity. For the most reactive functionalized system, detailed electronic and optical characterizations were carried out, including electronic density distribution, projected density of states (PDOS), electrostatic potential (ESP) maps, and simulated UV–Vis absorption spectra. The results demonstrate that surface termination significantly modulates the local reactivity profile and influences the efficiency of functionalization. Furthermore, the selected functionalized CD exhibits distinct electronic structure features, with modifications in orbital distribution and density of states that impact charge localization and potential interaction sites. Protonation effects were found to preserve the preferential reactivity toward the NO moiety and the releasing group, maintaining the electronic characteristics associated with radical formation. Overall, the findings provide a consistent theoretical framework for understanding how surface chemistry and electronic structure govern reactivity and functional performance in CD-based nanoplatforms designed for controlled NO delivery.

References:

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Acknowledgements:

This research benefited from computational resources provided by the Center for Scientific Computing (NCC/Grid-UNESP) of São Paulo State University (UNESP). The authors gratefully acknowledge the Coordination for the

Improvement of Higher Education Personnel (CAPES – Proc: 88887.105351/2025-00) and FAPESP (process nº 2025/09784-1) for financial support and for the scholarship granted. The authors also acknowledge INEO for the organization of the event and for the logistical and financial support provided. This work was further supported by FAPESP (process nº 2025/27044-5) and CNPq (process nº 408449/2024-1).

Palavras-chave: carbon dots; nitric oxide release; density functional theory; chemical reactivity; protonation effects; electronic structure.