PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

SPECTROSCOPY CHARACTERIZATION AND DFT MODELING OF THE SPONTANEOUS SYMMETRY BREAKING IN ZINC PHTHALOCYANINE AGGREGATES

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Zinc Phthalocyanine (ZnPC) is a highly relevant organic semiconductor for sustainable electronics and photonics due to its thermal stability and unique optoelectronic properties.[1-3] However, the natural tendency of this macrocyclic molecule to form aggregates (H-type) presents both challenges and opportunities for device design. This work presents a combined theoretical modeling and experimental characterization study focused on the supramolecular organization of ZnPC. Using Density Functional Theory (DFT) calculations, it was predicted that ZnPC aggregation induces a spontaneous symmetry breaking, resulting in an ordered structure with a helical conformation. To experimentally validate this theoretical prediction,

spectroscopic characterization techniques were employed, including Linear Optical Absorption, Photoluminescence, and Raman Scattering. Additionally, the application of advanced polarization- and chirality-sensitive techniques, such as Emission Ellipsometry and Raman Optical Activity (ROA), confirmed the preferential orientation and the induced chiral nature of the aggregated state. The obtained results not only validate the proposed theoretical model but also offer new perspectives for controlling the morphology and electronic properties of organic materials via aggregate engineering.

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Palavras-chave: zinc phthalocyanine; dft; supramolecular aggregation; raman optical activity; symmetry breaking.