PÔSTER - RESUMO - DISPOSITIVOS OPTOELETRÔNICOS

SIDE-CHLORO SUBSTITUTION: BRIDGING THEORETICAL AND EXPERIMENT INSIGHTS INTO ORGANIC ANISOTROPIC SYSTEMS TOWARDS OPTICAL DEVICES

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The investigation of anisotropic systems, specifically liquid-crystalline materials, occupies a critical position in the ongoing development and advancement of next-generation optically active devices, such as organic light-emitting diodes (OLEDs) [1]. A comprehensive understanding of the radiative decay dynamics within these specialized molecular systems is essential for understanding photophysical phenomena observed during operation, while also serving as an important guide for the strategic design of new synthetic pathways. In this work we investigate how structural modifications at the molecular level can dictate and modulate the macroscopic behavior of emerging organic semiconductor materials. We evaluated the influence of strategic introduction of chlorine substituents into a specific organic molecular framework on the photophysical and mesomorphic properties of the system. The methodology relies extensively on Density Functional Theory (DFT) [2] calculations to characterize molecular orbitals and map electronic transitions using the ORCA 6.1.0 package [3] and PBE0-D3BJ/Def2-TZVPP as the theory level. The resulting theoretical predictions were rigorously compared and validated against experimental data. The findings indicate that significant alterations in the molecular dipole moment,

mainly driven by the high electronegativity of the chlorine atom, is the main factor for the molecular self-assembly and spatial organization. Interestingly, despite these profound structural changes, the chlorine substituent was found to have a negligible influence on the intrinsic photophysical properties of the molecules. This study, which has been recently published [4], offers critical insights and a theoretical framework for the design of high-performance molecules tailored for the next generation of electro-optic devices.

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