PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

SUPPRESSION OF Π-STACKED AGGREGATES AND POWER-CONTROLLED EXCIPLEX FORMATION IN THIOPHENE–BENZENE–THIOPHENE MONOMERS

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Abstract

We present a comprehensive photophysical investigation of five thiophene–benzene–thiophene (TBT) monomers bearing distinct lateral side chains, elucidating how excitation power modulates their aggregation dynamics. Steady-state photoluminescence (PL) reveals two emissive contributions at 418 and 495 nm whose intensity ratio varies systematically with excitation powers from 8 to 3098 μW. Time-resolved PL assigns these bands to monomeric and aggregate-like species. Power-cycling experiments confirm complete spectral reversibility, excluding thermal or concentration-driven artifacts. Simulations

based on Fermi's Golden Rule combined with a two-species population model show that the zero-phonon transition energy remains invariant with excitation power, demonstrating that spectral evolution arises solely from population redistribution rather than energetic shifts. The lateral side chains suppress p-stacked aggregation while promoting excited–ground-state interactions that favor exciplex formation. These results establish a mechanistic basis for power-controlled emission in TBT systems and offer design guidelines for tuning excited-state interactions in p-conjugated materials.

Reference

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Acknowledgements

I thanks INEO, FAPESP (2025/27044-5) , FAPEMIG, CNPq (408449/2024-1) and CAPES for their assistance and support in the development of this work

Palavras-chave: power-dependent; phototoluminescence; molecular aggregation; exciplex.