PÔSTER - RESUMO - DISPOSITIVOS OPTOELETRÔNICOS

FROM SOLUTION TO DEVICE: AGGREGATION-INDUCED ENHANCED EMISSION AND TWISTED INTRAMOLECULAR CHARGE TRANSFER IN A PYRIDYLCARBODINITRILE FOR TUNABLE PHOTOLUMINESCENCE AND OLED APPLICATIONS

Carolina Vesga Hernández (cvesgah@gmail.com)

Dayvid Mello Nascimento (dayvid@aluno.puc-rio.br)

Rafael Dos Santos Carvalho (rffispuc@yahoo.com.br)

Arthur Rodrigues Jardim Barreto (arthurrjb@gmail.com)

Marlin Jeannette Pedrozo Penafiel (marlinpedrozo26@gmail.com)

Julia Rodrigues De Noronha (julianoronha@outlook.com)

Luís Maqueira (maqueira1382@gmail.com)

Davi Back (daviback@gmail.com)

Leandro H. Zucolotto Cocca (leandro.zucolotto@ufg.br)

Ricardo Queiroz Aucélio (aucelior@puc-rio.br)

Leonardo De Boni (deboni@ifsc.usp.br)

Marco Cremona (cremona@fis.puc-rio.br)

Jones Limberger (limberger@puc-rio.br)

The development of organic luminophores with tunable photophysical properties is crucial for advancing high-performance optoelectronic devices. In this work, a

series of phenylpyridylcarbonitrile (PPC) derivatives with donor–p–acceptor (D–p–A) architectures were synthesized and systematically investigated, aiming to correlate molecular structure with solvent-, aggregation-, and device-dependent emission behavior. Four PPC derivatives bearing distinct donor groups: methylphenyl (2M-PPC), biphenyl (BP-PPC), 9,9-dimethylfluorenyl (FL-PPC), and 3,5-dimethyl-4-methoxyphenyl (MT-PPC), were obtained and evaluated [1].

Among them, MT-PPC exhibited remarkable photophysical versatility, characterized by pronounced solvatochromism with an emission shift of 118 nm, indicative of twisted intramolecular charge transfer (TICT) states. Additionally, MT-PPC showed aggregation-induced enhanced emission (AIEE), with a nineteenfold increase in photoluminescence quantum yield upon aggregation. Thin films incorporating MT-PPC in an Bis(9,9-spirobifluorene-3-yl)-phenylphosphane oxide (SF3PO) host matrix displayed tunable emission as a function of dopant concentration, with lower concentrations leading to blue-shifted photoluminescence [1].

Organic light-emitting diodes (OLEDs) fabricated with MT-PPC at doping levels of 5%, 10%, and 20% demonstrated concentration-dependent electroluminescence, with emission maxima ranging from 438 to 460 nm. The devices were built in a conventional multilayer architecture consisting of an indium tin oxide (ITO) anode, a hole-injection layer of molybdenum trioxide (MoO3), a hole-transport layer of 1,1-bis[(di-4-tolylamino)phenyl]cyclohexane (TAPC), an exciton-blocking layer of 4,4',4"-tris(N-carbazolyl)triphenylamine (TCTA), the emissive layer composed of 9,9'-(sulfonylbis(4,1-phenylene))bis(9H-carbazole) (SF3PO) doped with MT-PPC, an electron-transport layer of 1,3,5-tri(m-pyrid-3-yl-phenyl)benzene (TmPyPB), a lithium fluoride (LiF) electron-injection layer, and an aluminum (Al) cathode [2]. All organic and metallic layers were sequentially deposited by thermal evaporation under high vacuum (~10-4 Pa), ensuring controlled film growth, well-defined interfaces, and reproducible device fabrication. The device containing 20% MT-PPC achieved a maximum luminance of 977 cd/m² and an external quantum efficiency of 0.80% [1]. The luminance and EQE values of the fabricated OLEDs still need to be optimized improving the device structure. However, these results highlight MT-PPC as a multifunctional luminophore with emission tunability across solution, solid-state films, and OLEDs, underscoring its potential for applications in sensors and advanced optoelectronic technologies.

The authors would like to thank FAPERJ, CAPES, CNPq (408449/2024-1), FAPESP (2025/27044-5) and INCT-INEO for partial financial support.

References:

[1] Vesga-Hernández, C., Carvalho, R. S., Barreto, A., Peñafiel, M. J. P., Noronha, J. R., Maqueira, L., Back, D., Nascimento, D. M., Cocca, L. H. Z., Aucélio, R. Q., Boni, L., Cremona, M., & Limberger, J. (2025). Journal of Photochemistry & Photobiology, A: Chemistry, 464, 116312. https://doi.org/10.1016/j.jphotochem.2025.116312

[2] Liu, X., Zhang, Y., Li, Z., Wang, Y., Chen, J., & Zhao, Z. (2020). Highly efficient blue-emitting OLEDs based on pyridine-containing emitters. Chemical Engineering Journal, 401, 126107. https://doi.org/10.1016/j.cej.2020.126107

Palavras-chave: pyridine-based luminophore; solid-state emission; organic light-emitting diodes (oleds).