

Analysis of interactions in donor-acceptor compounds and their application in organic light-emitting diodes (OLEDs)

Department of Physical Chemistry and Technology of Polymers

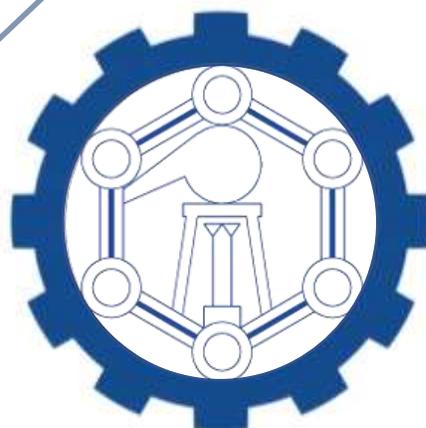
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List of Abbreviations:

AIE – Aggregation-induced emission

AIEE – Aggregation-induced emission enhancement or Aggregation-induced enhanced emission

DF – Delayed fluorescence

EA – Electron affinity

EBL – Electron blocking layer

EIL – Electron injection layer

EML – Emissive layer

EQE – External quantum efficiency

ETL – Electron transport layer

HBL – Hole blocking layer

HIL – Hole injection layer

HTL – Hole transport layer

HOMO – Highest occupied molecular orbital

IP – Ionization potential

IQE – Internal quantum efficiency

ISC – intersystem crossing

ITO – Indium-tin oxide

LUMO – Lowest unoccupied molecular orbital

OLED – Organic light-emitting diodes

PF – Prompt fluorescence

PLQY – Photoluminescence quantum yield

RISC – Reverse intersystem crossing

RTP – Room temperature phosphorescence

S₀ – Singlet ground state

S₁ – Singlet first excited state

SOC – Spin-orbital coupling

T₁ – Triplet first excited state

TADF – Thermally activated delayed fluorescence

ΔE_{ST} – Difference between energies of S₁ and T₁

List of Publications:

1. W. P. Silva, **N. O. Decarli**, L. Espíndola, K. Erfurt, A. Blacha-Grzechnik, P. Pander, M. Lapkowski and P. Data “Multifunctional Properties of D-A Luminophores Based on Acenaphthopyrido[2,3-b]pyrazine Core: Photophysics, Photochemistry, and Efficient Solution-Processed OLEDs.” *J Mater Chem C*. **2023**, 1, 3777. **doi:10.1039/D3TC02860G**
2. P. P. Abatti, **N. O. Decarli**, S. Gogoc, P. Data, I. H. Bechtold, E. Westphal and H. Gallardo. “Shedding Light on Highly Emissive 1,4-Dihydropyrrolo[3,2-b]pyrrole Derivatives: Synthesis and Aggregate-Dependent Emission.” *Chempluschem*, **2023**, e202300539. **doi:10.1002/cplu.202300539**
3. T. Hosono, **N. O. Decarli**, P. Z. Crocomo, T. Goya, L. E. de Sousa, N. Tohnai, S. Minakata, P. de Silva, P. Data and Y. Takeda. “The regioisomeric effect on the excited-state fate leading to room-temperature phosphorescence or thermally activated delayed fluorescence in a dibenzophenazine-cored donor-acceptor-donor system.” *J. Mater. Chem. C*, **2022**, 10, 4905-4913 **doi:10.1039/d1tc05730h**
4. **N. O. Decarli**, E. Zapp, B. S. de Souza, E. R. Santana, J. P. Winiarski and I. C. Vieira. “Biosensor based on laccase-halloysite nanotube and imidazolium zwitterionic surfactant for dopamine determination.” *Biochem Eng J.*, **2022**, 186, 108565. **doi:10.1016/j.bej.2022.108565**
5. S. Goto, Y. Nitta, **N. O. Decarli**, L. E. de Sousa, P. Stachelek, N. Tohnai, S. Minakata, P. de Silva, P. Data and Y. Takeda. “Revealing the internal heavy chalcogen atom effect on the photophysics of the dibenzo[a,j]phenazine-cored donor-acceptor-donor triad.” *J. Mater. Chem. C*, **2021**, 9, 13942-13953. **doi:10.1039/d1tc02635f**

1. Abstract

This study explores four series of compounds with different core structures, namely **PyBTA** ([1,2,3]triazolo[4,5-b]pyridine), **NQPy** (acenaphtopyrido[2,3-b]pyrazine), **TTT** (tris([1,2,4]triazolo)[1,3,5]triazine), and **JAP** (dibenzo[a,j]phenazine), for use in OLED devices. Various combinations of donor-acceptor molecules were characterized and successfully applied. For **PyBTA** compounds were developed three different isomers by changing the position of the methyl group, each of them with three distinct donors. Some of these compounds exhibited room-temperature phosphorescence (RTP), while others showed thermally activated delayed fluorescence (TADF) properties. In the photophysics of **PyBTZ-x-PTZ** and **PyBTZ-x-PXZ** were observed contributions from different conformers in the PF and DF emissions attributed to the axial and equatorial conformers of the **PTZ** and **PXZ** donors. **NQPy** derivatives showcased multifunctional properties, exhibiting TADF, RTP or RTP/TADF, which could be modulated by the choice of donor. Additionally, they demonstrated effectiveness in singlet oxygen generation and displayed characteristics of aggregation-induced emission (AIE) and AIE enhancement (AIEE). The **TTT** series of compounds were studied with and without the addition of methyl groups at distinct locations within the molecule, leading to significant variations in their photophysics. All three derivatives employed **PTZ** as the donor, and the presence of conformers was observed in the PF and DF emissions. The inclusion of a methyl group in the donor nearly extinguished the DF properties, whereas the addition of a methyl group at the phenyl spacer reduced the DF contribution in comparison to the derivative without the methyl group, but it still had an effective DF contribution. In addition, the **TTT** derivatives also effectively showed aggregation properties, such as AIEE. The regioisomers of **JAP** compounds displayed TADF or RTP properties depending on the position and the donor. Notably, the OLED efficiencies achieved up to 15.9% for **PyBTA-2-PTZ**, 15.3% for **NQPy-DMAC**, and 12.4% for **TTT-PTZ**, all of which were fabricated using a solution processing.