1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title:

Development of New MR-TADF Materials Containing Heteroatoms to Improve Stability for OLED Applications

1.1. Project goals

The project focuses on designing, synthesizing, and testing new stable and efficient organic compounds that emit visible light via electroluminescence in OLED devices. These compounds, intended for commercialization by Noctiluca SA, aim to outperform current fluorescent and phosphorescent emitters in terms of current efficiency and durability. By utilizing the TADF mechanism, the new materials will enable efficient blue pixel emission without relying on expensive and toxic heavy metals like iridium or platinum. This approach supports both improved device performance and sustainable material sourcing.

1.2. Outline

The project aims to develop novel MR-TADF organic compounds for use in OLED devices. These materials will be designed to improve current efficiency and stability, particularly in blue pixels, without relying on rare or toxic heavy metals. The compounds will be synthesized and tested in OLED structures, with the goal of commercial implementation by Noctiluca SA. The project addresses key limitations of current OLED emitters and supports sustainable innovation in display technology.

1.3. Work plan

I. Design of MR-TADF emitters – determination of key parameters using DFT methods (Gaussian, ORCA): absorption and emission wavelengths, singlet and triplet state energies, HOMO-LUMO orbital distribution, and chemical bond stability (BDE).

II. Synthesis – optimization of synthetic methods with respect to yield, selectivity, and product purity (>99.9%); preparation of material in quantities exceeding 500 mg.

III. Spectroscopic characterization – NMR analysis (^{1}H, ^{13}C), IR, UV-Vis absorption and emission (in solution and in thin film), measurements of PLQY, time-resolved spectra, and electrochemical parameters (cyclic voltammetry, absorption spectra).

IV. Fabrication and testing of OLED prototypes – evaluation of operational properties, including external quantum efficiency (EQE), current and luminous efficiency, full width at half maximum (FWHM) of emission, CIE coordinates, and operational lifetime (LT80, LT90, LT95).

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate)*

A. A. Zielinska, O. P. Kumar, H. U. Kim, Mariusz J. Bosiak, R. Braveenth, J. H. Kwon; Arylmethylated-acridine donor-based TADF emitters achieved over 36 % external quantum efficiency in the pure blue region, Materials Today Chemistry 2025, Materials Today Chemistry 44 (2025) 102528. https://doi.org/10.1016/j.mtchem.2025.102528

P. Keerthika, R. K. Konidena; Marching Toward Long-Wavelength Narrowband Emissive Multi-Resonance Delayed Fluorescence Emitters for Organic Light Emitting Diodes, Adv. Optical Mater. 2023, 11, 2301732. DOI: 10.1002/adom.202301732

C. Lv, X. Wang,Q. Zhang, Y. Zhang; Narrowband emission: organic thermally-activated delayed fluorescence materials and underlying mechanisms, Mater. Chem. Front., 2023, 7, 2809, DOI: 10.1039/d3qm00100h

X. Fan, X. Hao, F. Huang, J. Yu, K. Wang, X. Zhang; RGB Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes toward Realizing the BT.2020 Standard, Adv. Sci. 2023, 2303504, DOI: 10.1002/advs.202303504

H. Lee, R. Braveenth, S. Muruganantham, C. Y. Jeon, H. S. Lee, Jang Hyuk Kwon; Efficient pure blue hyperfluorescence devices utilizing quadrupolar donor-acceptor-donor type of thermally activated delayed fluorescence sensitizers, Nature Communications (2023) 14:419, DOI: 10.1038/s41467-023-35926-1

1.5. Required initial knowledge and skills of the PhD candidate

The candidate should have a solid foundation in organic chemistry, particularly in the synthesis and characterization of small molecules. Basic knowledge of photophysics and materials science, especially regarding optoelectronic properties of organic compounds. Familiarity with laboratory such and spectroscopy techniques i.e. NMR, UV-Vis, and fluorescence spectroscopy, as well as experience with thin-film preparation and device fabrication, will be advantageous.

1.6. Expected development of the PhD candidate's knowledge and skills

The PhD candidate will gain advanced expertise in organic synthesis, photophysical characterization, and OLED device engineering. They will develop skills in designing functional molecules, analyzing their optoelectronic properties, and integrating them into working devices. Through collaboration with industry partners and participation in interdisciplinary research, the candidate will also strengthen competencies in scientific communication, project management, and technology transfer. This training will prepare them for careers in both academic research and the high-tech materials industry.