1. Research project objectives/ Research hypothesis (in English)

This 24-month project aims to obtain purely organic TADF emitters to create high efficient blue TADF-OLED devices. TADF offers an enormous improvement in the efficiency and brightness of fluorescent OLEDs. The fluorescence observed from CT singlet excited state results in a broad emission spectrum, which is an obstacle for display applications, where high color purity is necessary. To solve this problem, multiple resonance (MR)-based TADF macrocycles were designed. A wise design strategy for efficient TADF compounds is highly desired. In the first step of the present project, the synthesis will be performed and guided by the best results from the theoretical quantum-chemical investigation. The synthesized macrocycle will be fully characterized and a detailed photophysics behavior study will be conducted. As the final step, the formation and full characterization of blue MR-TADF-OLED will be performed.

2. Research project methodology (in English)

Perfectly understanding the relationship between molecular structure and property is crucial and an important tool for the design of high-performance organic electronic devices.
The present research proposal will be divided into main tasks as following:
i) Design and theoretical quantum-chemical investigation of new blue TADF using Schrödinger software, by DFT calculation. To simulate the distribution of HOMOs and LUMOs and predict the excited energy levels;
ii) Synthesis of ambipolar macrocycles derived of the acceptor quinolino[3,2,1-de]acridine-5,9-dione acceptor and from the donors 4,4,8,8,12,12-hexamethyl-8,12-dihydro-4H-benzo[9,1]quinolizino[3,4,5,6,7-defg]acridine and diphenylamine.
iii) Fully characterization of the target TADF using NMR spectroscopy, high-resolution mass spectrometry (HRMS) and thermogravimetric analysis (TGA) and X-ray crystallography;
iv) Electrochemical and spectroelectrochemical by UV-Vis-NIR, EPR, Raman and Fluorescence investigations, for the study of the structural changes of investigated molecules. The electrochemical energy values such as band gap and HOMO-LUMO levels will be obtained from the cyclic voltammetry (CV) analysis to select emitters with potential application in OLED devices;
v) The photophysical investigation, such as oxygen effect on fluorescence intensity, fluorescence solvatochromism, time-resolved spectra, power dependence of delayed fluorescence and fluorescence decay, to understand the structure-property relationship of TADF parameters;
vi) Formation and characterization of blue MR-TADF-OLED devices towards high EQEs and narrow-fluorescence;

3. Expected impact of the research project on the development of science, civilization and society (in English)

Nowadays, lighting is using more than 15% of the total electricity of the world, being responsible for 5% of worldwide greenhouse gas emissions. OLED devices are the most eco-friendly form of lighting on the planet; they are transducers of electrical energy to light conversion. Flexible OLED devices are a great promise to revolutionize the lighting industry. Therefore the present project corresponds to the EU Environment Action Programme to 2020, where one of the three key objectives is to turn the Union into a resource-efficient, green, and competitive low-carbon economy: Priority Scientific Trends set forth in the National Scientific, Technical and Innovative Policy Foundations up to the year 2020 - *"Założenia polityki naukowej, naukowo-technicznej i innowacyjnej państwa do 2020 r."* – the document, locating itself in such thematic groups as Info: optoelectronics, computational science Techno: new materials and technologies and nanotechnologies and Basics: chemistry and solid-state physics.
The dissemination of obtained results will be by publication in worldwide scientific journals, aiming at high-impact factor journals. The results will also be presented at national and international conferences.