

Diaza-BF₂-embedded N-polycyclic aromatic hydrocarbons – game changer in the domain of NIR TADF emitters

There is a high probability that you are using an organic light emitting diode (OLED) device while reading this text on the display of your computer or smartphone. However, the potential of these energy-saving light sources is much broader - including night-vision devices, biological sensors, anti-cancer therapies and photovoltaics. In the presented areas, near-infrared (NIR) light emitters range can be applied. There are many dyes that exhibit such emission through fluorescence, but their yield is limited to 25%. The process of reverse intersystem crossing (rISC) in the excited molecule gives the possibility to increase the yield up to 100%. The observed effect of rISC is delayed fluorescence; the phenomenon itself is an endothermic process - hence the name - thermally activated delayed fluorescence (TADF). This idea was implemented for third generation of OLEDs, that became economically competitive with the technologies used so far. Moreover, utilizing of purely organic emitters does not require the use of toxic and difficult to utilize metal complexes, therefore it corresponds to the current assumptions of the 'green economy'.

Among the developed NIR TADF emitters, a drastic decrease of the external quantum efficiency (EQE) is noticeable due to the shift of the emission maximum towards lower energies (NIR). Changing the approach from trying to tune a single parameter to a comprehensive view of all properties can be a solution to this problem and such concept, I propose in this project. The basic assumption in the design of the presented scaffolds is ambipolarity - spatial separation of the electron donor and acceptor parts. The structural combination of nitrogen-doped polycyclic aromatic hydrocarbons (N-PAHs) with boron complexes incorporated into the phenazine fragment gives a high probability to shift emissions towards red light. Furthermore, such an approach will allow for the effective separation of HOMO-LUMO orbitals and an increase of external quantum efficiency (EQE) and photoluminescence quantum yield (PLQY) comparing to known NIR TADF emitters.

As part of the synthetic tasks, I will focus on obtaining double and quadruple diaza-BF₂ complexes with the architecture of donor-acceptor (D-A) and donor-acceptor-donor (D-A-D), respectively. This topology minimizes the overlap of the HOMO-LUMO orbitals. Which is the basis for achieving a small singlet-triplet energy difference (ΔE_{ST}) conditioning TADF. Moreover, introducing BF₂ units into the acceptor fragment, and then expanding its π skeleton will affect the bathochromic shift of the emission spectra. The implementation of a curved N-PAH donor system will also be crucial. Non-planar geometry and an additional fragment improving systems solubility are necessary from the viewpoint of the functionalization and application of these compounds. The project represents a highly multidisciplinary, therefore the last two research tasks concern the structural and photophysical analyzes of the obtained complexes and the fabrication of OLED devices using them as an emission layer, which will be a proof of concept. These tasks will be implemented in cooperation with the group of Prof. P. Data.

Undoubtedly, the indicated research problem requires a broader view, and the conception proposed in this project, encompassing the improvement of efficiency and the ability to tune the properties of structural motifs, may be a breakthrough in the design of efficient NIR TADF emitters.