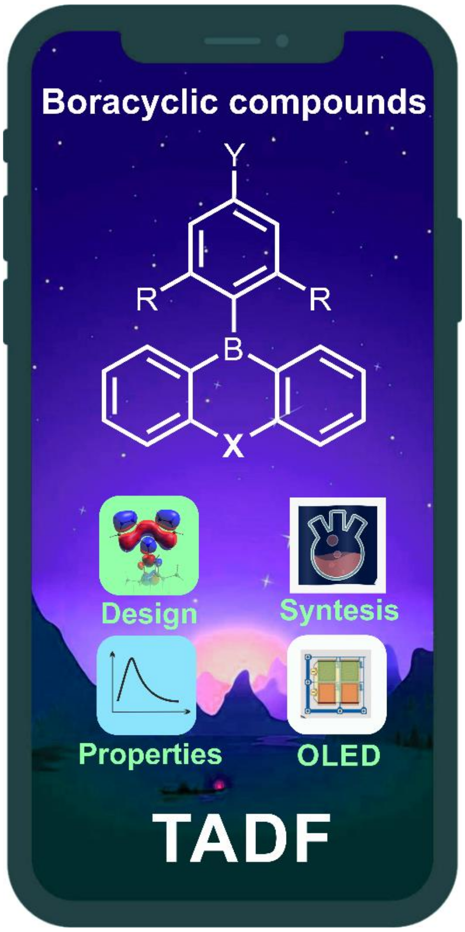
Tuning acceptor strength and conformational flexibility of boracyclic cores as a tool for synthesis of efficient TADF emitters

Organic Light-Emitting Diodes (OLEDs) are optoelectronic devices which convert electric energy to light. One of their most important advantages is high luminous efficiency which implies low energy consumption. From the point of potential applications, a wide palette of colors, wide viewing angles, sunlight-readability, high contrast as the light on the screen comes from each individual pixel rather than backlight, and attractive mechanical properties, e.g., opening the possibility for construction of flexible displays and curved screens, are very important. In the emissive layer, being the heart of working OLED, emitter molecules are excited by recombined hole-electron pairs, *i.e*., excitons. Hence, the chemical structure and resulting optical and physicochemical properties of the emitter molecule are the most important factors influencing OLED performance. Only 25% of generated excitons are singlets, whilst remaining 75% are triplet excitons. Typical fluorescent molecules emit light only due to interaction with singlet excitons. Therefore, the so-called Internal Quantum Efficiency (IQE) of the 1st generation OLEDs cannot exceed 25%. In order to achieve higher IQE values (theoretically up to 100%), triplet excitons need to be effectively harvested. For that purpose, 2nd generation OLEDs, comprising phosphorescent dye emitters (typically, coordination compounds with transition metal centres such as iridium and platinum). However, such phosphorescence-based diodes (PhOLEDs) exhibit important limitations arising from low chemical stability of emitters as well as very high cost of aforementioned noble metals.



In this context the use of TADF phenomenon is very promising as it allows for achieving high IQE values, theoretically reaching upper limit of 100%. Importantly, TADF emitters are usually typical organic molecules, which do not contain heavy metal atoms in their structures. They serve as the basis for the construction of 3rd generation OLEDs which are currently the subject of intensive studies, engaging research groups from both universities and industry. Unfortunately, the use of known TADF emitters still poses problems related to low stability, decrease of quantum yield upon voltage increase (roll-off) and wide emission bands which affects luminous efficiency, color purity and lifespan, especially in the case of blue OLEDs. Since the proper design of TADF emitter molecule is a non-trivial task, the number of such structures is still rather limited. Therefore, the project is aimed at design and obtaining novel, efficient and stable emitters for the use in 3rd generation OLEDs. Those materials will be based on cyclic organic boron compounds featuring enhanced electron-acceptor properties. It is assumed that their combination with suitable donor fragments will result in increase of luminance efficiency. The design of structures featuring higher chemical stability with respect to known materials plays also an important role. The practical utility of obtained emitters will be evaluated based on testing prototype OLEDs whose performance parameters will meet the formulated requirements.