Abstract

Developing new organic materials for optoelectronic applications such as OLED and OPV continues to be a challenge due to the market demand for more efficient devices that operate with minimum energy consumption. Designing purely organic molecules exhibiting TADF properties may be an excellent strategy for obtaining efficient OLED devices. The design of TADF emitters covers mainly the combinations of electron-acceptor (A) and electron-donor (D) units in twisted D-A structures, obtaining spatially separated HOMO and LUMO orbitals and small singlet-triplet energy gap, which can allow efficient RISC process in molecules.

This work brings the design and synthesis of different A, belonging to various classes of compounds and commonly D moieties (diphenylamine, carbazole, phenothiazine, phenoxazine, acridine derivatives, and azepine derivatives), displaying different configurations of D-A structures to investigate the photophysical and electrochemical properties and consequently suitability to optoelectronic applications. The final compounds were synthesized mainly using N-C and C-C cross-coupling reactions between the brominated acceptors and donors, obtaining moderate to good yields. The acceptor design strategy covered mainly the construction of N-rich systems, such as acenaphtopyridopyrazine, naphthalene benzimidazole, diquinoxaline, diphenazine, derivatives of pyridobenzotriazole isomers, benzopyridoimidazoisoquinolinone, and perylene dianhydride/tetraesthers and triphenylphosphanimine.

All the acceptors were connected with common donors, and their molecular structures were characterized by ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) and High-Resolution Mass Spectrometry (HRMS). The electrochemical properties were investigated by cyclic voltammetry (CV), and the energies of HOMO and LUMO levels were estimated from oxidation and reduction potentials, respectively. Additionally, the susceptibility of some compounds to the electrochemical polymerization process was displayed. The photophysical parameters were investigated by UV-Vis and photoluminescence in solution and in the solid state in Zeonex matrix. The profile of the emission was examined in different solvent polarities to understand the nature of the emission (CT and/or LE) of the compounds. Moreover, aggregation-induced emission (AIE) properties were investigated in THF solutions with different water fractions for the acenaphtopyridopyrazine and triphenylphosphanimine derivatives. The properties of the obtained materials indicated that the compounds can be excellent candidates for applications in optoelectronic devices.