SYNTHESIS AND PHOTOPHYSICAL PROPERTIES OF NOVEL PYRIMIDINE-BASED DONOR-ACCEPTOR EMITTERS

Irina Fiodorova[1*], Rokas Skaisgiris[2], Toma Šapalaitė[1], Tomas Serevičius[2], Sigitas Tumkevičius[1], Saulius Juršėnas[2]

[1]Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania
[2]Institute of Photonics and Nanotechnology, Faculty of Physics, Vilnius University, Sauletekio 3, LT-10257 Vilnius, Lithuania.
**irina.fiodorova@chgf.vu.lt*

TADF compounds are perfect candidates as the third generation emitters for OLED devices due to low synthesis cost (no noble metals atoms), emission yield reaching near unity [1] and efficient utilization of triplet excitons [2]. Triplet upconversion in TADF compounds is enabled by lowering the singlet-triplet energy gap (ΔE_{ST}) until the thermally activated reverse intersystem crossing becomes evident [3]. Minimization of ΔE_{ST} can be achieved by decoupling HOMO and LUMO in compounds constructed of donor (D) and acceptor (A) aromatic or heteroaromatic units. Recently, compounds containing pyrimidine heterocycle as an A unit have been demonstrated to be promising for TADF applications [3-5]. As a continuation of our work in the field of pyrimidine TADF emitters, we present herein results on the synthesis and photophysical characterization of novel pyrimidine derivatives bearing carbazole, acridane and phenoxazine moieties as D units (Fig. 1).

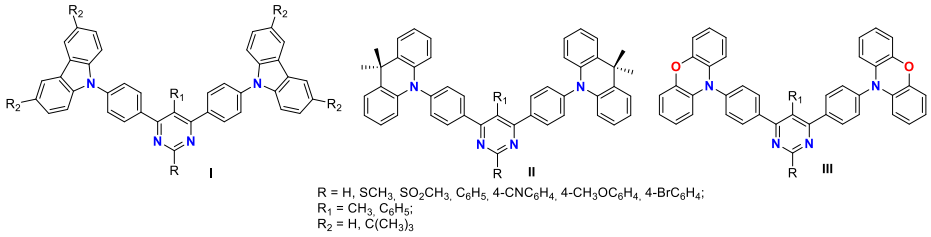

Fig. 1. General structures of pyrimidine-based emitters.

Synthesis of the pyrimidine-based emitters **I-III** and intermediates was carried out starting from easily accessible 4,6-diiodo-5-methyl(or phenyl)-2-methylthiopyrimidines by a combination of palladium-catalyzed Suzuki-Miyaura and Liebeskind-Srogl cross-coupling arylation, and Buchwald-Hartwig amination reactions. Optical properties of the synthesized compounds **I-III** were assessed by DFT calculations and investigated by absorption, time integrated and time-resolved fluorescence spectroscopies and fluorescence quantum yield and lifetime measurements. Details on the synthetic peculiarities and fluorescence properties of the synthesized materials will be presented in the report.

References

1. H. Kaji, H. Suzuki, T. Fukushima, K. Shizu, K. Suzuki, S. Kubo, T. Komino, H. Oiwa, F. Suzuki, A. Wakamiya, Y. Murata, C. Adachi. Nat. Commun. **6** (2015) 8476.
2. L.-S. Cui, A. J. Gillett, S.-F. Zhang, H. Ye, Y. Liu, X.-K. Chen, Z.-S. Lin, E. W. Evans, W. K. Myers, T. K. Ronson, H. Nakanotani, S. Reineke, J.-L. Bredas, C. Adachi, R. H. Friend. Nat. Photonics **14** (2020) 636.
3. T. Serevičius, R. Skaisgiris, J. Dodonova, K. Kazlauskas, S. Juršėnas, S. Tumkevičius. Phys. Chem. Chem. Phys. **22** (2020) 265.
4. T. Serevičius, R. Skaisgiris, I. Fiodorova, G. Kreiza, D. Banevičius, K. Kazlauskas, S. Tumkevičius, S. Juršėnas. J. Mater. Chem. C **9** (2021) 836.
5. T. Serevičius, R. Skaisgiris, J. Dodonova, L. Jagintavičius, D. Banevičius, K. Kazlauskas, S. Tumkevičius, S. Juršėnas. *ACS Appl. Mater. Interfaces*. **12** (2020) 10727.