St. Petersburg
hν 2021
Molecular Photonics

Terenin Memorial Symposium

5th International Symposium on Molecular Photonics

dedicated to the memory of Academician A.N. Terenin (1896–1967)

May 6–7, 2021, Peterhof, St. Petersburg, Russia

BOOK OF ABSTRACTS

Key lectures

(in order of presentation)

Oral lectures

(in order of presentation)

Posters

(in order of presentation)

Memorial section

Program Committee

Theoretical insight of the delayed luminescence mechanism of new push-pull systems based on diazine derivatives

Kurtsevich A.E.[1*], Gadirov R.M.[1]

1 – National Research Tomsk State University

** koall1996@yandex.ru*

Organic light-emitting diodes (OLEDs) are of considerable scientific interest. This is due to the advantages of OLED over alternative light emitting devices. Among these advantages are high contrast, unlimited space for the choice of emitting materials (which allows you to create a device with the emission of any color), the ability to create flexible and transparent displays for devices wearable electronics.

Various approaches are used to create emitting structures. In particular, extensive studies have demonstrated that D–(π)–A structures are useful for developing high-efficiency emitters, because such push–pull systems usually show strong intramolecular charge-transfer (ICT) emission and their optoelectronic properties can be facilely modulated through tuning the electron donor (D) and/or acceptor (A) strengths.

A series of novel pyrazine quinoxaline derivatives D–A and D–π–A structures is synthesized. The photo- and electroluminescent properties of the obtained compounds were studied [1]. In this report, we provide a theoretical explanation of the mechanisms of the processes of delayed luminescence occurring in the presented structures.

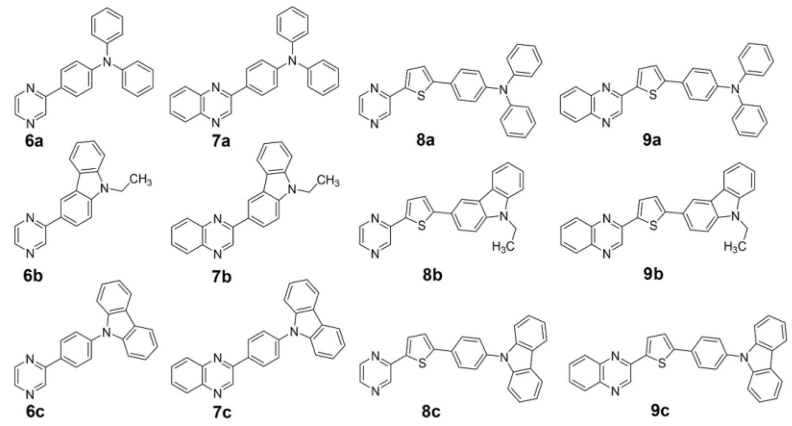

Figure 1: Structures of the studied compounds [1]

All calculations were carried out in the quantum-chemical software package Orca 4.2.1 [2, 3] using stationary and time-dependent density functional theory (DFT and TD-DFT). The geometry of the ground and first excited states was simulated; a diagram of the energy levels of molecules for triplet and singlet states was constructed. All compounds are characterized by a close to orthogonal arrangement of the donor and acceptor fragments of the molecule in the excited state. This leads to a low spatial overlap of the HOMO and LUMO, which favorably affects the quantum yield of delayed fluorescence. Analysis of Jablonski diagrams in comparison with experimental data has shown [1] that the test compound delayed fluorescence occurs by several mechanisms, including both the thermally activated delayed fluorescence (TADF) through the high triplet state (so-called "hot-excitons" mechanism – HE) and triplet-triplet annihilation (TTA). In the first case the energy gap between S_1 and T_2 states was close to zero, when for the TTA cases the S_1 state was approximately halfway between T_1 and T_2 states. The fact that delayed fluorescence occurs via the HE mechanism is explained by the different nature of the T_1 and T_2 states. This leads to little interaction between them. So the process of nonradiative relaxation in the T_1 state is extremely slowed down.

References

[1] Verbitskiy E. V. et al. The effect of molecular structure on the efficiency of 1, 4-diazine–based D–(π)–A push-pull systems for non-doped OLED applications //Dyes and Pigments. – 2021. – V.187. – p.109124.
[2] Neese, F. (2012) The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2, 73–78.
[3] Neese, F. (2017) Software update: the ORCA program system, version 4.0, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 8, e1327.