AMPL-2021

PULSED LASERS AND LASER APPLICATIONS

September 12–17, 2021
Tomsk, Russia

ABSTRACTS

GENERAL SPONSOR

Special Systems. Photonics, St. Petersburg, Russia

CONFERENCE ORGANIZERS

Institute of Atmospheric Optics SB RAS
Institute of High Current Electronics SB RAS
Tomsk State University
Tomsk Polytechnic University

CONFERENCE SPONSORS

Ministry of Education and Science of Russian Federation, Russia
Russian Academy of Sciences, Russia
Siberian Branch of Russian Academy of Science, Russia
Laser Association, Russia

CONFERENCE SPONSORS

TOPAZ Research and Inculcation Enterprise, Tomsk, Russia
Young Scientists Counsil IAO SB RAS, Tomsk, Russia
SP Equipment, Novosibirsk, Russia
Azimut Photonics, Moscow, Russia
LOTIS TII, Minsk, Belarus
Special Systems. Photonics, St.-Petersburg, Russia
CLZ Ltd, Moscow, Russia
Leningrad Laser Systems, St.-Petersburg, Russia

MEDIA SPONSORS

Atmospheric and Oceanic Optics Journal, Tomsk, Russia
Photonics Journal, Moscow, Russia

Scientific & Technical Translations
STT
PUBLISHING
Tomsk, 2021

current in combination with an ICCD camera, the study of the generation of REs with reference to the dynamics of streamer formation was performed.

The reported study was performed within the framework of the State assignment of the IHCE SB RAS, Project No. 0291-2021-0014 (FWRM-2021-0014) as well as was funded by RFBR, Project No. 20-02-00733.

Y-13

PHOTOPHYSICAL INVESTIGATION AND THEORETICAL MODELING OF STRUCTURE ON THE EFFICIENCY OF SUBSTITUTED DIAZINES AS EMITTERS FOR OLEDS

E.V. Verbitskiy[1,2], A.E. Kurtcevich[3], L.G. Samsonova[3], and R.M. Gadirov[3]

[1]Institute of Organic Synthesis UB RAS, 22 Kovalevskaya St., 620108, Ekaterinburg, Russia, charushin@ios.uran.ru;
[2]Ural Federal University, 19 Mira St., 620002, Ekaterinburg, Russia, contact@urfu.ru;
[3]Tomsk State University, 36 Lenina Ave., 634050, Tomsk, Russia, koall1996@yandex.ru

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.

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.

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. 109124.
2. *Neese F.* The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2012. **2**. P. 73–78.
3. *Neese F.* Software update: the ORCA program system, version 4.0, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2017. 8, e1327.