Contribution ID: **172** Type: **Poster**

Spectral properties of the new boron-containing dyes in composite thin films fabricated using thermal vacuum deposition method

Friday 7 November 2025 11:40 (5 minutes)

The development of organic light-emitting diodes (OLEDs) towards higher efficiency and lifetime depends on creating new efficient organic molecules which can be evaporated using thermal vacuum deposition method. Here we present the studies of the electronic structure of new luminescent difluoroborate complexes of benz[c,d]indole derivatives. The one-component and composite Alq3-dyes thin films were fabricated using thermal vacuum deposition method.
The full interpretation of the absorption and fluorescence spectra of dyes solutions, one component and composite thin films has been done using the results of quantum-chemical calculations. The equilibrium molecular geometry and electronic structure of the lowest electron transitions of the dye molecules were performed on the software package Gaussians16 (DFT/B3LYP).
High fluorescence quantum yields of dyes in solutions and thin composite films can be explained by the calculated high dipole moments of first electron transitions and rigid molecule's structures. Efficient electron excitation energy transfer from the Alq3 matrix to dye molecules occurs at a dye concentration of about 1%. At the same time, these dyes have a low quantum yield in single-component thin films because of the formation of H-aggregates.
Due to high fluorescence quantum yields and good photostability the investigated compounds are promising candidates as emitters both in light-emitting layers of OLEDs and in sensor applications.

Acknowledgment
This work has received funding from the Ministry of Education and Sciences of Ukraine and Research Council of Lithuania, project "Exploitation of the solid-state enhanced long-lived emission of organic emitters for the detection of nitroaromatic explosive compounds"; agreements No S-LU-24-6, No M58-2024.

Type of presence

Presence at Taras Shevchenko National University

Author: NAVOZENKO, Oleksandr (Department of Experimental Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv, Akademika Glushkova Av. 4, 03127, Kyiv, Ukraine.)

Co-authors: LOSYTSKYY, Mykhaylo (Department of Experimental Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv, Akademika Glushkova Av. 4, 03127, Kyiv, Ukraine.); Dr BEZVIKONNYI, Oleksandr (Department of Polymer Chemistry and Technology, Faculty of Chemical Technology, Kaunas University of Technology, K. Baršausko st. 59, LT-51423 Kaunas, Lithuania and Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063, Riga, Latvia.); Dr MYKOLA, Shandura (Institute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Murmanska Str., 02660 Kyiv, Ukraine.); GRAZULEVICIUS, Juozas Vidas (Department of Polymer Chemistry and Technology, Faculty of Chemical Technology, Kaunas University of Technology, K. Baršausko st. 59, LT-51423 Kaunas, Lithuania)

Presenter: NAVOZENKO, Oleksandr (Department of Experimental Physics, Faculty of Physics, Taras Shevchenko National University of Kyiv, Akademika Glushkova Av. 4, 03127, Kyiv, Ukraine.)

Session Classification: Poster Session