National Research Tomsk State University

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

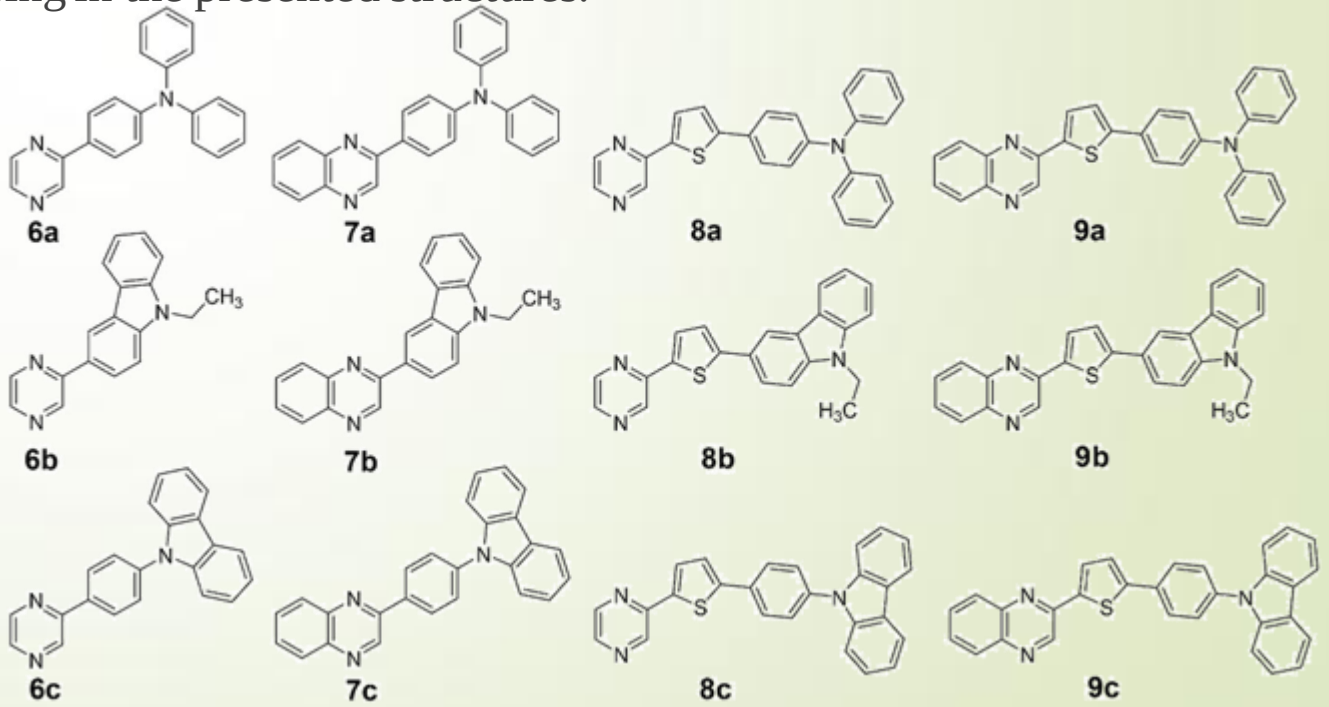
Kurtsevich A.E.[1*], Gadirov R.M.[1]

1 – National Research Tomsk State University

** koall1996@yandex.ru*

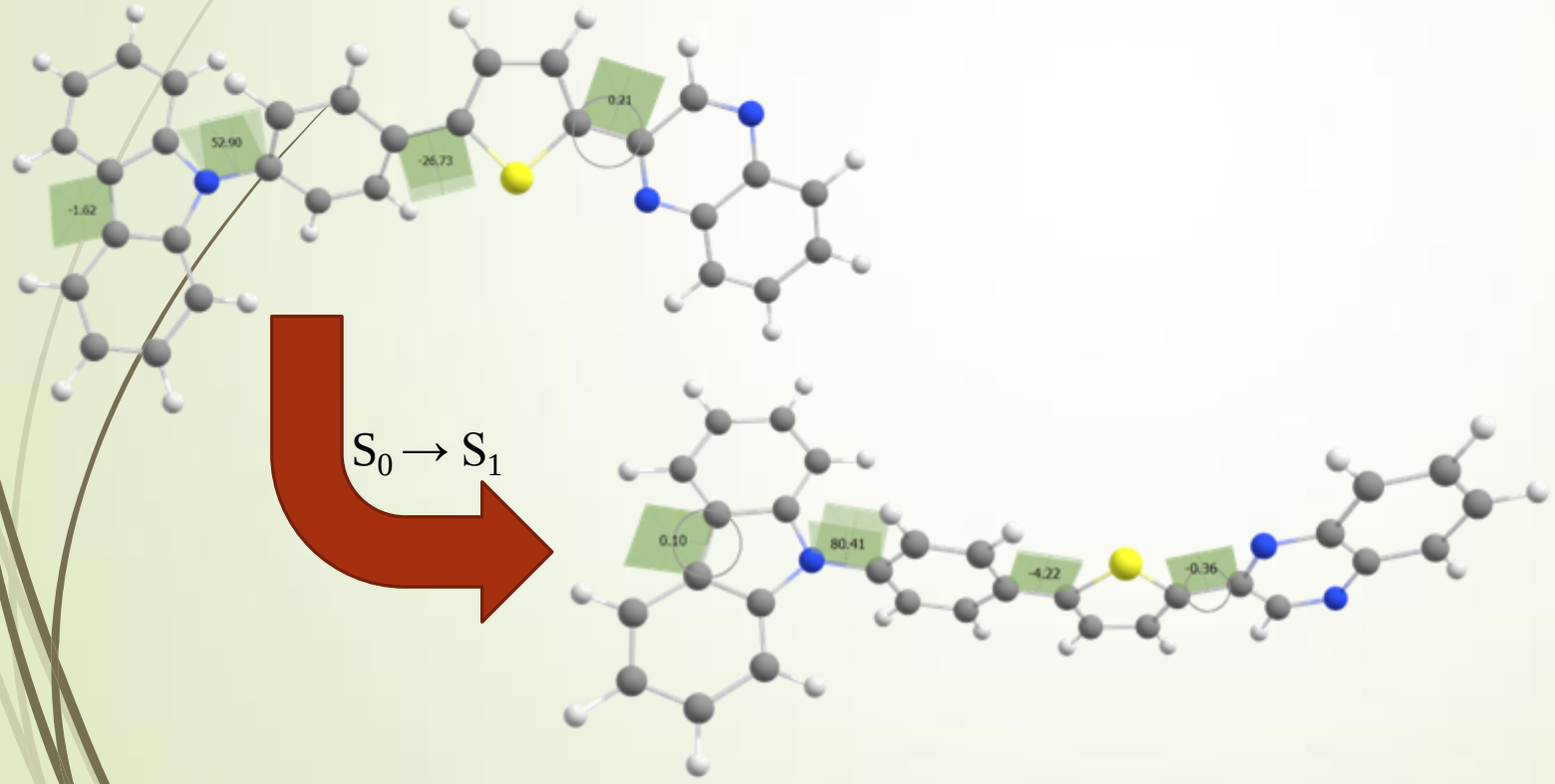
Purpose and Tasks

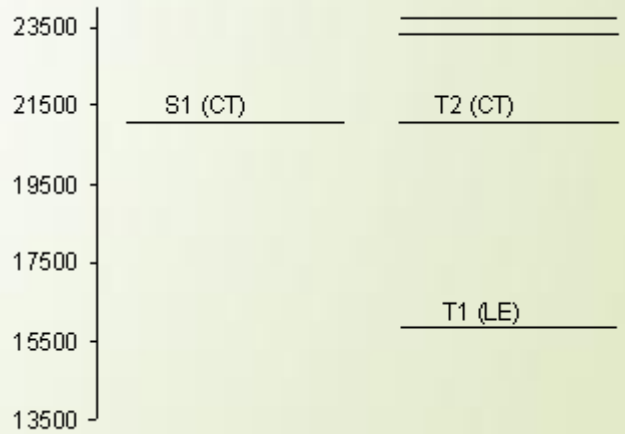
- A series of novel pyrazine quinoxaline derivatives D – A and D – π – A structures is synthesized. The photo- and electroluminescent properties of the obtained compounds were studied.
- There was some unclear effects in photoluminescence spectra.
- This report is aimed for a theoretical explanation of the mechanisms of the processes of delayed luminescence occurring in the presented structures.



Calculations results

- All calculations were carried out in the quantum-chemical software package Orca 4.2.1 using stationery and time-dependent density functional theory (DFT and TD-DFT). All calculations were performed at B3LYP / 6-31G(d, p) and CAM-B3LYP / 6-31G(d, p) levels of theory.





Conclusion

- 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 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. Thus, the process of nonradiative relaxation in the T_1 state is extremely slowed down.

Thank you for your attention