

1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Synthesis and characterization of luminescent compounds containing selenium atoms in their structure.

1.1. Project goals

The research carried out during the doctorate will be aimed at developing new luminescent emitters of visible light with selenium atom/atoms in their structure. The project involves the synthesis of new compounds or modification of known compounds containing oxygen or sulfur atoms by exchanging them for selenium atoms. Organoselenium compounds included in the project will be respectively:

- a) new derivatives of known compounds possessing carbazol/phenothiazine/phenoxazine as a donor group, which will be replaced with phenoselenazine;
- b) new derivatives of known emitters by the modification of their structure through the attachment of additional substituents;
- c) new organoselenium emitters possessing a structure that will evolve on the basis of the conducted research.

1.2. Outline

A significant development in the market of new generation emitters started in 2012 from the work of H. Uoyamy and C. Adachi, in which new compounds, exhibiting for the first time thermally activated delayed fluorescence (TADF), were presented. The derivatives were groundbreaking in the field of luminescent molecules due to high emission efficiencies. In the paper, several emitters were obtained. By slight structure modifications, like the number of substituents or isomerization, they exhibited different emission maxima in the OLED devices based on them. In the following years, many derivatives that were created exhibited TADF, as well as fluorescence and phosphorescence based on structures that do not contain heavy metals, like in the case of the previous generation of emitters.

Till now, only a few examples of organoselenium compounds have been used as emitters. These structures are build-up from aromatic rings connected through selenium, nitrogen and boron¹, phenoselenazine^{2,3}, and donors possessing selenium as substituent⁴. They exhibit new and interesting properties, different than analogical compounds containing oxygen or sulfur presented in the attached literature. Through adequate emitter design, compounds with improved stability, efficiency and particular wavelength emission can be obtained. The main goal of the project is the synthesis of modified emitters by replacing carbazole, phenothiazine or phenoxazine with phenoselenazine, modification of known compounds possessing selenium in their structure and the synthesis of new organoselenium emitters.

1.3. Work plan

Year I

- Designing new organic emitters containing selenium.
- Development of synthetical procedures to obtain and purify the donor parts of the designed compounds.
- Analyses of newly obtained compounds, including NMR, UV-Vis, and IR spectra, GC, HPLC, and fluorescence measurements.

Year II

- Synthesis and purification of the designed organoselenium compounds.
- Analyses of newly obtained compounds and fluorescence measurements.
- Evaluation of the emission of obtained compounds by PL emission spectra.

Year III

- Further synthesis, purification, and characterization of compounds containing selenium.
- Evaluation of the type of emission of obtained compounds by PL emission spectra.
- Primary selection of the synthesized derivatives.
- Attempt to construct the prototype of OLED diode for TADF emitters.

Year VI

- Final modifications and measurements.
- Preparation of the doctoral dissertation.

During the Ph.D. studies, the obtained results will be published and presented at national and international conferences.

1.4. Literature

1. Pratik, S.; Coropceanu, V.; Brédas, J., ACS Materials Letters, 2022, 4, 440.
2. C. L. Kim, J. Jeong, D. R. Lee, H. Jang, S.-T. Kim, M.-H. Baik, J. Y. Lee. J. Phys. Chem. Lett. 2020 11, 5591.
3. De Sa Pereira, D.; Lee, D. R.; Kukhta, Nadzeya A.; Lee, K. H.; Kim, C. L.; Batsanov, A. S.; Lee, J. Y.; Monkman, A. Journal Mat. Chem. C, 2019, 7, 10481.
4. Song, L., Meng, X., Zhao, J., Han, M., & Zheng, D. Spectrochimica Acta Part A (2022). 264, 120296.

1.5. Required initial knowledge and skills of the Ph.D. candidate

- Knowledge in the field of organic chemistry, in particular the synthesis of organoselenium compounds.
- Practical skills enabling efficient laboratory work.
- Experience in analytical methods used to isolate and characterize organic compounds - IR, NMR, UV-Vis, and chromatographic techniques

- General predispositions to scientific work – motivation, proper work planning, and diligence.

1.6. Expected development of the PhD candidate's knowledge and skills

- Expanding the knowledge of organic chemistry, especially in the field of emitter synthesis.
- Increasing the knowledge of fluorescent, phosphorescent, and TADF emitters.
- Learning various analytical methods to characterize the synthesized emitters.
- Acquiring the ability to deal with difficult and stressful situations.