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

Synthesis of New Electron Injection Materials (EIL) for the Emissive Layer in OLED Diodes

1.1. Project goals

The project aims to design, synthesize, and implement new electron injection layer (EIL) materials for OLED devices, focusing on sodium-, lithium-, and potassium-based compounds. Unlike the extensively studied emissive layers, EIL materials have seen little innovation over the last 20 years despite their critical role in lowering energy barriers for electron injection and improving device lifetime. The goal is to develop innovative, cost-effective, and environmentally friendly materials that significantly increase OLED durability, reduce energy consumption, and extend operational lifetimes. The project will deliver patentable compounds and enable their commercialization through collaboration with Noctiluca S.A., enhancing Poland's competitiveness in the global OLED materials market.

1.2. Outline

The project involves the development of new electron injection layer (EIL) materials for OLED devices, based on sodium, lithium, and potassium compounds. The aim is to create innovative, durable, and environmentally friendly materials that reduce energy consumption and improve OLED reliability. The project includes the synthesis and testing of new compounds, followed by their implementation in collaboration with Noctiluca S.A., enabling commercialization and strengthening Poland's position in the global OLED materials market..

1.3. Work plan

The workplan spans eight semesters and integrates scientific research with implementation tasks:

Semesters I-II:

- Literature review, selection of key parameters influencing electron mobility.
- DFT calculations for at least 30 candidate EIL materials (dipole moment, electron affinity, HOMO/LUMO levels, bond dissociation energies).
- Initial syntheses of selected compounds, NMR/IR confirmation, and spectral/thermal characterization.

Semesters III–V:

- Continued synthesis on small scale for at least 10 alkali-metal-based structures.
- Determination of HOMO/LUMO energies, TGA/DSC analyses, vacuum sublimation studies.
- Prototype OLED testing with synthesized ElLs.
- Optimization of device architectures and performance (EQE, current and luminance efficiency, CIE coordinates, LT80–LT95 lifetime).
- Preparation of patent applications and scientific publications.

Semester VI:

- Scale-up synthesis from milligram to multi-gram quantities (>500 mg per material, up to tens/hundreds of grams).
- Testing in prototype OLEDs at larger scale.
- Optimization of cathode/electron transport interfaces.
- Industrial verification in collaboration with Noctiluca S.A.

Semesters VII–VIII:

- Summarizing results and preparing PhD dissertation.
- Final patent applications and publications.

- Technology transfer, customer testing, and commercialization.
- Promotion at international conferences and industry events.

1.4. Literature (max. 10 listed, as a suggestion for a PhD candidate)

- 1. T. Chiba, Y. Puand J. Kido, Solution-processable electron injection materials for organic light-emitting devices, J. Mater. Chem. C, 2015, DOI: 10.1039/C5TC02421H
- 2. A. P. Kulkarni, C. J. Tonzola, A. Babel, S. A. Jenekhe, Electron Transport Materials for Organic Light-Emitting Diodes, Chem. Mater. 2004, https://doi.org/10.1021/cm049473l
- 3. S. H. Jeon, Y. M. Cho, T. Kim, S. Kang, Discovering new M-quinolate materials: theoretical insight into understand the charge transport, electronic, self-aggregation properties in M-quinolate materials (M = Li, Na, K, Rb, Cs, Cu, Ag, and Au), J Mater Sci, 2019, DOI:10.1007/s10853-019-03584-8
- 4. D. Singh, V. Nishal, S. Bhagwan, R. K. Saini, I. Singh, Electroluminescent materials: Metal complexes of 8-hydroxyquinoline A review, Materials & Design, 2018, https://doi.org/10.1016/j.matdes.2018.06.036
- 5. F. A. Angel, R. Gao, J. U. Wallace, C. W. Tang, Silver-induced activation of 8-hydroxyquinolinato lithium as electron injection material in single-stack and tandem OLED devices, Organic Electronics, 2018, DOI:10.1016/j.orgel.2018.05.023
- S. Ohisa, T. Karasawa, Y. Watanabe, T. Ohsawa, Y. Pu, T. Koganezawa, H. Sasabe, J. Kido, A Series of Lithium Pyridyl Phenolate Complexes with a Pendant Pyridyl Group for Electron-Injection Layers in Organic Light-Emitting Devices, ACS Applied Materials & Interfaces, 2017, https://doi.org/10.1021/acsami.7b13550

1.5. Required initial knowledge and skills of the PhD candidate

The candidate should have a solid foundation in organic chemistry, particularly in the synthesis and characterization of small molecules. Basic knowledge of photophysics and materials science, especially regarding optoelectronic properties of organic compounds. Familiarity with laboratory such and spectroscopy techniques i.e. NMR, UV-Vis, and fluorescence spectroscopy, as well as experience with thin-film preparation and device fabrication, will be advantageous.

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

The PhD candidate will gain advanced expertise in organic synthesis, photophysical characterization, and OLED device engineering. They will develop skills in designing functional molecules, analyzing their optoelectronic properties, and integrating them into working devices. Through collaboration with industry partners and participation in interdisciplinary research, the candidate will also strengthen competencies in scientific communication, project management, and technology transfer. This training will prepare them for careers in both academic research and the high-tech materials industry.