Tytuł projektu

Synteza wydajnych fluoroforów jako sond molekularnych – związki o potencjalnym zastosowaniu w diodach OLED

Project title

The synthesis of highly fluorescent spectral probes - potential compounds for OLED materials

Dyscyplina /Area of science

Nauki chemiczne

PROJECT DESCRIPTION

Project goals

- The synthesis of the precursors of fluorophores and their conversion to compounds carrying boron atom.
- The measurements of the photophysical properties for obtained compounds.
- Modification of the fluorophores with variable substituents and groups with increasing steric effect to tune charge transfer properties.
- Tests of the synthesized compounds towards sensing based on techniques of supramolecular chemistry.
- Measurements of the properties in variable polarity environment and at variable temperatures to study their dynamics.
- Cocrystalization of selected compounds with suitable counterparts and studies of aggregation of molecules in solid.

Outline

Due to the social impact the luminescent materials are one of the most needed in the industry. These are used in many fields as, for example, bioimaging, OLED and molecular sensing. Thus, their structure should be known in detail regarding their geometry but also for their intermolecular interactions. These two properties would help designing new materials that, for example, could be used in TADF[1] emitters increasing the effectiveness of the luminescence.

The intermolecular interactions are important for the design and for tuning properties of new materials. These forces are a) hydrogen bonding, b) halogen bonding, c) hydrophobic interaction, d) pi-pi stacking and other. These, together with intramolecular effects, can be used in crystal engineering and molecular aggregation in solution. Mentioned interactions are in line with the application of fluorophores in analytics. That is due to the fact that both, the fluorescence quenching and aggregation-induced

emission are preferred for the on-off mechanisms of molecular reporting. Also, the shift of the spectral characteristics or the change of the fluorescence life-time can also be useful.

It is expected that the steric and electronic effects within fluorophore and in the interacting molecule would tune the properties and aggregation of molecules[2-5] influencing their photophysical properties.[6-7] The PhD project will be guided at Nicolaus Copernicus University and in cooperation with Wrocław University of Science and Technology and University of Nantes in France and University of Łódź. The research is supported by National Science Centre (Harmonia project).

Work plan

1. The synthesis of chosen precursors and fluorophores that belong to several series of B-carrying molecules.
2. The substitution by groups capable to introduce the needed properties, as for example, hydrogen, halogen bonding or pi-pi stacking interactions.
3. Functionalization of molecules in a systematic way to tune their aggregation by steric effects in solution and in the crystal.
4. Correlation of the molecular structure with photophysical properties in solid state.

Literature

1 T.-T. Bui, F. Goubard, M. Ibrahim-Ouali, D. Gigmes and F. Dumur, Beilstein J. Org. Chem., 2018, 14, 282–308.
2 B. Ośmiałowski, K. Mroczyńska, E. Kolehmainen, M. Kowalska, A. Valkonen, M. Pietrzak and K. Rissanen, J. Org. Chem., 2013, 78, 7582–7593.
3 B. Ośmiałowski, E. Kolehmainen and M. Kowalska, J. Org. Chem., 2012, 77, 1653–1662.
4 B. Ośmiałowski, E. Kolehmainen, S. Ikonen, A. Valkonen, A. Kwiatkowski, I. Grela and E. Haapaniemi, J. Org. Chem., 2012, 77, 9609–9619.
5 B. Ośmiałowski, E. Kolehmainen, R. Dobosz, R. Gawinecki, R. Kauppinen, A. Valkonen, J. Koivukorpi and K. Rissanen, J. Phys. Chem. A, 2010, 114, 10421–10426.
6 B. Jędrzejewska, A. Grabarz, W. Bartkowiak and B. Ośmiałowski, Spectrochim. Acta A Mol. Biomol. Spectrosc., 2018, 199, 86–95.
7 B. Jędrzejewska, A. Skotnicka, A. D. Laurent, M. Pietrzak, D. Jacquemin and B. Ośmiałowski, J. Org. Chem., 2018, 83, 7779–7788.

Required initial knowledge and skills of the PhD candidate

- ➔ Analytical thinking
- ➔ Eager to learn and work hard
- ➔ Understanding of organic synthesis and methods for separation and purification
- ➔ Ability to work in the laboratory (synthesis and basic spectral measurements)

Zgłaszający projekt/ Author of the project	
dr hab. inż. Borys Ośmiałowski, prof. UMK stopień/tytuł, imię, nazwisko	borys.osmialowski@umk.pl e-mail
	Wydział Chemii UMK jednostka organizacyjna
Proponowani promotorzy i mentorzy/prospective supervisors	
1) promotor główny/ main supervisior	
dr hab. inż. Borys Ośmiałowski, prof. UMK	borys.osmialowski@umk.pl e-mail
	Wydział Chemii UMK jednostka organizacyjna
2) promotor pomocniczy / co-supervisor	