PhD position:
Purely organic room-temperature phosphorescent chromophores for near-infrared organic light-emitting diodes

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Context and project:

The phenomenon of room-temperature phosphorescence (RTP) in purely organic materials has garnered significant attention due to its diverse applications, including anticounterfeiting, *in vivo* imaging and Organic Light-Emitting Diodes (OLEDs).[1] Compared to the more traditional fluorescence where the emission originates from an excited singlet state, phosphorescence requires intersystem crossing to populate the triplet state prior to radiative deexcitation. In purely organic molecules, intersystem crossing is formally prohibited by spin selection rules but can be achieved through spin-orbit coupling, which mixes singlet and triplet states. A major challenge in purely organic RTP chromophores is overcoming the energy-gap law to maintain strong emission in the near-infrared region (NIR, 700-1000 nm). This is particularly arduous as non-radiative deactivation of the triplet state significantly increases with bandgap narrowing. Consequently, only a handful of NIR RTP organic emitters have been identified.[2] Surmounting this hurdle holds the potential to pave the way for next-generation NIR OLEDs.[3]

In light of these challenges, this PhD project proposes the development of new purely organic chromophores exhibiting far-red to NIR phosphorescence. Based on a previous study on RTP chromophores derived from 2-bromo-7-carbonylfluorene[4] and a preliminary theoretical analysis, novel chromophores with low triplet energy and high spin-orbit coupling were designed. These chromophores feature rigid thiophene-based conjugated π-systems, composed of fused cycles, ensuring improved electronic delocalization for red-shifted optical properties. Throughout the project, the PhD candidate will synthesize new organic conjugated molecules, perform their structural characterization and investigate their optical properties in solution and solid state. Analysis of the structure-properties relationship will enable us to optimize their optical properties and provide new molecular engineering guidelines for enhancing NIR RTP. Additionally, deuteration of the most promising chromophores will present a powerful tool to diminish non-radiative pathways, thereby increasing the phosphorescence quantum yield.[5] Finally, efficient NIR RTP chromophores will be incorporated in OLEDs devices.

Presentation of the lab:

MOLTECH-Anjou (https://moltech-anjou.univ-angers.fr/), UMR CNRS 6200 of the University of Angers, is a laboratory of 90 chemists and physicists with a scientific activity centered on the development of organic molecular materials or organic-inorganic hybrids, in support of highly visible axes such as organic electronics, stimulable materials, self-assembled materials, materials for energy, functionalized nanostructured surfaces and photonics. For 20 years, MOLTECH-Anjou has continuously contributed to the development of organic photovoltaics and enabled significant advances. Since 2018, the unit has benefited from a new technical platform, unique in the West of France and dedicated to the manufacture of electronic devices.

Profile of the applicant:

The candidate must hold a Master/Engineer degree in Chemistry, Physical Chemistry, Materials Science or associated fields, with experience in organic synthesis. Previous experience on

the synthesis and study of luminescent materials is not required but appreciated. Good lab skills and scientific rigor are greatly appreciated. Throughout the PhD program, the candidate will acquire skills in organic chemistry, fluorescence/phosphorescence spectroscopy, material chemistry and possibly electrochemistry and device fabrication.

Funding:
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References:

[1] S. Hirata, *Adv. Opt. Mater.* **2017**, *5*, 1700116.
[2] G. D. Gutierrez, G. T. Sazama, T. Wu, M. A. Baldo, T. M. Swager, *J. Org. Chem.* **2016**, *81*, 4789–4796.
[3] Y. Xiao, H. Wang, Z. Xie, M. Shen, R. Huang, Y. Miao, G. Liu, T. Yu, W. Huang, *Chem. Sci.* **2022**, *13*, 8906–8923.
[4] J. Xu, A. Takai, Y. Kobayashi, M. Takeuchi, *Chem. Commun.* **2013**, *49*, 8447–8449.
[5] S. Hirata, K. Totani, J. Zhang, T. Yamashita, H. Kaji, S. R. Marder, T. Watanabe, C. Adachi, *Adv. Funct. Mater.* **2013**, *23*, 3386–3397.