MOLTECH-Anjou laboratory, UMR 6200 CNRS University of Angers
Supervision by **Flavia Pop**, CR CNRS, **flavia.pop@univ-angers.fr**

PhD position at MOLTECH-Anjou laboratory starting on October 1st 2023
Funding: EUR-LUMOMAT and University of Angers

Helicene and quasi-circulene diketopyrrolopyrroles (DPP) photoconductors

The project proposes to explore novel chromophores based on diketopyrrolopyrrole (**DPP**) decorated with helical chirality of dithia-[7]helicenes (**dtH**) and dithia-quasi-[8]circulenes (**dtQC**) type (Figure 1). The (opto)electronic properties of these molecules could be modulated through the DPP by using different types of aromatic units and their solubility can be adjusted using different alkyl substituent on the N atoms.[1] Substituents on the amide motifs represent one way to render DPPs chiral. The importance of the chiral centre position with respect to the DPP chromophore has recently been highlighted in series of phenyl, thiophene and pyridine DPPs.[2] The asymmetric carbon atom directly linked the N atom of the DPP core renders these chiral DPPs active in circular dichroism (CD) and fluorescent in the solid state. The interest of incorporating such chiral DPPs in the active layer of photovoltaic devices has been recently highlighted on DPPs decorated with chiral and H-bonding N-subtituents[3] and by the international partner of the project (D. Amabilino, ICMAB, Spain) by mapping the supramolecular structures of thin films of chiral DPPs.[4] The **dTH** and **dtQC** proposed in here possess two thiophene rings in the helical structures that induce complete selectivity of their synthesis. They are both obtained from the same intermediate by cross coupling and oxidative dehydrocyclisation reactions. Recent preliminary reporting on the stereostability and resolution of the enantiomers, represent valuable assets and a strong starting point for the project.[5]

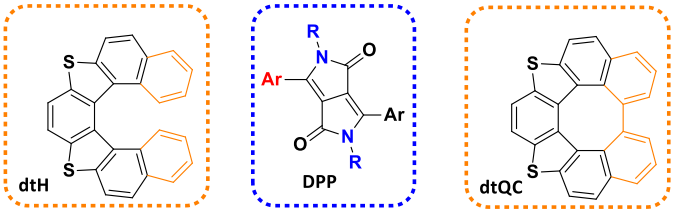

Figure 1. Key units of the project.

The project is dedicated to the investigation of new materials with crossroad properties resulting from the association of chirality and high molar absorptivity in chromophores. Secondly, the project wants to bring contributions in the field of chiral semiconductors by bringing insights into the requirements needed for active materials and the role the chirality to improve structural order in thin films and thus efficiency of photovoltaic devices. Moreover, due to their chirality, these materials will show selectivity towards circularly polarized light (CPL) absorption and thus activated photoconductivity when irradiated with CPL.

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Researched skills

The candidate will be responsible of the synthesis, purification and characterization of the precursors and of final chiral chromophores. She/He will be involved in their characterization by spectroscopy (absorption, emission, CD absorption and CPL emission), cyclic voltammetry and occasionally by single crystal diffraction. Furthermore, aggregation of the new molecules will be studied in solution and on surfaces, and the properties of the supramolecular aggregates will be investigated. The microscopy study of chiral aggregates will be performed in the partner's laboratory at the ICMAB, Barcelona, Spain. Accordingly, two shorts stays, of 4 months each, will be carried out in the ICMAB laboratory during the second and the third year of thesis. The photovoltaic characterization will be performed in the international partner's lab and by collaboration with the members of the Moltech-Anjou laboratory.

The candidate should have a master degree in chemistry and an interest in organic and supramolecular chemistry and chirality. Any knowledge in theoretical chemistry, spectroscopy, chiroptical methods and crystallography will be highly appreciated.

All applications, sent to flavia.pop@univ-angers.fr, should include a cover letter, a CV and the contact of at least one referent person.

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[1] Pop, F.; Lewis, W., Amabilino, D.B. *CrystEngComm.* **2016**, *18*, 8933–8943.
[2] Mastropasqua Talamo, M.; Pop, F.; Avarvari N. *Chem. Commun.* **2021**, *57*, 6514–6517.
[3] Militzer, S.; Nishimura, N.; Avila-Rovelo, N.R.; Matsuda, W.; Schwaller, D.; Mesini, P.J.; Seki, S.; Ruiz-Carretero, A. *Chem. Eur. J.* **2020**, *26*, 9998–10004.
[4] Killalea, C.E.; Samperi, M.; Siligardi G.; Amabilino, D.B. *Chem. Commun.* **2022**, *58*, 4468−4471.
[5] Baudillon, M.; Cauchy, T.; Vanthuyne, N.; Avarvari, N.; Pop, F. *Org. Chem. Front.* **2022**, *9*, 4260–4270.