# Master 2 internship offer:
# New pyranopyran-based conjugated cores for organic electronics

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## Context:

The development of new organic π-conjugated materials has garnered significant attention and has led to substantial advancements in organic electronics over the past three decades. Through key innovations, such as the introduction of new chromophores (**Y6** for organic photovoltaics (OPV))[1] or of new concepts (thermally activated delayed fluorescence (TADF)[2] in organic light-emitting diodes (OLEDs)), the performances of organic devices have dramatically improved. However, organic electronics still lag behind their inorganic counterparts in terms of performance. Furthermore, despite the impressive efficiencies achieved by **Y6** and its derivatives, its practical application is hindered by complex synthesis and high production costs, with a commercial price of 4500€/g (Ossila). This underscores the ongoing need to design new conjugated molecules to close the performance gap between organic and inorganic electronics while keeping production costs minimal for a faster transition to renewable energy.

The combination of electron-donating **D** and withdrawing **A** groups to obtain charge transfer material is one of the most promising approaches for designing new NFA and TADF materials. In particular, structures that combine a strong donor core with two acceptor groups in an **A-D-A** architecture have demonstrated significant potential in OSC[3] or OLEDs.[4]

To advance beyond existing structures, we conducted a preliminary Density Functional Theory (DFT)/Time-Dependent DFT (TD-DFT) study using Gaussian to design novel conjugated cores based on the pyranopyran motif. While pyran-based chromophores have shown promising performances in OPV or organic photodetectors,[5,6] pyranopyrans have yet to be explored in organic electronics. The two bithieno-fused pyranopyran isomers exhibit exceptionally high calculated HOMO energy level values of -4.78 eV and -5.02 eV, respectively. These values originate from the combination of low aromatic stabilization energies and the donating capacity of the added oxygen atoms.

Building on this theoretical foundation, this internship aims to synthesize and study new pyranopyran-based building blocks, as well as the quadrupolar chromophores obtained by adding two electron-withdrawing groups A, for next-generation OSCs and OLEDs. After synthesis, optical and electrochemical characterization of new chromophores, promising molecules will be used as active materials in OSCs and OLEDs. These results will contribute to the identification of organic chromophores that can enhance light absorption, charge separation, and stability, leading to solar cells with higher power conversion efficiencies and longer operational lifetimes, as well as improved light emission for more energy-efficient lighting and displays. Hence, this internship aims to respond to the affordable and clean energy goal of the Sustainable Development Goals (https://sdgs.un.org/goals) and will be funded by EU GREEN (https://eugreenalliance.eu/mission-vision/).

## Candidate:

We are looking for a passionate and motivated student studying Chemistry, Physical Chemistry, Materials Science or associated fields, with experience in organic synthesis. He/she should have a strong interest in the organic synthesis of π-conjugated molecules for organic electronics. Good lab skills and scientific rigor are greatly appreciated. Throughout the internship, the student will develop his/her skills in organic synthesis (following experimental protocols, purification by crystallization and column chromatography, structural characterization by NMR, MS and XRD) and learn about the characterization of π-conjugated molecules (absorption and fluorescence spectroscopy, electrochemistry) and possibly the fabrication of organic electronic 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, stimuli-responsive 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.[7,8] 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.

Within MOLTECH-Anjou, the intern will join the Kemtronix team and will be supervised by Dr. Maxime Remond and Dr. Philippe Blanchard.

## References:


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[3] C. Yan, S. Barlow, Z. Wang, H. Yan, A. K.-Y. Jen, S. R. Marder, X. Zhan, "Non-fullerene acceptors for organic solar cells" *Nat. Rev. Mater.* **2018**, *3*, 1–19.

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