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Topic: *Supramolecular Polymers for Organic Thermoelectrics*

The self-assembly of small molecules through non-covalent but directive interactions is key to form of 1D wire-like or 2D nanosheets supramolecular objects that exhibit various properties. [1] Our group has been active in this field with the development of an organic platform called Toluene Bis-Amide (TBA), forming elongated ribbons in solution (Figure 1). These defect-less assemblies are very promising systems for charge transport on long distances, such as in field effect transistors or in thermoelectric devices.[2] (Organic) Thermoelectrics is a phenomenon in which the semiconductor converts heat into electricity, making this technology particularly relevant in the context of energy generation through green processes (Figure 2). [3] A good thermoelectric semiconductor must effectively conduct charges and should not conduct heat. 1D or 2D self-assembled materials are very promising because i) they usually present defect-less structure (good charge conductivities), self-healable characteristics and ii) thanks to their non-covalent nature, they should prohibit heat transport.

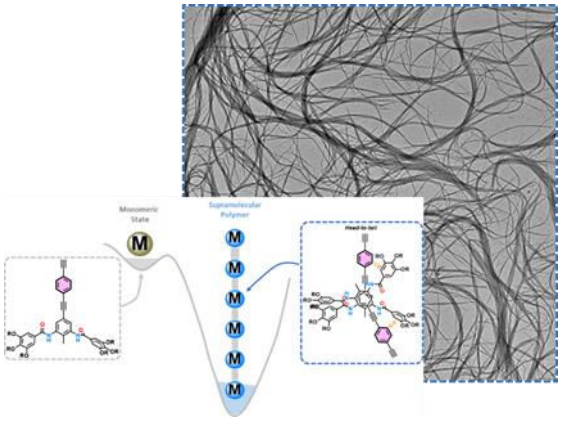
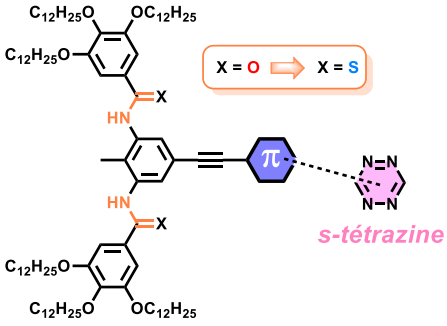


Figure 1 Our previous investigations on TBA platforms

The objective of the PhD track is to design innovative organic supramolecular small molecules assemblies that fulfill those criteria. To conduct charges (electrons), the supramolecular TBA moiety will be connected to an electron transporter, namely the s-tetrazine (Scheme 1). In particular, we will investigate the influence of the assembling functions (amide vs thioamide) on the supramolecular processes and on the thermoelectric merit. **At the interface** of multiple research domains, ranging from **organic synthesis** of aromatic systems to **spectroscopic measurements** or **device fabrication**, this work would require to:

Figure 2 Example of clothing equipped with thermoelectric generators (doi: 10.1016/j.apenergy.2016.08.150)

1/ synthetize functional heteroaromatic systems.
2/ characterize the physical-chemistry properties of the materials (optical, electrochemical, self-assembly behavior, rheology, small angle X-ray scattering, TEM, AFM)
3/ fabricate devices and incorporate those organic materials into devices to investigate their charge and heat conductivities. The PhD will have the opportunity to carry out some measurements with our international partner Pr. ORGIU facilities in Québec.



TBA

Scheme 1 Objectives and Target molecules

This PhD topic is by essence multidisciplinary and rely on a strong international collaboration **(E. Orgiu, INRS, Québec)** and would allow the PhD student to acquire sets of complementary skills and expertises in particular in synthesis and in physical-chemistry characterizations.

Feel free to contact either of us for more information: olivier.galangau@univ-rennes.fr and/ or stephane.rigaut@univ-rennes.fr

[1] Galangau, O. Angew. Chem. Int. Ed. **2023**, e202313696 (open access ⇨ doi.org/10.1002/anie.202313696)
[2] Sirringhaus, H. Adv. Mater. **2014,** 26, 1319.
[3] a) Fenwick, O.; Orgiu, E. Mol. Syst. Des. Eng. **2017**, 2, 47. b) Bubnova, O.; Khan, Z. U.; Malti, A.; Braun, S.; Fahlman, M.; Berggren, M.; Crispin, X. Nat. Mater. **2011**, 10, 429.