Molecular Materials for Room Temperature Thermoelectrics

Objective. This research project aims to study and adapt Molecular Materials for future use in Thermoelectric Generators. We seek to better understand the ability of our nanomaterials in converting heat into electrical energy. The project will involve synthesizing new molecular materials, characterizing their electric and thermoelectric properties, for rationalizing their performances, and ultimately design new materials with improved performances. The ultimate goal is to develop cost-effective and environmentally friendly thermoelectric materials for sustainable energy conversion applications.

Context. Intense research efforts are currently devoted to the search of efficient and eco-friendly energy sources and conversion technologies. In this context, the thermoelectric production, which consist in transforming heat loss into electrical energy, have gained significant attention.[1] This technology relies on ThermoElectric Materials ("TEM") that are able to generate a difference in electric potential when submitted to a temperature difference applied to their ends. The most well-known TEM are inorganic materials (metallic chalcogenides), which are used for high-temperature applications, such as for recovering waste heat from steel furnaces. Recent studies on organic polymers show that such TEMs could exploit the temperature difference between human skin and the environment to power low-consumption wearable electronics (*e.g.* for powering bio-sensors).[2] However, significant challenges remain to develop fully operational and marketable generators based on these materials. The main bottleneck is the low performance of these systems. in particular a relatively low energy conversion efficiency (with power conversion efficiencies in the range 1 - 3 % and Seebeck coefficients usually < 100 $\mu V.K^{-1}$ for temperature differences as high as 100 K).[3]

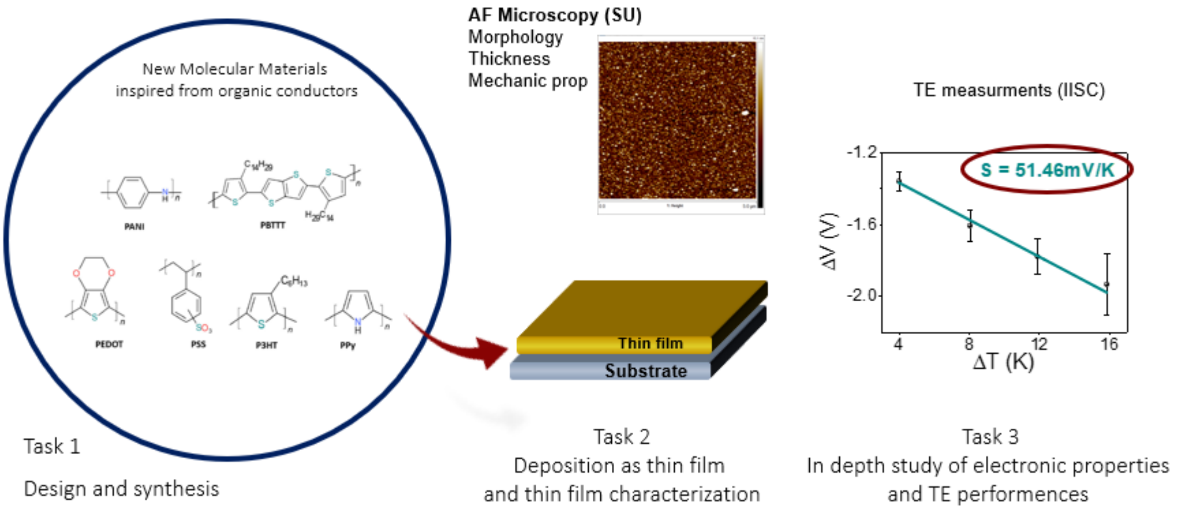
Very recently, we discovered with the Kaliginedi group (at IISc-Bangalore) a family of materials which exhibits outstanding thermoelectric power, in particular high Seebeck coefficients (up to 50,000 $\mu V.K^{-1}$) for temperature differences as low as 16 K, near room temperature. Since the power factor of Thermo-electric generators depends on the square of the Seebeck coefficient, it is very likely that such TEMs could achieve conversion efficiencies much higher than those reported for current devices. To date, we do not fully understand the origin of the high performances of this new family of materials, and there is a need for in-depth investigation to rationalize and further optimize their properties.

Scientific Approach. The first task in the Ph.D. student will consist in acquiring the synthetic know-how to prepare the new materials. Then the student will synthesize derivatives with different subcomponents to better understand the role of each of these elements in the electronic properties and TE performances. The materials will be prepared as thin films to anticipate their integration into thermoelectric generators (in the frame of established collaborations at SU) by microscopy and spectroscopy techniques, in order to evaluate their mechanical properties and some of their electronic properties. The PhD student will take part to these measurements under supervision of scientific and technical staff, and he/she should gain expertise on some of the techniques. This will constitute a second task in the PhD work. Finally, in-depth electronic characterization and evaluation of the TE features of

[1] M. Feng et al., *Renew. Sust. Energ. Rev.*, **2023**, 187, 113723. https://doi.org/10.1016/j.rser.2023.113723.
[2] S. Zhu et al., *Energies*, **2022**, 15, 3375. https://doi.org/10.3390/en15093375
[3] H. Jin et al., *Angew. Chem. Int. Ed.*, **2019**, 58, 15206. https://doi.org/10.1002/anie.201901106

the materials (including thermal conductivity measurements) will be carried out at IISc Bangalore. We expect the student to participate to these measurements during short stays that will be organized during the second and third years of the Ph.D. One of the objectives of the Ph.D. work is to validate some hypotheses we built on the role of the subcomponents. A second objective is to further improve the electrical conductivity of our thin films by changing the nature of the materials subcomponents, while maintaining low thermal conduction, which are two conditions to obtained good TE performances. At the end of his/her PhD the young doctor will have gained knowledge in synthesis and material characterization, involving the use of diverse advanced techniques. He/she should be able to evolve in a multidisciplinary domain to further pursue his/her carrier in Material Science.

Host Institutions. The IISc Bangalore is the first ranked research Institution in India and SU is one of the French leading University. V. Kaliginedi has a very strong expertise in molecular electronics and the characterization of the electrical and thermoelectric properties of molecule and materials…. R. Lescouëzec (IPCM) has a strong expertise in the design of Molecular Materials showcasing unusual electronic properties. Dr. L Fillaud (LISE) has an expertise in molecular electronic and electropolymerization.



Candidate Profile. We seek for a curious, dynamic and highly motivated master student who has a keen interest in working on an interdisciplinary project. Given the collaborative nature of the project, the candidate should demonstrate good communication and teamwork skills for interacting and favouring the link between supervisors and colleagues with different expertise fields. Strong problem-solving abilities, adaptability, and a proactive approach are essential for navigating the diverse challenges of the research project. Knowledge in organic/inorganic synthesis, or in material characterization should be beneficial to the project.

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