Minisymposium
Thermoelectricity

Vendredi 11 octobre 2024 9h30-11h30

Amphithéâtre Henri Benoît

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Is the field of organic thermoelectrics stuck?

With the increasing popularity of organic thermoelectrics, the interest in doping strategies for organic semiconductors has increased dramatically over the past decade. Here we use a meta-analysis of reported performance indicators of organic thermoelectric materials. Based on this, we show that despite the superlinear increase in the number of publications on this topic, surprisingly no clear upward trend in power factor can be observed in the same time range. In the second part, we discuss possible strategies to break this deadlock. Particularly promising approaches include controlling the distribution of dopant atoms in the host material, both on a microscopic and macroscopic scale. A combination of kinetic Monte Carlo simulations and experiments enable us to understand under which conditions these strategies can result in an increase in performance indicators.

Mariano Campoy Quiles

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On the thermal conductivity of semiconducting polymers

The thermal conductivity is the main parameter defining how heat propagates in a solid. It is of paramount importance for heat dissipation in electronics and transmission lines, but also in thermoelectrics. Despite its importance, little attention has been paid to its actual value, in part due to the general belief that the thermal conductivity in organic semiconductors “should be” small. Literature shows, however, values spanning more than two orders of magnitude.

In this talk, we will show a combined experimental/theoretical study, in which we have measured the thermal conductivity for a large polymer library and discovered the coexistence of two fundamentally distinct regimes [1]. Semicrystalline conjugated polymers behave as conventional theory predicts, with increasing order leading to an increase in thermal conductivity, and this correlates also with an increase in charge carrier mobility. In other words, thermal and electrical transport go hand in hand. On the other hand, materials that do not show long range order in GIWAXS behave very differently, not following the same classic theory. As a consequence, for the latter, charge carrier mobility and thermal conductivity appear to be anticorrelated. We rationalize our results using Spearman statistics as well as theoretical calculations, which allow us to provide simple and exploitable design rules for materials that are able to decouple thermal and electronic transport, namely, texture/orientation and monomer/sidechain weight. Some of these design rules are tested by measuring the thermal conductivity of thiophene based materials as a function of molecular weight and Mw distribution (modal vs bimodal).
Finally, following our initial test on the effect of doping on thermal conductivity [2], we have undergone a study with 8 different polymers and 5 different doping systems to develop a more general understanding of the thermal conductivity of doped polymers for thermoelectrics [3].

Séminaires organisés par M. Brinkmann en amont de la soutenance de GUCHAIT Shubhradip 14h le meme jour.

References for Mariano Campoy Quiles:

[1] “On The Thermal Conductivity of Conjugated Polymers for Thermoelectrics” X. Rodríguez-Martínez, F. Saiz, B. Dörling, S. Marina, J. Guo, K. Xu, H. Chen, J. Martin, I. McCulloch, R. Rurali, J. S. Reparaz, M. Campoy-Quiles. Adv. Energy Mater., 2024, 2401705. (2024) DOI: 10.1002/aenm.202401705
[2] “Reduction of the Lattice Thermal Conductivity of Polymer Semiconductors by Molecular Doping”, O. Zapata-Arteaga, A. Perevedentsev, S. Marina, J. Martin, J. S. Reparaz, M. Campoy-Quiles, ACS Energy Letters, 5, 9, 2972–2978 (2020). DOI: 10.1021/acsenergylett.0c01410
[3] “Microstructural changes dominate the thermal conductivity variations upon doping in conjugated polymers”, J. Guo, K. Xu, J. Asatryan, M. J. Alonso Navarro, O. Zapata-Arteaga, M. Craighero, M. M. Ramos, J. L. Segura, J. Martín, C. Müller, J. S. Reparaz, M. Campoy-Quiles, in preparation (2024)