DS 25: Focus Session: Organic-based Hybrid Thermoelectrics II

Time: Wednesday 11:15–12:45 Location: CHE 89

Invited Talk DS 25.1 Wed 11:15 CHE 89

Organic thermoelectrics: fundamentals, challenges and recent results — •Martijn Kemerink — Centre for Advanced Materials, Universität Heidelberg, Germany

The potential use in thermoelectric applications of heavily doped organic semiconductors has led to a dramatic increase in research on these materials. In this talk, I will use recent results by ourselves and others to highlight some of the potential and some of the challenges of organic thermoelectrics (OTE). Specifically, I will focus on three aspects, being the role of the material morphology, the influence of doping on the energy landscape experienced by the mobile charge and the formal description thereof.

The topic of morphology will be addressed for systems containing either one or two semiconductors. In the former, it will be shown how processing-induced structural anisotropy can lead to a non-trivial simultaneous increase in electrical conductivity and thermopower. For the latter, the degree of phase separation will be shown to play the key role in determining whether the semiconductor blend behaves as an effective medium or not, which gives the unique opportunity to reach record-high thermopowers, albeit at the cost of a reduced but still finite electrical conductivity. Experimental results are interpreted by semi-analytical and numerical modeling that allows to identify strategies for fundamental and application-oriented research.

DS 25.2 Wed 11:45 CHE 89

Electronic Transport in Polymer Thin Films for Thermoelectric Applications — •Marie Siegert[1], Mahima Goel[2], Mukundan Thelakkat[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg — [2]Applied Functional Polymers, University of Bayreuth — [3]ZAE Bayern

The interest in thermoelectric materials has greatly gained traction over the last decades due to their immense potential in waste heat recovery. Recently, the focus has shifted towards organic materials as a sustainable, low-cost alternative to inorganic semiconductors. Especially polymers hold great promise, as they can be solution processed at large scales and display low thermal conductivities. However, the improvement of their electrical conductivity σ, while retaining their Seebeck coefficient S, imposes a major challenge upon implementation in efficient thermoelectrics. Hence, we compare two possible strategies on improving the charge carrier transport in such disordered systems. At first, σ of organic composite films has been investigated, combining the well studied polymer PEDOT:PSS with crystallites of the low-dimensional molecular metal TTT_2I_3, which shows superior charge carrier transport over a wide temperature range[1]. Secondly, doped polymer films utilizing an oxidized hole conductor as dopant have been electrically characterized by means of σ and S. Both approaches will be evaluated with respect to the enhancement in σ and the underlying transport mechanisms. First estimations of the resulting power factors indicate future strategies to further enhance the electronic properties and thus, the figure of merit. [1] Huewe et al. *Adv. Mat.* 29 (2017).

Invited Talk DS 25.3 Wed 12:00 CHE 89

Tuning the Thermoelectric Performance of Hybrid Polymer/Nanoparticle Composites via Stoichiometric Control — •Katherine A. Mazzio[1], Danny Kojda[1], Britta Ryll[1], Jens Niederhausen[1], Rodrigo Rubio-Govea[1,2], Klaus Habicht[1,3], and Simone Raoux[1,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Institut für Chemie, Humboldt Universität zu Berlin, Berlin, Germany — [3]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [4]Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany

Hybrid materials consisting of inorganic nanostructures embedded in conducting polymer matrices have emerged as promising systems for room temperature thermoelectric applications. They are attractive due to their intrinsic low thermal conductivities, the ability to engineer interfaces for energy filtering effects and phonon scattering, and their ability to take advantage of high-throughput and solution processable manufacturing. When synthesizing hybrid materials, one can think of them as a three phase system consisting of the organic material, the inorganic material, and the interface. Our goals revolve around controlling each of these components independently, and in this contribution, I will detail our recent efforts towards this end. Ultimately, we aim to develop an understanding of how to use solution-based synthesis to influence thermoelectric device properties.

DS 25.4 Wed 12:30 CHE 89

Radical Ion Doped Organic Single Crystals for Thermoelectric Applications — •Maximilian Frank[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern eV), 97074 Würzburg

The successful application of organic semiconductors in lighting or photovoltaics would not have been possible without doping. Motivated by this, we will deal with the implementation of doped molecular crystals in thermoelectrics (TE) which promise the recovery of substantial amounts of waste heat generated upon primary energy consumption [1]. It is desirable to use materials with large Seebeck coefficient S, high electrical conductivity σ, and low thermal conductivity κ, which can be summarized in the dimensionless figure of merit at given temperature $zT = \frac{\sigma S^2}{\kappa} T$. In this sense, long-range ordered molecular crystals offer an interesting approach by their low thermal conductivities generic to van-der-Waals bound systems combined with moderate mobilities for electrons and holes. We use high quality polyaromatic single crystals to systematically alter their bandfilling and, thus, their electrical transport properties by electrochemical doping. The variations in electrical conductivity as well as Seebeck coefficient will be discussed as function of doping. The results will be critically evaluated in regard of the independent optimization of the thermoelectric parameters and, thus, of the implementation of doped single crystals and thin films in TE applications.

[1] C. Forman, et al., Renew. Sust. Energ. Rev. 2015, 57, 1568