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Thermoelectricity in Disordered Organic Semiconductors under the Premise of the Gaussian Disorder Model and its Variants DAN MENDELS, NIR TESSLER, TECHNION, ORGANIC MATERIALS AND DEVICES TEAM — Charge transport in disordered organic systems has been in recent decades mainly discerned from the perspective of a variety of phenomenological models prominent of which those stemming from the Gaussian Disorder Model. But while the use of these models has been prevalent, uncertainty regarding the extent of their validity remains due to the large number of free parameters they consist and their frequent deficiency to consistently account for large sets of experiments while keeping model input parameters and distributions unchanged. In the presented study, we have investigated using Monte Carlo simulations the thermoelectric properties of disordered organic semiconductors under the premise of the Gaussian Disorder Model and its variants. Doing so enabled the provision of additional dimensions for comparison between the aforementioned theoretical frameworks and real systems, beyond those based on extensively studied charge transport properties, and the provision of a frame-of-reference for rising interest in these systems for thermoelectric applications. To illustrate the potential existing in the implementation of combined transport and thermoelectric investigation, strategies will be discussed to experimentally deduce the DOS shape, infer whether a system's activation energy originates from its energetic disorder or a polaron activation energy (while deducing the given polaron activation energy), and discerning whether a system's energetic disorder is spatially correlated or accompanied by off-diagonal disorder.

Dan Mendels
TECHNION

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