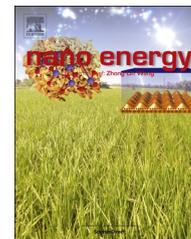




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RAPID COMMUNICATION

# Effect of host-mobility dependent carrier scattering on thermoelectric power factors of polymer composites



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## Abstract

The interfacial carrier scattering was thought to be ineffective in enhancing thermoelectric (TE) properties of polymer hybrids and there was also a lack of fundamental understanding of carrier scattering at polymer/polymer interfaces. Here we unravel the mechanism behind the role of polymer/polymer interfacial scattering on the TE properties through integration of computation and experiments. We discover that the effect of interfacial scattering at polymer/polymer interfaces on TE properties of polymer hybrids is strongly dependent on the carrier mobility of host polymers besides interfacial barriers. Only when the host carrier mobility is above a threshold, the effect of interfacial scattering on TE enhancement can be significant. Simulation suggests that the host mobility threshold is  $\sim 1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  for PEDOT-based polymers. The polymer hybrid system of poly(3,4-ethylenedioxythiophene) (PEDOT) nanowires/PEDOT was successfully employed to verify the theoretical results. These findings offer groundbreaking knowledge on polymer/polymer interfacial carrier-transport and will advance the design and fabrication of high-efficiency organic thermoelectric materials.

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## Introduction

Thermoelectric (TE) materials convert thermal energy to electricity and vice versa. The conversion efficiency is governed by the TE figure of merit ( $ZT$ ),  $ZT = S^2\sigma T/\kappa$ , where  $S$  is the Seebeck coefficient,  $\sigma$  is the electrical conductivity,  $\kappa$  is the thermal conductivity, and  $T$  is the absolute temperature at operation [1]. Organic TE materials are very attractive since they are composed of earth-abundant elements (and thus low cost), lightweight, and easy to process [2]. Because organic materials (e.g. conjugated polymers) usually present intrinsically low thermal conductivity [3-6], enhancing the power factor  $S^2\sigma$  is crucial to achieve high  $ZT$  for efficient energy conversion. Several state-of-art methods have been employed for enhancing the power factors of conjugated polymers, including doping control [7-13], the addition of carbon nanofillers (e.g. carbon nanotubes (CNTs) [14-21], graphene [2,22-25]) and high-TE-performance inorganic semiconductors [26-28], metal coordination polymers [29], metal-organic frameworks (MOFs) [30] and polymer blends [31,32]. Recently, the conducting polymer, highly doped poly(3,4-ethylenedioxythiophene) (PEDOT), has been intensively studied as a promising organic TE material [7-12]. The thermoelectric power factor is significantly improved by engineering the doping levels and morphology of PEDOT [7-13].

It is paramount to significantly increase  $S$  so as to maximize  $S^2\sigma$ . It has been well reported that the carrier scattering can significantly improve the Seebeck coefficient of inorganic TE materials for enhanced power factor and  $ZT$  [33]. However, there is a lack of fundamental understanding and consensus on the significance potential of interfacial carrier scattering for enhancing the Seebeck coefficient and thus power factor of fully organic TE materials. Previous attempts using polymer blends have not yet uncovered a significant improvement to the Seebeck coefficient via such a mechanism [31,32]. Therefore, it is worth to explore the potential of carrier scattering for enhancing TE properties in fully organic materials.

In this work, we for the first time explore the mechanism behind the role of interfacial carrier scattering on the TE transport (Seebeck coefficient) of polymer/polymer hybrids through theoretical calculations and experimental verification. We theoretically simulated the host mobility-dependent carrier scattering effect by calculating Seebeck coefficient enhancement as a function of host carrier mobility. Experimental results were employed to confirm these theoretical findings.

## Experimental

### Transport property calculation

The carrier scattering induced Seebeck coefficient enhancement as a function of host carrier mobility is presented by the Seebeck coefficient ratio of  $S_1/S_0$ , where  $S_1$  is the Seebeck coefficient of the host polymer after interfacial carrier scattering (with polymer nanowire), and  $S_0$  is the Seebeck coefficient of the host without fillers. It was calculated by taking the relaxation time approximation [34]. Detailed simulation process can be found in [Supporting information](#).

## Linear carrier mobility measurements

A electrolyte-gated organic electrochemical transistor (OECT) method was used to measure the linear carrier mobility of highly doped PEDOT:PSS as reported in the literature [35,36]. Ion gel was used to introduce a higher density of charge carriers. As shown in [Figure S2](#), transistors with a channel length ( $L$ ) of 50  $\mu\text{m}$  and width ( $W$ ) of 6 mm were fabricated in a side-gate configuration on the glass substrate. Au was used for source, drain, and gate electrodes. Ion gels based on poly(vinylidene fluoride-co-hexafluoropropylene) (P(VDFHFP)) and the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ( $[\text{EMI}^+][\text{TfSA}^-]$ ) were used as the dielectric layer [35,36]. The thickness of PEDOT:PSS layer is 20-50 nm, and the thickness of ion gel dielectric layer is  $\sim 6 \mu\text{m}$ . The validity of measurement, operation procedures, calculation process and other experimental details of the linear mobility measurement by the electrolyte-gated OECT method can be found in [Supporting information](#).

## Work function measurements

Kelvin probe work function measurements were performed on an SKP SPV-LE 450 Scanning Kelvin Probe Surface Photovoltage instrument from KP Technology. KP measurements were performed in air with a probe oscillation frequency of 78 kHz.

## Thermoelectric characterization

The Seebeck coefficient  $S$  was measured following the method previously reported [37]. The electrical conductivity measurement was conducted using the van der Pauw method.  $I$ - $V$  sweeps were performed using a Keithley 6221 current source and a Keithley 2182 A nanovoltmeter.

Detailed information regarding theoretical calculations, carrier mobility measurements, work function measurements, and thermoelectric property measurements can be found in [Supporting information](#).

## Results and discussions

Organic materials are usually disordered and show much lower carrier mobility (typically,  $\mu < 0.1 \text{ cm}^2/\text{Vs}$ ) and mean free path (MFP) than inorganic materials. However, recent research presents that the carrier transport in conjugated polymers can be significantly facilitated by engineering polymer morphology (e.g. conformation of conducting chains) or synthesizing novel conducting polymers etc. [14,35,36,38]. As the carrier mobility increases, the carrier MFP is believed to increase significantly. For instance, it has been intensively reported that highly doped PEDOT polymers perform their metallic or semi-metallic transport properties [10,39,40]. To some extent, their carrier transports may be different from typical organic semiconductors (hopping transport), while they are more likely to be similar to that in some inorganic semiconductors (e.g. band-like transport [41,42]). So we first modeled the effects of host carrier mobility  $\mu$  and interfacial barrier  $E_b$  on the Seebeck coefficient in the polymer/polymer hybrids.

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