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The figure numbers correspond to the figures in the paper \

Figure 1. Impact of regioregularity on thermoelectric properties of polymer films. (a) Chemical structures for RR and RRa P3HT. Blends prepared with a different composition of RRa to RR P3HT. (b) Power law fits to Seebeck coefficient–electrical conductivity curves of RR-RRa blends indicate a nonuniversal power law dependence.
Figure 2. WAXS of undoped and iodine-doped P3HT. X-ray scattering pattern of (a) undoped P3HT and (b) iodine-doped P3HT. (c) Intensity ratio for the π–π stacking peak to the lamellar stacking peak shows a reduction with increasing RRa P3HT content. This ratio was calculated based on the intensity of Gaussian distribution fits of the peaks with the highest intensity for both types of polymer packing.

Figure 3. Probing polymer–dopant distance through NIR. (a) Experimental NIR spectra of doped P3HT blends show a redshift for iodine-doped RR P3HT with regard to iodine-doped RRa P3HT. (b) Simulated NIR spectra also show a redshift for doped RR P3HT and blends with the highest content of the same.

Figure 4. Kinetic analysis and diffusion rate of iodine dedoping of RR and RRa P3HT show a contribution from multiple structural entities. (a) Electrical conductivity of polymer blends with different RR to RRa content as a function of time. (b) RRa P3HT fits to a single exponential decay rate, indicating dedoping of one type of domain. (c) RR P3HT fits to two exponentials, indicating dedoping of two types of domains. (d) Diffusion coefficient of RR and RRa P3HT show that RRa P3HT has a faster diffusion rate within this doping-level range.

Figure 5. Experimental data and simulations estimate polymer–dopant distances. Experimental data of the Seebeck coefficient (α) and electrical conductivity (σ) fit to simulated data. Simulated data of pure components were simulated using a polymer–dopant distance of 0.8 nm for RR P3HT and 0.3 nm for RRa P3HT. Thermoelectric properties of P3HT blends were simulated by combining the DOS values of each component.

Supplementary Figure 1. Polymer DOS for individual components and polymer blends. Regiorandom (RRa) P3HT blend has a single DOS. Regioregular (RR) has a crystalline DOS and an amorphous DOS. All blends have a total polymer DOS made of the individual DOS for each constituent. The dopant DOS affects polymer DOS depending on the doping level.

Supplementary Figure 2. Experimental-simulations fit and associated error of simulations for polymer blends of regioregular and regiorandom P3HT.

Supplementary Figure 3. Deconvolution of scattering pattern by using multiple Gaussian distributions to fit the data. For regioregular P3HT (0% RRa), the fit includes narrow distributions for (100) and (010) peaks and one or more broad distributions for both peaks. Regiorandom P3HT (100% RRa) has a sharp peak for (100) and a sharp peak for (010). It also has a broad shoulder peak in the (100) region.

Supplementary Figure 4. X-ray scattering pattern of undoped and doped P3HT blends with different regioregularity. The (100) peak of undoped Regiorandom P3HT has a right shoulder. The data shows that all samples have similar intensity, except for a slight variation in the background of the doped samples.5

Supplementary Figure 5. Simulated diffusion rate for different polymer-dopant distances and their effect in offset of energy levels between the polymer and the dopant(ΔE). The data shows a faster diffusion rate for higher polymer-dopant distances at low-medium doping levels (top). At high doping levels, shorter polymer-dopant distances have a faster diffusion rate. Although polymer-dopant distance affects diffusion rates, the effect of ΔE is more significant and persists across different doping levels. For small and large Rmin (bottom), a change in ΔE makes the diffusion rate vary significantly across different doping levels.