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Tuning the charge conductivity and thermoelectric properties of oriented F4TCNQ-P3HT films by controlled dopant intercalation

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This contribution focuses on the impact of crystallinity, structure and orientation on the doping efficiency and resulting thermoelectric (TE) properties of oriented regioregular poly(3-hexylthiophene) films doped with F4TCNQ.[1] We use the rubbing temperature (T_R) as a handle to tune the film's structure and investigate by a combination of UV-Vis-NIR spectroscopy, Transmission Electron Microscopy (Electron Diffraction), Electron Spin Resonance (EPR), charge conductivity and thermopower measurements, how the structural variety impacts charge conductivity and TE properties. [2]

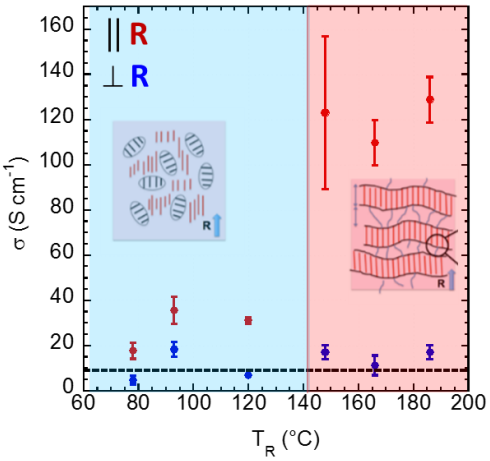

*Figure 1: Evolution of the charge conductivity measured along and perpendicular to the rubbing direction **R** for P3HT films rubbed at different T_R and doped with F_4TCNQ*

As a main result, the semi-crystalline structure of aligned P3HT films obtained for T_R>144°C shows superior conductivity and TE efficiencies (power factor) as compared to the smectic-like phase (50°C≤T_R≤125°C) because of both a higher in-plane orientation and a higher doping level. [3] Electron Diffraction on doped oriented films of the smectic-like and the semi-crystalline phases highlight differences in the intercalation mechanism of F_4TCNQ in the layers of alkyl side chains. We demonstrate the counter-intuitive idea that doping can promote ordering of P3HT backbones along the chain direction within individual π-stacks. Correlations between the order parameter and the anisotropy in charge transport and Seebeck coefficient are revealed. The angular dependence of characteristic polaronic and anionic bands helps quantify the amount and the orientation distribution of the intercalated dopants. Optimal TE performances are obtained for thin films rubbed at 186°C with conductivities of up to 160 S/cm and power factors of 56 μW m^{-1} K^{-2} along the rubbing direction versus a few μW m-1 K-2 for non-oriented films.

References

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