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Quantitative assessments of the effect of microstructure on transport in organic semiconductors

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From the fundamental standpoint, organic semiconductors are fascinating as they are neither crystalline nor amorphous and their microstructure plays a central role in governing charge transport. I will show that understanding disorder is the key to determining charge transport mechanism. We are particularly interested in cumulative disorder (paracrystallinity), where the lattice parameter takes on a Gaussian distribution about its mean value. The disorder parameter g allows us to rank materials quantitatively on a continuous scale, from a perfectly crystalline material ($g < 1\%$) to an amorphous one ($g > 10\%$). Surprisingly, even the polymers that are considered to have the highest crystallinity (PBTTT) have a g in the pi-stacking direction close to that of an amorphous material ($\sim$7%). Furthermore, comparison of X-ray diffraction data and optical absorption data provides insight into the nature of the disordered phase as well. Using first principle calculations and tight binding methods, I will show that paracrystallinity in the pi-stacking direction provides a fundamental mechanism for the existence of an exponential distribution of localized tail states in the gap. The larger the degree of disorder the higher the trap density and the deeper their energy. Using disorder as a ranking parameter, I will discuss the differences in transport between small molecule and polymer films as well as their respective inherent limitations and bottlenecks.