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A general relationship between disorder, aggregation and charge transport in conjugated polymers

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The large variety of semiconducting polymers is a result of the synthetic capabilities to tune the optoelectronic properties of materials. Such variability also leads to a wide range of microstructures when solid films of conjugated polymers are cast from solution. Indeed, the large number of degrees of conformational freedom of these macromolecules and their weak intermolecular interactions result in complex microstructures - displaying a coexistence of amorphous and ordered phases with varying degrees of order. Understanding the limitations of charge transport in conjugated polymers is difficult owing to the unusual range of disorder they exhibit. These microstructures highlight the necessity to study the contributions of electronic processes at various length scales. In this talk, I will describe X-ray diffraction studies that show a large amount of disorder in semiconducting polymers while optoelectronic measurements show charges stay in the semi-ordered regions. Considering a particular system, P3HT with variable molecular weight, very similar transitions are observed in the behavior of the lattice disorder parameter (paracrystallinity) and charge mobility. Additionally, a comprehensive comparison of structure-property data across a wide range of materials uncovers strong similarities between seemingly diverse families of conjugated polymers. These insights allow the grouping of materials and identification of the importance of short-range ordered aggregates in transport. This generalization explains the seemingly contradicting high performance of recently reported, poorly ordered polymers and suggests molecular design strategies to further improve the performance of future generations of organic electronic materials. Specifically, the key to designing high mobility polymers is not in increasing crystallinity but rather in increasing their tolerance to an inevitably large amount of disorder within the aggregates by allowing more efficient intra- and intermolecular charge transport/transfer at the segmental level.