Revealing Order and Disorder in Films and Single Crystals of a Thiophene-Based Oligomer by Optical Spectroscopy

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Abstract:

Depending on processing conditions, ordered microstructures of conjugated oligomers or polymers exhibit variable amounts of grain boundaries, lattice disorder and amorphous (disordered) regions. These structural details can be determined very precisely, their correlations with optical or electronic properties, however, are very difficult to establish, because e.g., optical spectra are usually averaged over regions with different degrees of disorder. In an attempt to facilitate the interpretation of optical spectra, we performed systematic studies on thin films and µm-sized single crystals of thiophene-based conjugated molecules, which allow identifying the relative contributions of ordered and disordered regions in optical emission spectra. A detailed multi-peak analysis of the emission spectra showed that the peak positions, the energy of the emitted photons, were always the same, independent if highly ordered or rather disordered samples were examined. However, the relative emission intensity changed significantly between samples, in particularly, for single crystals the purely electronic 0-0 transition nearly vanishes, i.e. it is essentially optically forbidden as theoretically predicted. These changes in emission probability provide a possibility to quantify the degree of structural order in semiconducting conjugated systems.