Semiconducting molecular crystals: Bulk in-gap states modified by structural and chemical defects

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Charge transport in organic molecular crystals is strongly influenced by the density of localized in-gap states (traps). Thus, a profound knowledge of the defect states’ origin is essential. Temperature-dependent space-charge limited current (TD-SCLC) spectroscopy was used as a powerful tool to quantitatively study the density of states (DOS) in high-quality rubrene and pentacene single crystals. In particular, changes of the DOS due to intentionally induced chemical and structural defects were monitored. For instance, the controlled exposure of pentacene and rubrene to x-ray radiation results in a broad over-all increase of the DOS. Namely, the ionizing radiation induces a variety of both chemical and structural defects. On the other hand, exposure of rubrene to UV-excited oxygen is reflected in a sharp peak in the DOS, whereas in a similar experiment with pentacene oxygen acts as a dopant, and possible defects are metastable on the time-scale of the measurement, thus leaving the extracted DOS virtually unchanged.