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Influence of exciton transfer on the optical cycle of α-PTCDA

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Abstract

The optical properties of single crystals of α-3,4,9,10-perylene-tetracarboxylic-dianhydride are analysed in terms of the transfer of Frenkel excitons coupled to an effective internal vibrational mode of the molecule, including the full microscopic crystal geometry with two molecules per unit cell. The resulting linear optical properties agree quantitatively with the refractive index and extinction coefficient measured on polycrystalline thin films, and the energy dependence of the anisotropic dielectric tensor is similar to ellipsometry data. A generalization of this model to Frenkel excitons propagating with different wave vectors results in a minimum of the exciton dispersion at the surface of the Brillouin zone. These low-lying states are obvious candidates for the origin of the red-shifted photoluminescence (PL), and the calculated radiative lifetime coincides with the measured decay time of the dominating PL channel at low temperature.

Author Keywords: PTCDA; Frenkel exciton; Photoluminescence; Charge-transfer exciton

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