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Energy band dispersion in well ordered N,N′-dimethyl-3,4,9,10-perylenetetracarboxylic diimide films

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The electronic properties of well ordered N,N′-dimethyl-3,4,9,10-perylenetetracarboxylic dimide (DiMe-PTCDI) films prepared on sulfur passivated GaAs(001) substrates were studied by means of photoemission spectroscopy. From the photon energy dependence of normal emission spectra an intermolecular energy band dispersion of about 0.2 eV was determined for the highest occupied molecular orbital (HOMO). Simulation of the density of states reveals that the HOMO band has a single π-character. The observed energy band dispersion thus originates from the intermolecular π-π interaction and is modeled using the tight binding model. The analysis provides a value of 0.04 eV for the transfer integral. The inner potential was treated as a fitting parameter such that the expected periodicity of the dispersion in the reciprocal space was obtained. ©2004 *American Institute of Physics*

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