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Ab initio Evaluation of the Charge-Transfer Integrals and Band Structures of Phenanthroline-based Molecular Crystals[1] H. LI, J.-L. BREDAS, Georgia Institute of Technology, C. LENNARTZ, BASF Aktiengesellschaft, Germany — Ab initio calculations are carried out to study the charge-transport properties of phenanthroline-based molecular crystals, BCP and Bphen. The charge-transfer integrals in the two crystalline structures and in a quasi-1D chain model for BCP are evaluated based on: (i) a tight-binding approximation for dimers; (ii) the band structures of the periodic systems. In these compounds, the LUMO/LUMO+1energies of the isolated molecules are very close, which results in the LUMO and LUMO+1orbitals both having significant contributions to the LUMO level in the dimer. In this case, the usual definition based on the electronic coupling between the two LUMO orbitals from each molecule cannot be applied to describe the charge-transfer characteristics in the dimer. A new definition of "effective transfer integrals" based on "mixed states" was proposed (H. Li, J.L. Bredas, and C. Lennartz, J. Chem. Phys. 126 (2007) 164704) to address this problem. Within the tight-binding approximation, the "effective transfer integrals" for both hole and electron transfers are found to be in very good agreement with the valence and conduction band dispersions obtained from plane-wave DFT calculations. We acknowledge many stimulating discussions with Veaceslav Coropceanu and Demetrio da Silva Filho.

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Hong Li
School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

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