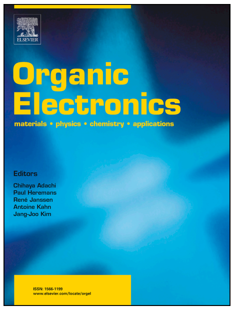

Relating stacking structures and charge transport in crystal polymorphs of the pyrrole-based π-conjugated molecule

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Relating Stacking Structures and Charge Transport in Crystal Polymorphs of the Pyrrole-Based π-Conjugated Molecule

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Abstract

We present a theoretical study on charge transport in crystal polymorphs of the pyrrole-based π-conjugated molecule, the dipyrrolyldiketone difluoroboron complex. The ab initio all-electron fragment molecular orbital calculations were carried out to evaluate electronic couplings for charge transfer in three crystal polymorphs. The electron and hole carrier mobilities were estimated on the basis of the master equation combined with the Marcus theory. We found that utilizing the polar diketone difluoroboron unit as the π-conjugated molecule results in the large molecular interactions and electronic couplings. We demonstrate the impact of crystal packing structures on the anisotropy of charge transport, highlighting the dimensionality of charge-transfer networks varying from zero-dimensional behavior of charge localization to three-dimensional behavior of isotropic charge transport. We further elucidate the effects of different π-π stacking modes on the electronic couplings and intermolecular interactions, which underlie the relationship between the crystal packing structures and charge transport.

Keywords: charge transport, crystal polymorphism, dipyrrolyldiketone difluoroboron complex, electronic coupling, fragment molecular orbital method

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