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A Strategy for Reducing Dynamic Disorder in Small Molecule Organic Semiconductors by Suppressing Large Amplitude Thermal Motions

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Abstract : Large-amplitude intermolecular vibrations in combination with complex shaped transfer integrals generate a thermally fluctuating energetic landscape. The resulting dynamic disorder and its intrinsic presence in organic semiconductors is one of the most fundamental differences to their inorganic counterparts. Dynamic disorder is believed to govern many of the unique electrical and optical properties of organic systems. However, the low energy nature of these vibrations makes it difficult to access them experimentally and because of this we still lack clear molecular design rules to control and reduce dynamic disorder. Applying a novel technique based on electron diffraction we encountered strong intermolecular, thermal vibrations in every single organic material we studied (14 up to date), indicating that a large degree of dynamic disorder is a universal phenomenon in organic crystals. In this paper a new molecular design strategy will be presented to avoid dynamic disorder. We found that small molecules that have their side chains attached to the long axis of their conjugated core have been found to be less likely to suffer from dynamic disorder effects. In particular, we demonstrate that 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothio-phene (C8-BTBT) and 2,9-di-decyl-dinaphtho-[2,3-b:20,30-f]-thieno-[3,2-b]-thiophene (C10DNTT) exhibit strongly reduced thermal vibrations in comparison to other molecules and relate their outstanding performance to their lower dynamic disorder. We rationalize the low degree of dynamic disorder in C8-BTBT and C10-DNTT with a better encapsulation of the conjugated cores in the crystal structure which helps reduce large amplitude thermal motions. The work presented in this paper provides a general strategy for the design of new classes of very high mobility organic semiconductors with low dynamic disorder.

Keywords : charge transport, C8-BTBT, C10-DNTT, dynamic disorder, organic semiconductors, thermal vibrations
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