Accurate analysis of anisotropic carrier mobility and structure-property relationships in organic BOXD crystalline materials

Supplementary Material

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Figure S 1. a) Molecular structure of single molecular BOXD-o-1. b) Crystal structure of BOXD-o-1. c) Primary relative position of the bi-molecular in π-stacking. d) Primary relative position of the bi-molecular in herringbone-arrangement.

Figure S 2. a) Molecular structure of single molecular BOXD-o-2. b) Crystal structure of BOXD-o-2. c) Primary relative position of the bi-molecular in π-stacking. d) Primary relative position of the bi-molecular in herringbone-arrangement.
Figure S 3. a) Molecular structure of single molecular BOXD-p. b) Crystal structure of BOXD-p. c) Primary relative position of the bi-molecular in $\pi$-stacking. d) Primary relative position of the bi-molecular in herringbone-arrangement.

Figure S 4. a) Molecular structure of single molecular BOXD-D. b) Crystal structure of BOXD-D. c) Primary relative position of the bi-molecular in $\pi$-stacking.
Figure S 5. a) Molecular structure of single molecular BOXD-T. b) Crystal structure of BOXD-T. c) Primary relative position of the bi-molecular in π-stacking. d) Primary relative position of the bi-molecular in herringbone-arrangement.

Figure S 6. Calculated reorganization energies of five molecular structure.
Figure S 7. The bi-molecular orbital overlap direction of primary electron transfer paths in π-stacking.
Figure S 8. The bi-molecular orbital overlap direction of primary electron transfer paths in herringbone arrangement.
Figure S 9. The bi-molecular orbital overlap direction of primary hole transfer paths in \( \pi \)-stacking.
Figure S 10. The bi-molecular orbital overlap direction of primary hole transfer paths in herringbone arrangement.