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Supporting Information

Terminal π-π Stacking Determines Three-Dimensional Molecular Packing and Isotropic Charge Transport in an A-π-A Electron Acceptor for Non-Fullerene Organic Solar Cells

Guangchao Han,[ab] Yuan Guo,[ab] Xiaoxian Song,[c] Yue Wang,[c] Yuanping Yi[ab]*

[a] Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

[b] University of Chinese Academy Sciences, Beijing 100049, China

[c] State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, China.

*Corresponding authors. E-mail: ypyi@iccas.ac.cn

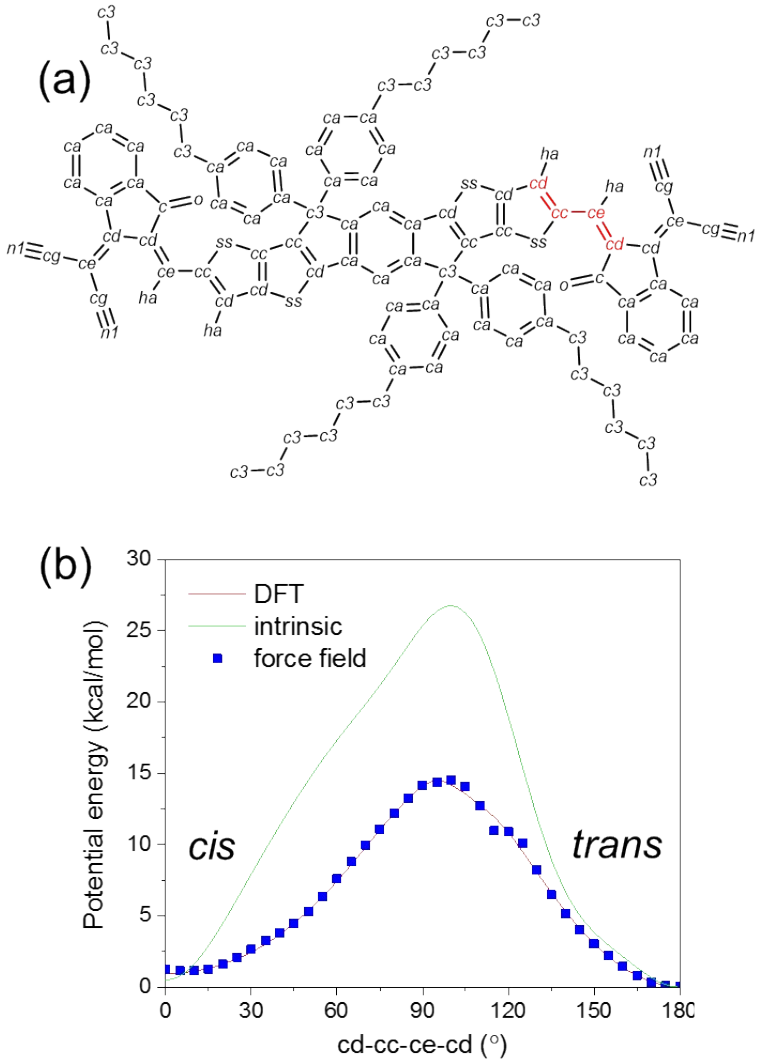

Figure S1. (a) Definition of atomic types for ITIC using the general AMBER force filed (GAFF). The hidden hydrogen atoms on the c3 atoms are defined as hc. (b) Potential energy for cd-cc-ce-cd calculated by DFT and GAFF along with the fitted intrinsic torsion potential.

The torsion potential between the fused-ring backbone and IC (cd-cc-ce-cd) was fitted according to DFT calculations and inserted in the GAFF using the force matching approach as follows:

(1) Scanning total potential energies every 5° from 0° to 180° by constrained geometry optimizations by DFT at the B3LYP/6-311G** level;
(2) Evaluating non-bonded energies for the same set of points by the incomplete force field with the torsion angle in question switched off;
(3) Calculating intrinsic torsion potential from the difference of the energies obtained in steps (1) and (2), and fitting it using the periodic potential;
(4) Inserting the fitted intrinsic potential in the force field parameter file to repeat the reference DFT scan.

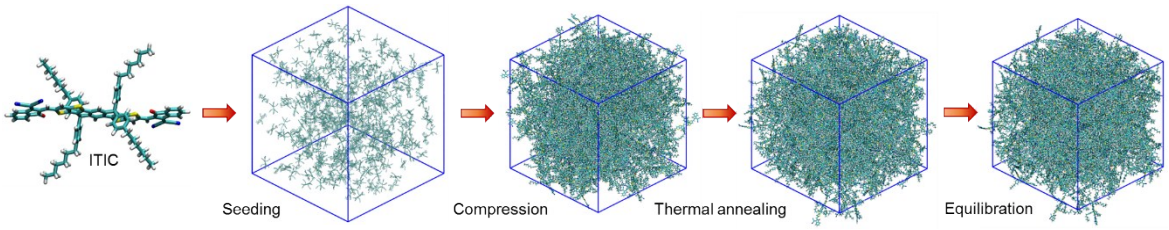

Figure S2. Workflow of molecular dynamics simulation of the ITIC film.

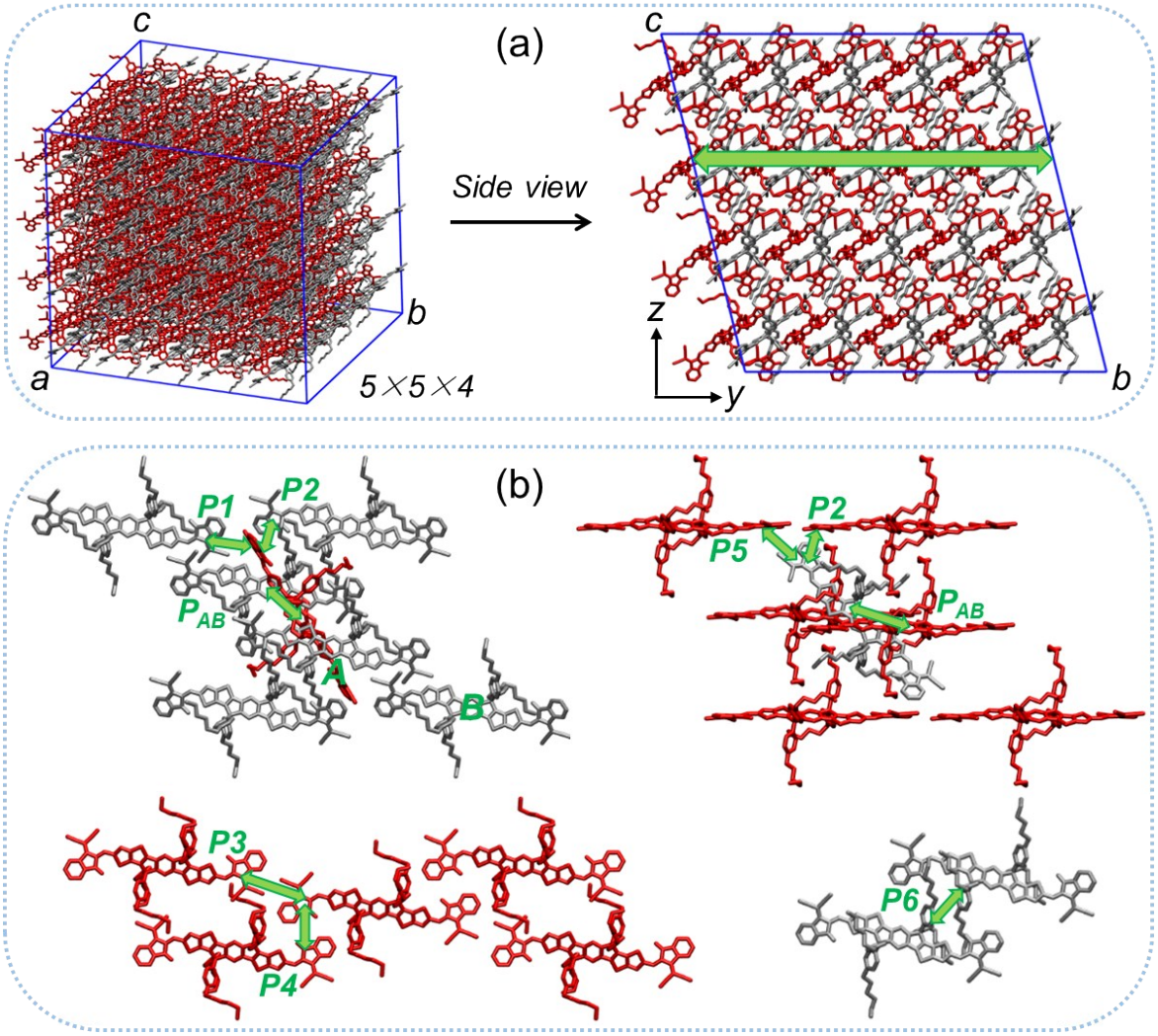

Figure S3. (a) 5×5×4 supercell of the ITIC crystal. (b) Illustration of possible molecular pairs (P1-P6 and P_{AB}) in the ITIC crystal.

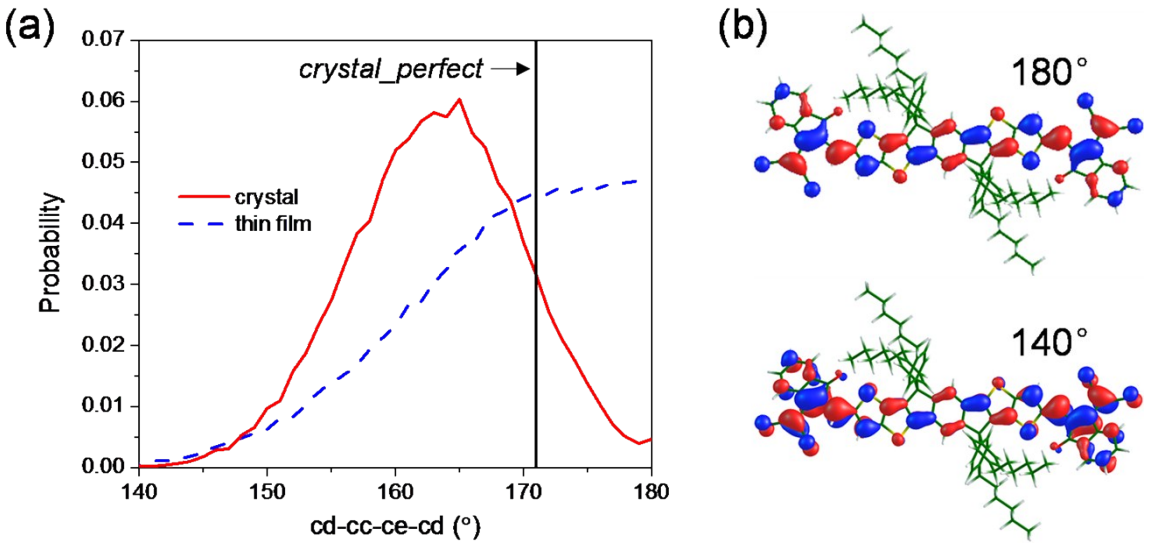

Figure S4. (a) Distribution of the cd-cc-ce-cd torsion angle for ITIC in the simulated thin film and (b) the LUMO of ITIC with the torsion angle set to 140° and 180° calculated by DFT at the B3LYP/6-31G** level.

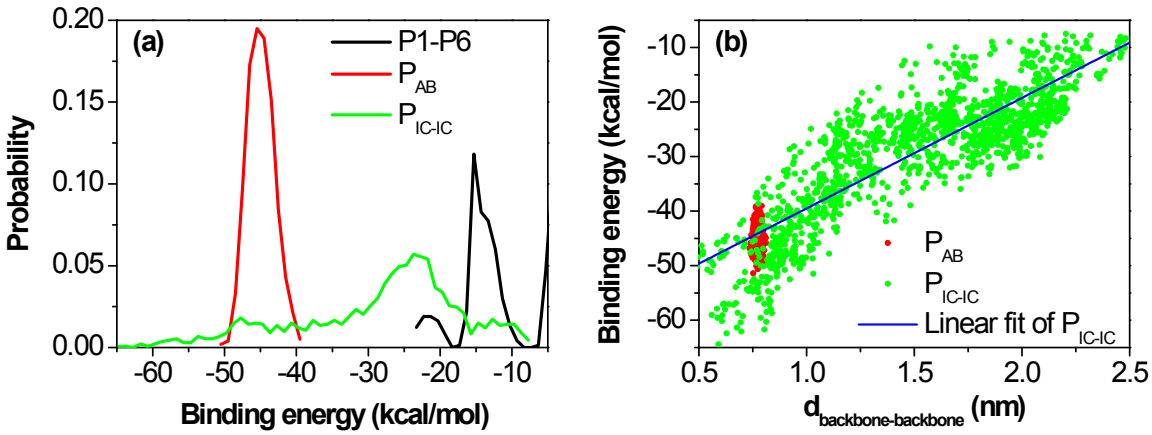

Figure S5. (a) Distribution of binding energies for molecular pairs P_{AB}, P1-P6, and P_{IC-IC} calculated by the force field. (b) Binding energies vs the backbone-backbone center-of-mass distances for P_{AB} and P_{IC-IC}.

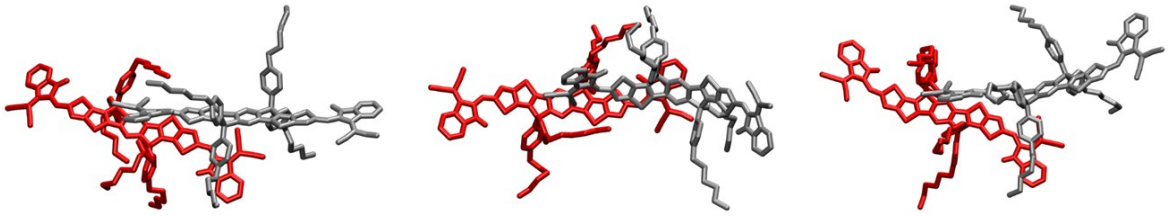

Figure S6. Three representative molecular pairs similar to P_{AB} in the simulated thin film.

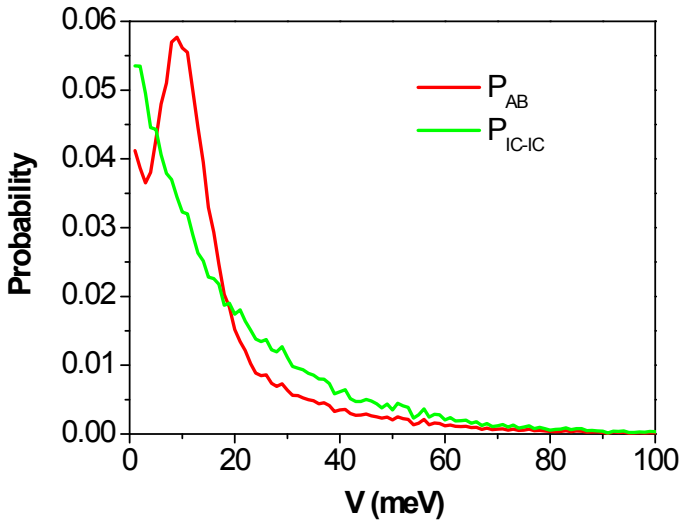

Figure S7. Distribution of electronic couplings for P_{AB} and $P_{IC\text{-}IC}$.