Supplementary Information

Regioisomeric control of charge transport polarity for indigo-based polymers

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Supplementary Information

1. Computer simulations

Geometry optimization of model compounds was performed based on the density functional theory (DFT) using the B3LYP hybrid function[1] and the 6-31G* basis set and the Gaussian 09W package[2] on the Shared Hierarchical Academic Research Computer Network (SHARCNET) of Canada.

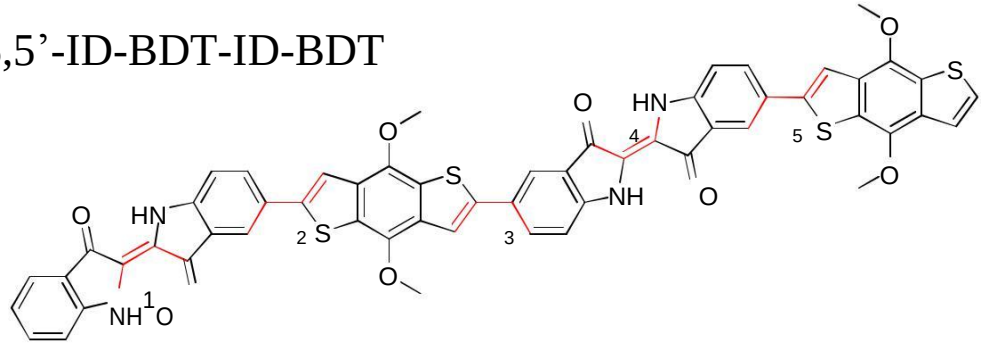
The route used for all calculations was the following:

opt=tight freq b3lyp/6-31g(d) guess=save geom=connectivity int=ultrafine

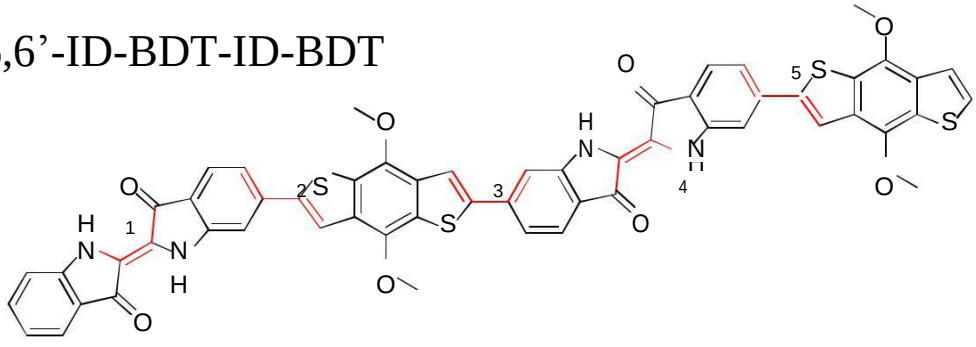
The obtained key dihedral angles of two model compounds, 5,5'-ID-BDT-ID-BDT and 6,6'-ID-BDT-ID-BDT are summarized in Table S1.

Table S1. Summary of computer simulation results of model compounds, 5,5'-ID-BDT-ID-BDT and 6,6'-ID-BDT-ID-BDT.

5,5'-ID-BDT-ID-BDT



6,6'-ID-BDT-ID-BDT



Model compound	Dihedral angle ( )				
	1	2	3	4	5
5,5'-ID-BDT-ID-BDT	0	24.8	26.4	0	24.8
6,6'-ID-BDT-ID-BDT	0	25.5	25.6	0	25.3

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2. Additional data

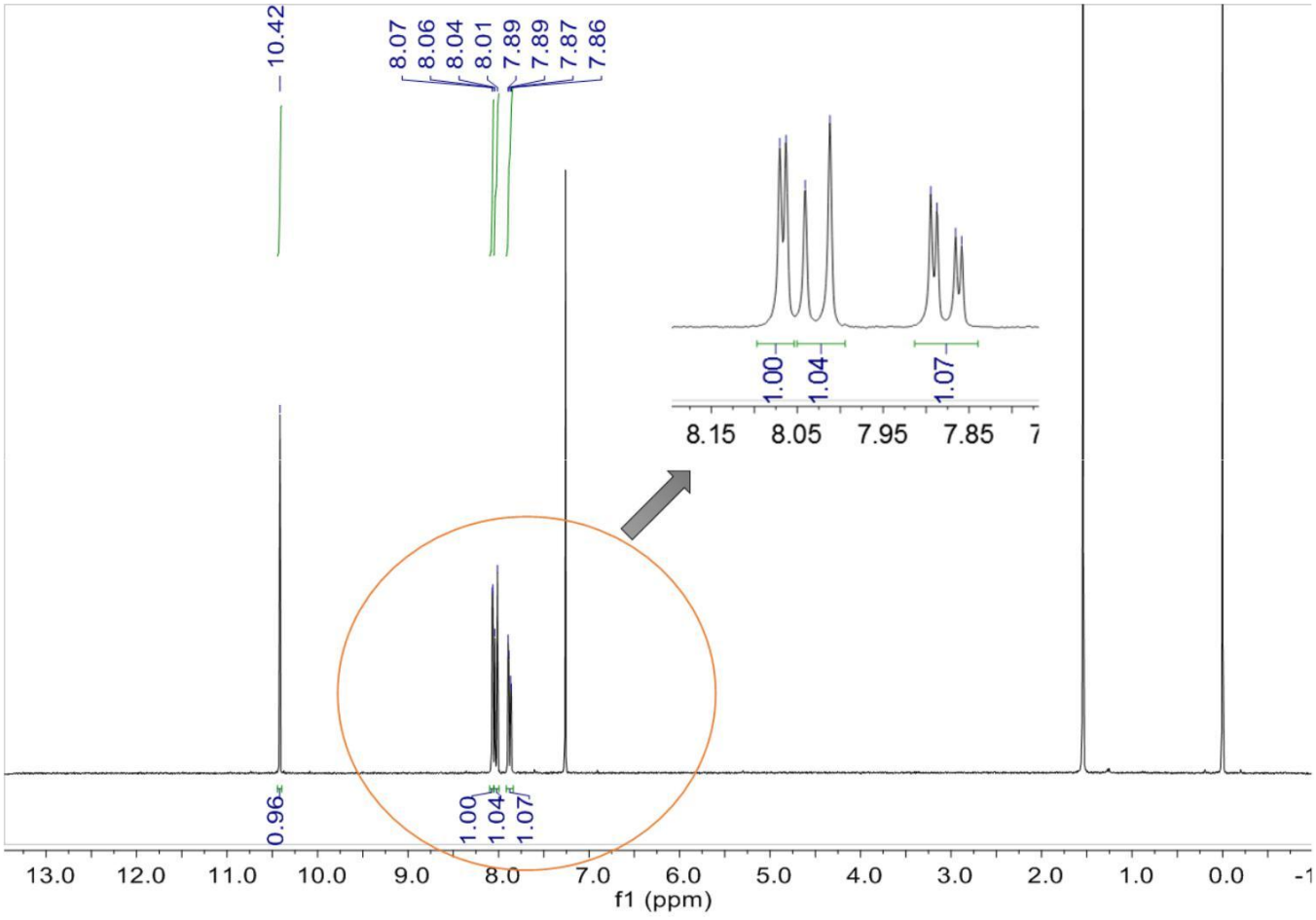

Figure S1. The 300 MHz ^{1}H NMR spectrum of 5-bromo-2-nitrobenzaldehyde (**1**) measured in $CDCl_3$.

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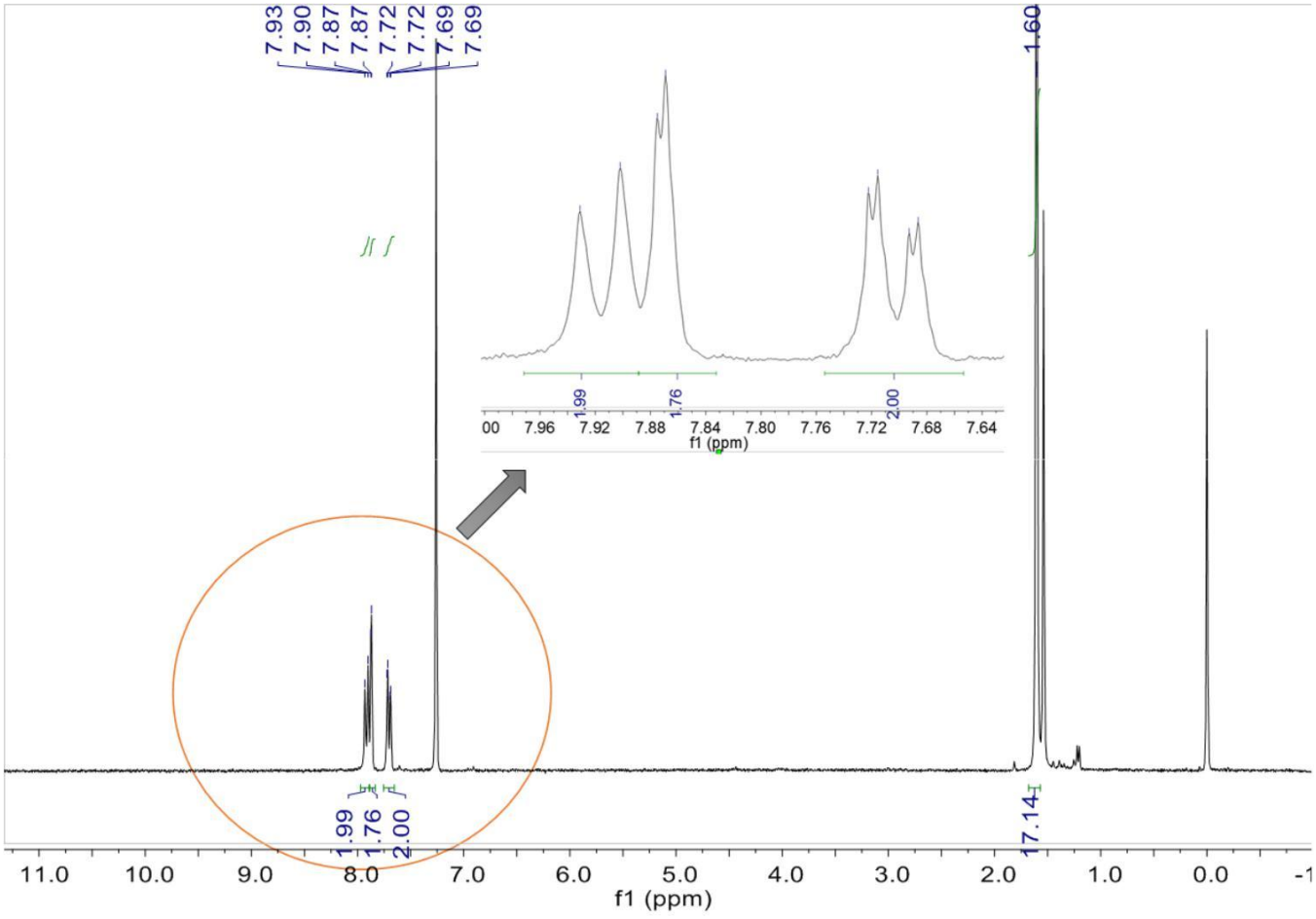

Figure S2. The 300 MHz ^{1}H NMR spectrum of di-*tert*-butyl 5,5'-dibromo-3,3'-dioxo-[2,2'-biindolinylidene]-1,1'-dicarboxylate (**3**) measured in $CDCl_3$.

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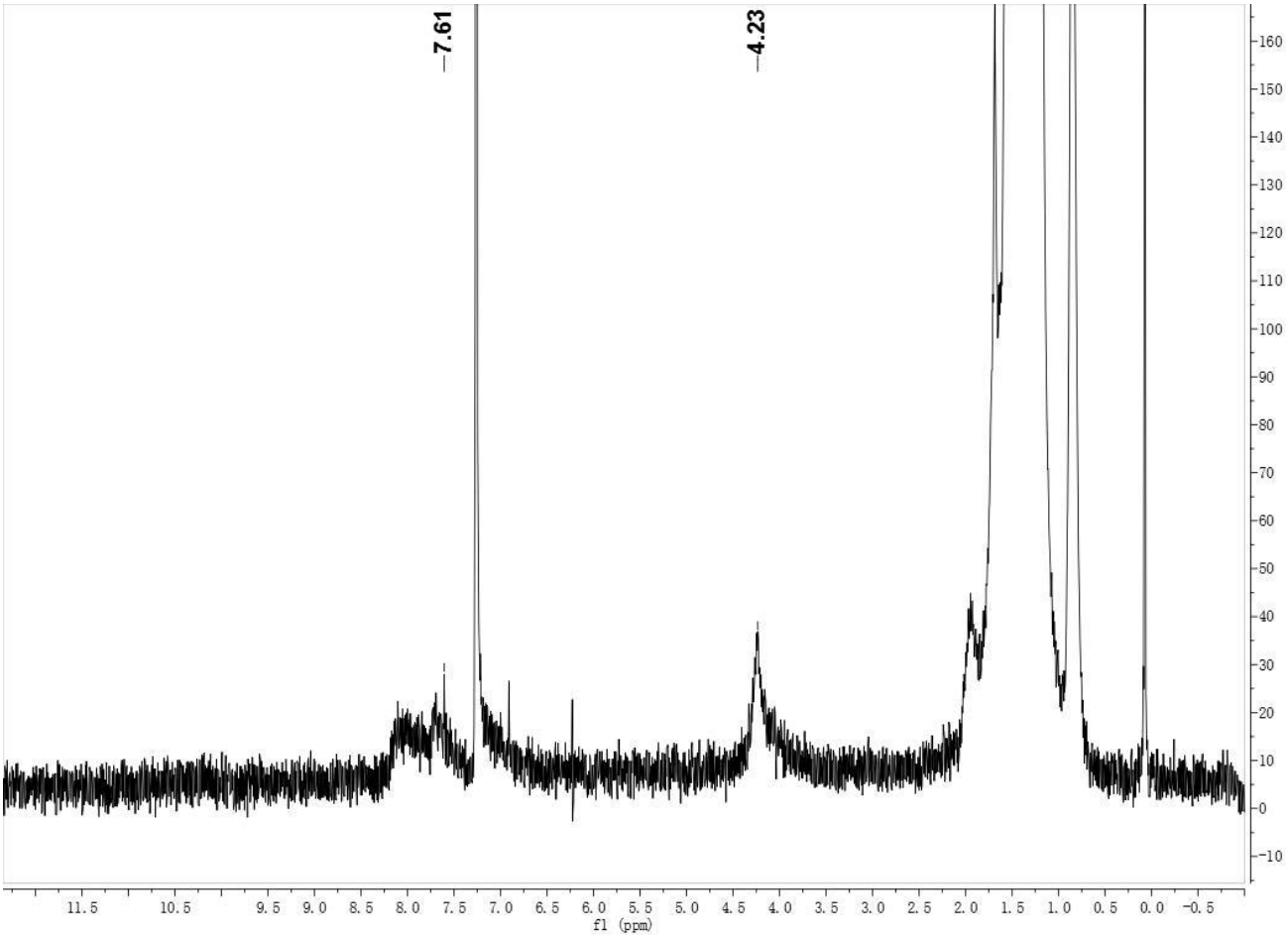

Figure S3. The 300 MHz ^{1}H NMR spectrum of **5,5'-PIDBDT** measured in $CDCl_3$.

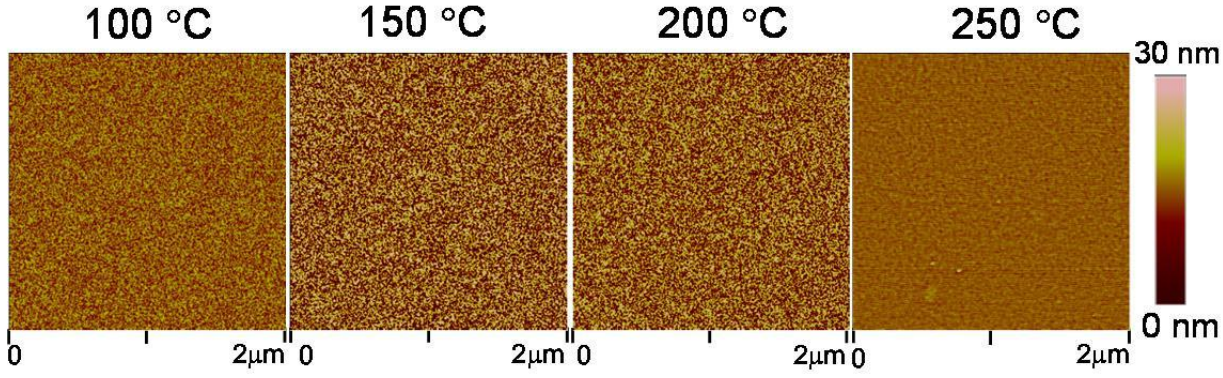

Figure S4. AFM images (2 μm × 2 μm) of polymer thin films on SiO_2/Si substrates annealed at 100 C, 150 C, 200 C and 250 C.

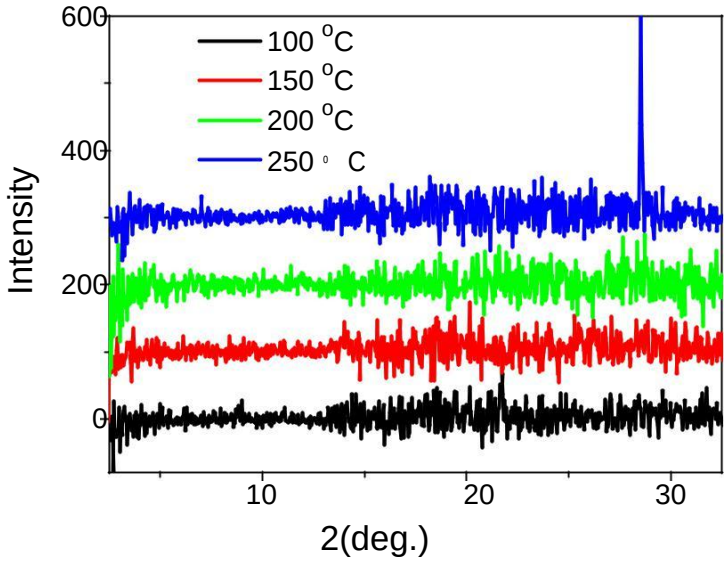

Figure S5. XRD diagrams obtained from spin-coating polymer thin film on SiO_2/Si substrates annealed at 100 C, 150 C, 200 C and 250 C. Note: The peak at 2 = ~28 ° for the 250 C-annealed sample is the (111) peak of the Si substrate.

3. References

1. (a) A. D. Becke, Phys. Rev. A, 1988, 38, 3098. (b) C. Lee, W. Yang and G. G. Parr, Phys. Rev. B, 1988, 37, 785.

2. (a) Æ. Frisch, Gaussian 09W Reference, Gaussian, Inc., Wallingford, CT, 2009. (b) Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.