

Electronic Supplementary Information

Dithieno[3,2-b:2',3'-d]silole-based low band gap polymers: the effect of fluorine and side chain substituents on photovoltaic performance

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1. X-ray Diffraction

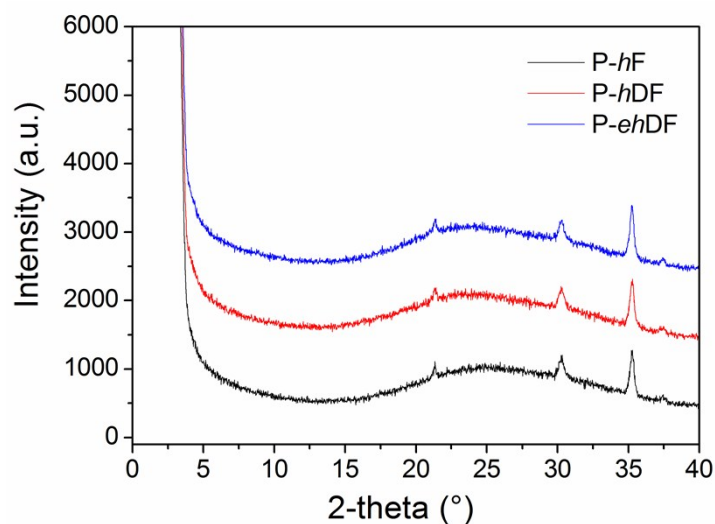


Fig. S1. Out-of-plane XRD patterns of **P-hF**, **P-hDF** and **P-ehDF**. Curves are offset for clarity.

2. TGA and DSC

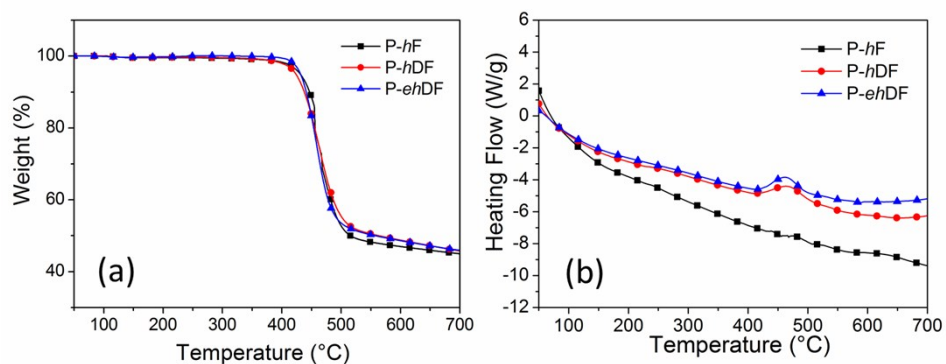


Fig. S2 TGA (a) and DSC (b) curves of the polymers with a heating rate of $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen atmosphere.

3. Computational Study

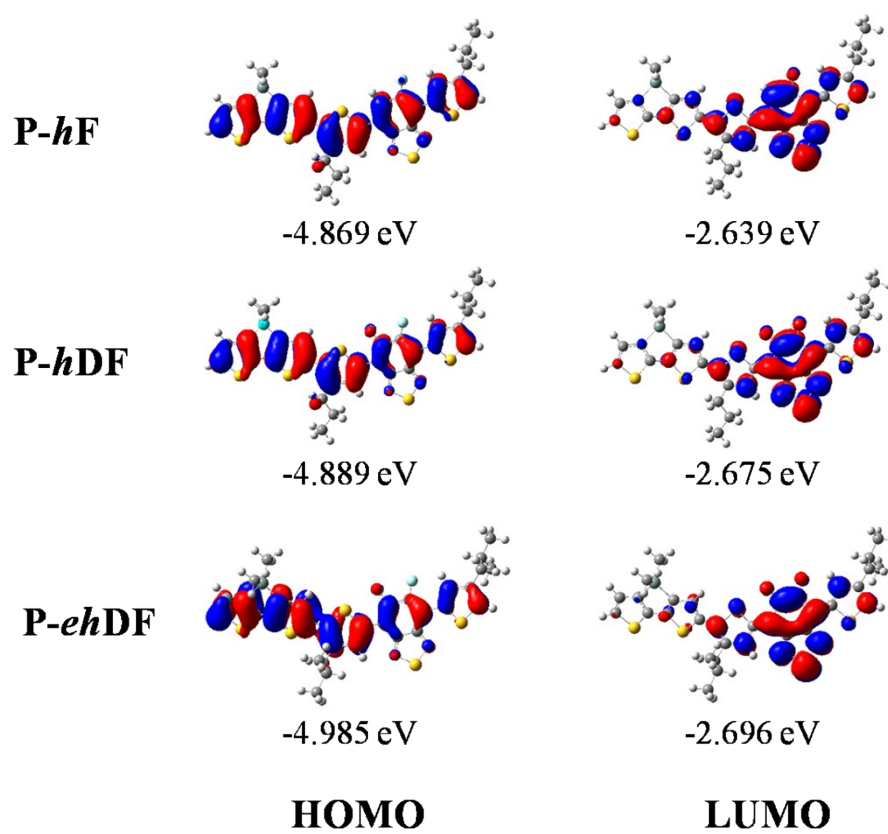


Fig. S3. The energies and distributions of the frontier molecular orbitals of the polymers¹.

4. Detailed device parameters of PSCs

Table S1. PSCs performance with device configuration
ITO/PEDOT:PSS/polymer:PC₇₁BM/Ca/Al

Active layer	ratio	DIO (%)	V_{OC} (V)	J_{SC} (mA cm ⁻²)	FF (%)	PCE (%)
P-hF :PC ₇₁ BM	1:1	0	0.620	14.04	53.5	4.66
	1:1	0.5	0.553	15.51	58.8	5.04
	1:1	1	0.546	15.52	58.6	4.97
	1:1	2	0.543	15.91	55.8	4.82
	1:1.5	0.5	0.551	14.35	59.1	4.67
	1.5:1	0.5	0.594	10.87	44.4	2.87
P-hDF :PC ₇₁ BM	1:1	0	0.683	10.90	64.0	4.76
	1:1	0.5	0.623	12.57	64.2	5.03
	1:1	1	0.593	15.98	64.8	6.14
	1:1	2	0.602	14.67	66.9	5.91
	1:1.5	1	0.605	11.24	62.5	4.25
	1.5:1	1	0.623	12.28	62.5	4.78
P-ehDF :PC ₇₁ BM	1:2	0	0.805	8.01	62.6	4.03
	1:2	1	0.753	4.72	56.2	2.00
	1:2	2	0.749	5.11	52.4	2.01
	1:1	0	0.827	6.05	54.3	2.72
	1:1.5	0	0.811	7.40	59.5	3.57
	1:3	0	0.753	8.81	44.8	2.97

5. Hole mobility

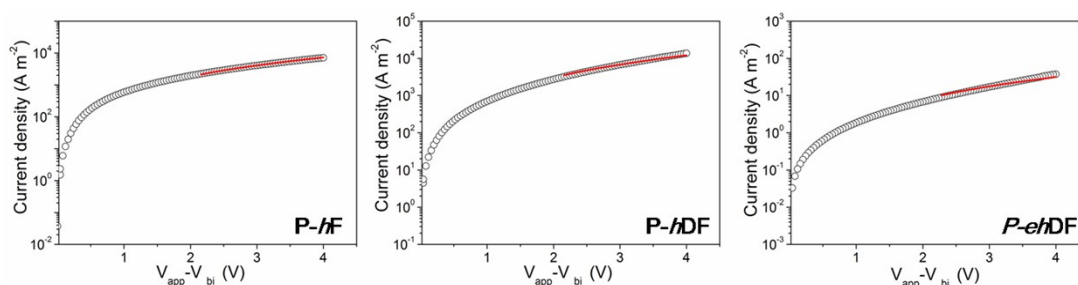


Fig. S4. Current density–voltage (J - V) curves for polymer:PC₇₁BM based device (the symbols are experimental data for transport of hole, and the red line is fitted according to the space-charge-limited-current model). The devices were constructed as ITO/PEDOT:PSS (40 nm)/polymer:PC₇₁BM (110 nm)/MoO₃ (10 nm)/Al (100 nm).

References:

1. 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, 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 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.