Supporting information for

Synthesis and Photovoltaic Performance of Donor–Acceptor Copolymers Based on Thieno[3,2-b]quinoxaline

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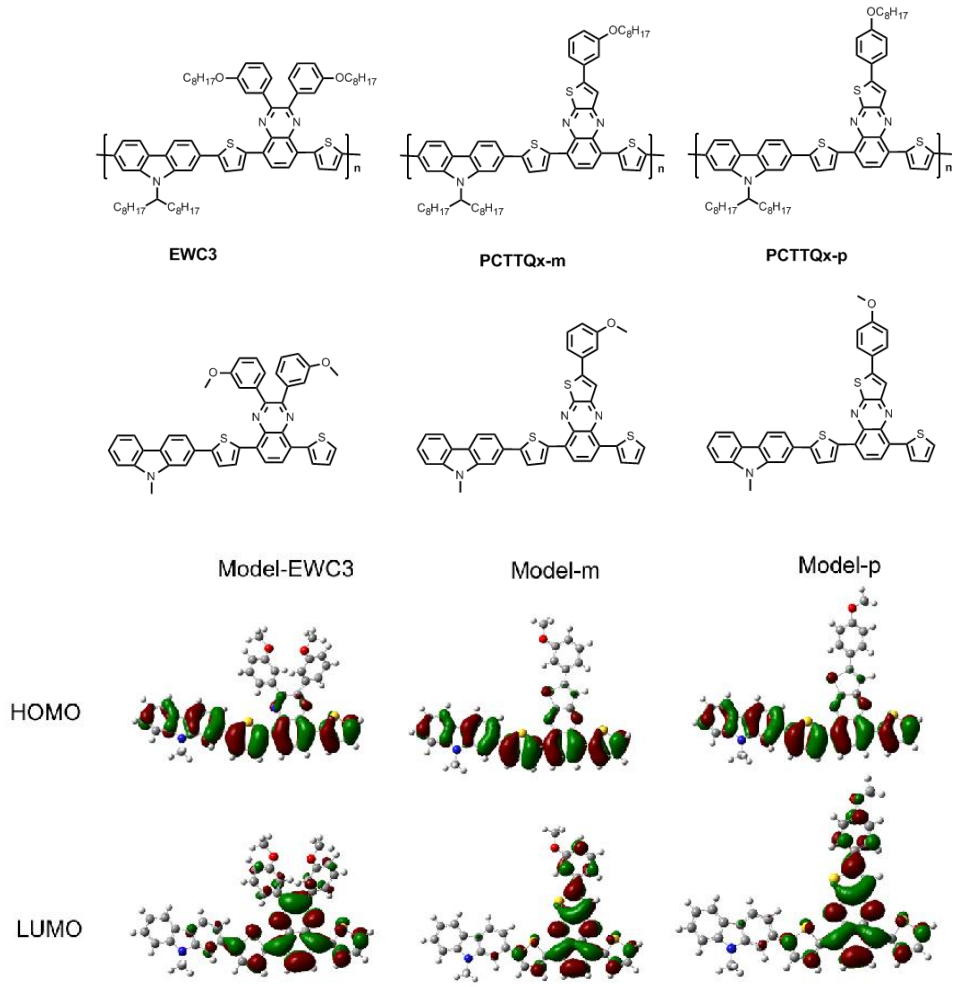

Fig. S1. HOMO and LUMO surface plots for model compounds of EWC3,[1] PCTTQx-m and PCTTQx-p.

Table S1 Calculated HOMO and LUMO energy levels for Model-EWC3, Model -m and Model -p.

	HOMO(eV)	LUMO(eV)	E_g(eV)
Model-EWC3	-4.85	-2.16	2.69
Model-m	-4.86	-2.39	2.47
Model-p	-4.84	-2.35	2.49

Molecular geometries of model compounds of EWC3, PCTTQx-m and PCTTQx-p were optimized using density functional theory at B3LYP/6-31G(d) level.[2] To simplify the calculation, the alkoxy groups of phenazine are replaced by methoxy groups and alkyl groups on carbazole are replaced by methyl groups. As shown in **Fig. S1**, Their HOMO orbitals are delocalized along the conjugated backbones while their LUMO orbitals are mainly located on the quinoxaline derivates unit. The calculated HOMO energy levels for Model-EWC3, Model-m and Model-p are very close, while the calculated E_g of Model-m and Model-p are clearly lower than that of Model-EWC3.

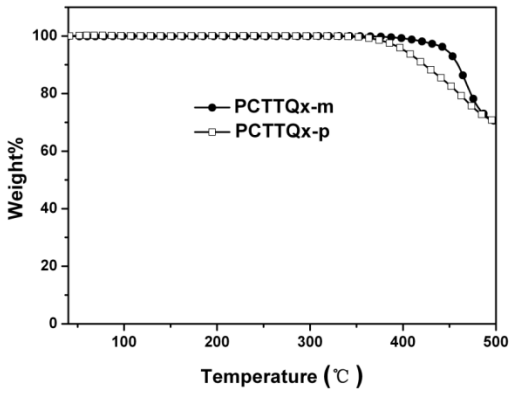

Fig. S2. TGA curves of copolymers with a heating rate of 10 ^{o}C min^{-1} in N_2.

Reference:

1. E. Wang, L. Hou, Z. Wang, Z. Ma, S. Hellström, W. Zhuang, F. Zhang, O. Inganäs and M. R. Andersson, *Macromolecules*, 2011, **44**, 2067-2073.
2. Gaussian 03, Revision B.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.