Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Organic Cocrystal based on Phthalocyanine with Ideal Packing Mode towards High-Performance Ambipolar Property

Shuyu Li†[a], Lei Zheng†[b], Yion Chan[c], Bin Li[b], Yajing Sun[b], Lingjie Sun[b,d], Chun Zhen[b], Xiaotao Zhang*[a], Wenping Hu[b,d]

[a] *Institute of Molecular Aggregation Science of Tianjin University, Tianjin 300072, China*

[b] *Tianjin Key Laboratory of Molecular Optoelectronic Sciences, Department of Chemistry, School of Science, Tianjin University, Tianjin 300072, China*

[c] *2608, No. 23, Guangqu Road, Chaoyang District, Beijing, China*

[d] *Joint School of National University of Singapore and Tianjin University, International Campus of Tianjin University, Fuzhou 350207, China*

[*] Corresponding Authors: zhangxt@tju.edu.cn

Supplemental Figures

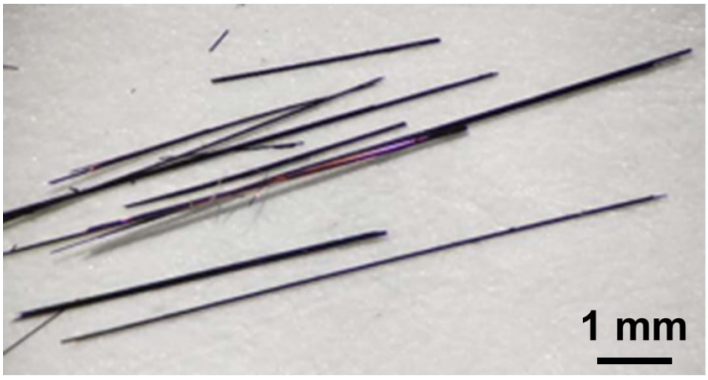

Fig. S1 Large crystal photo of ZnPc–F_{16}CuPc cocrystal.

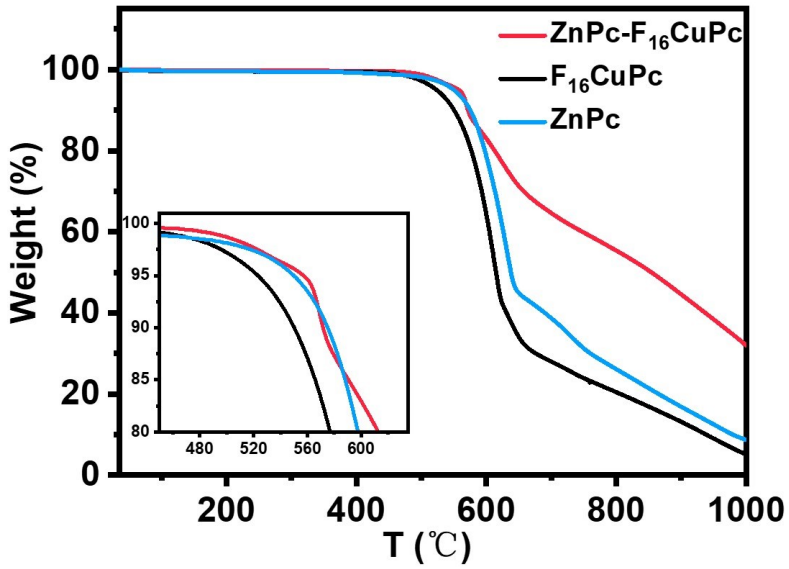

Fig. S2 TGA spectra of ZnPC, F_{16}CuPc and ZnPc–F_{16}CuPc.

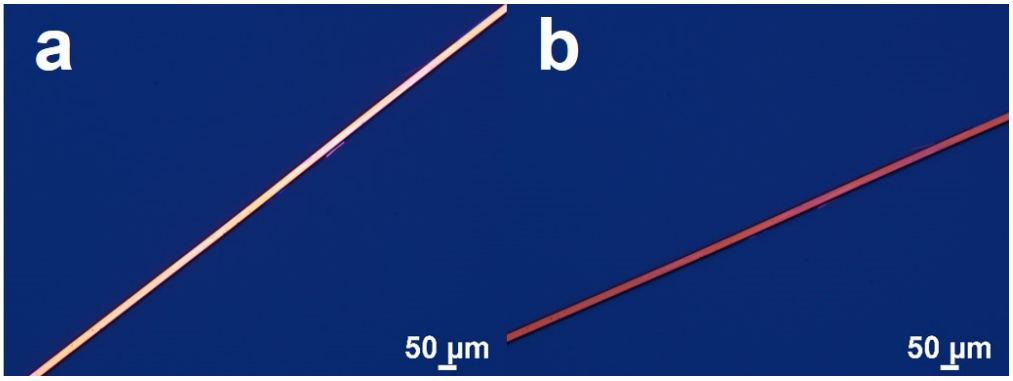

Fig. S3 Polarized optical microscope images of ZnPc–F_{16}CuPc cocrystal on the Si substrate with angles: (a) 0°, (b) 20°

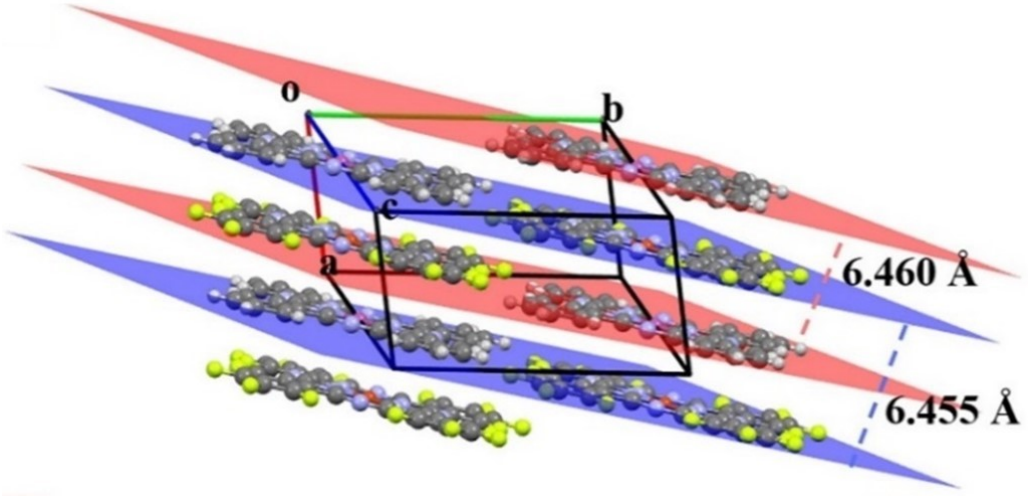

Fig. S4 The distance in ZnPc–F_{16}CuPc cocrystal.

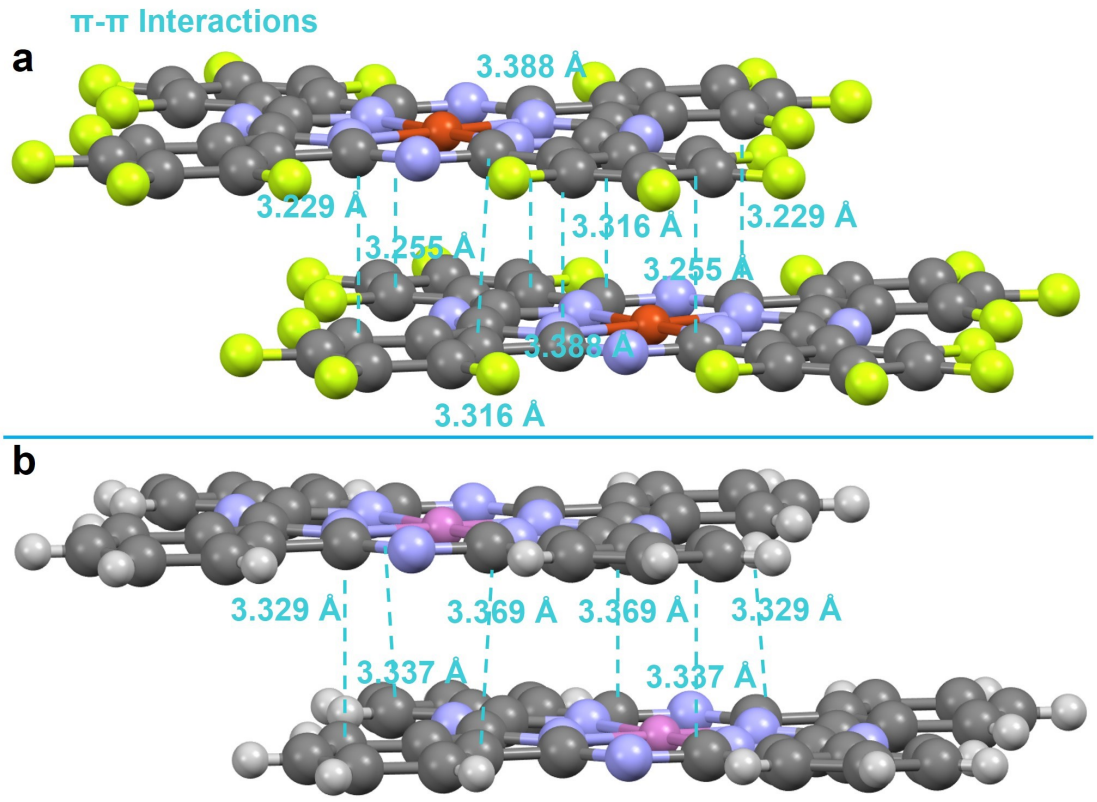

Fig. S5 The π-π interactions in (a) F_{16}CuPc and (b) ZnPc.

Fig. S6 Photo images of the typical bending configurations of a ZnPc–F_{16}CuPc needlelike cocrystal.

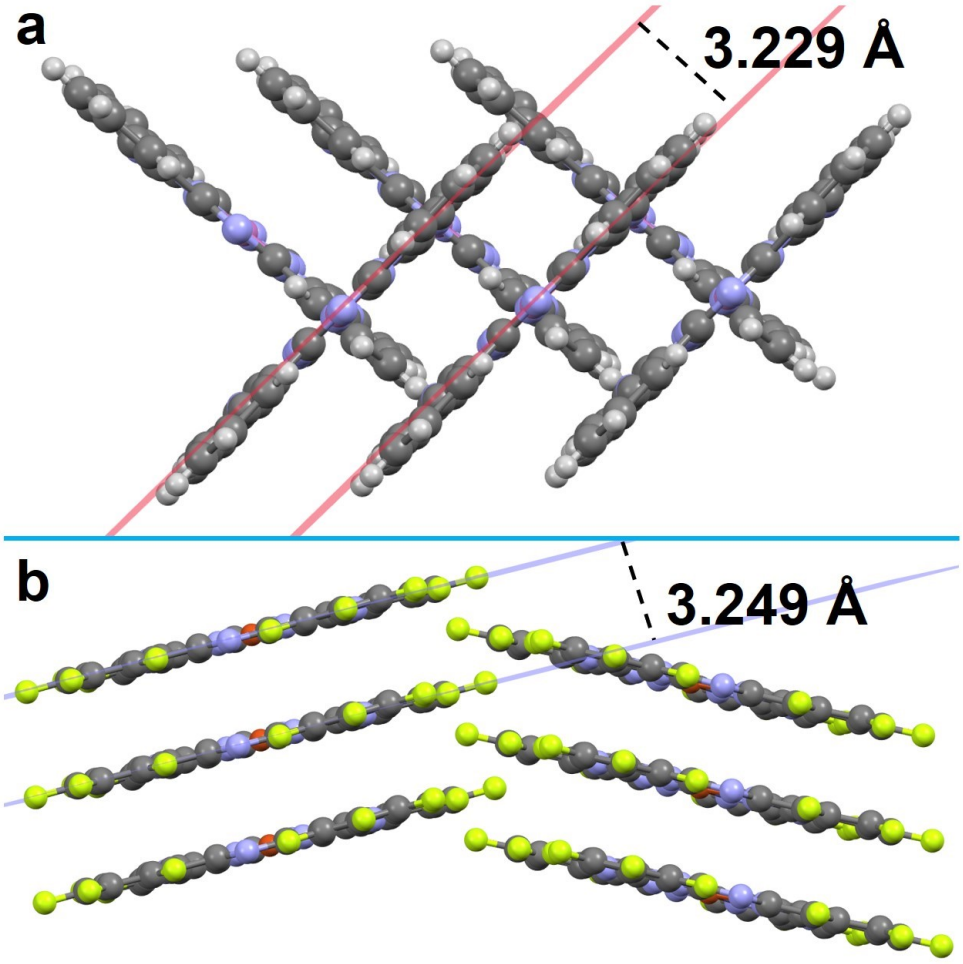

Fig. S7 The distance between (a) ZnPc molecules in ZnPc single crystal and (b) F_{16}CuPc molecules in F_{16}CuPc single crystal.

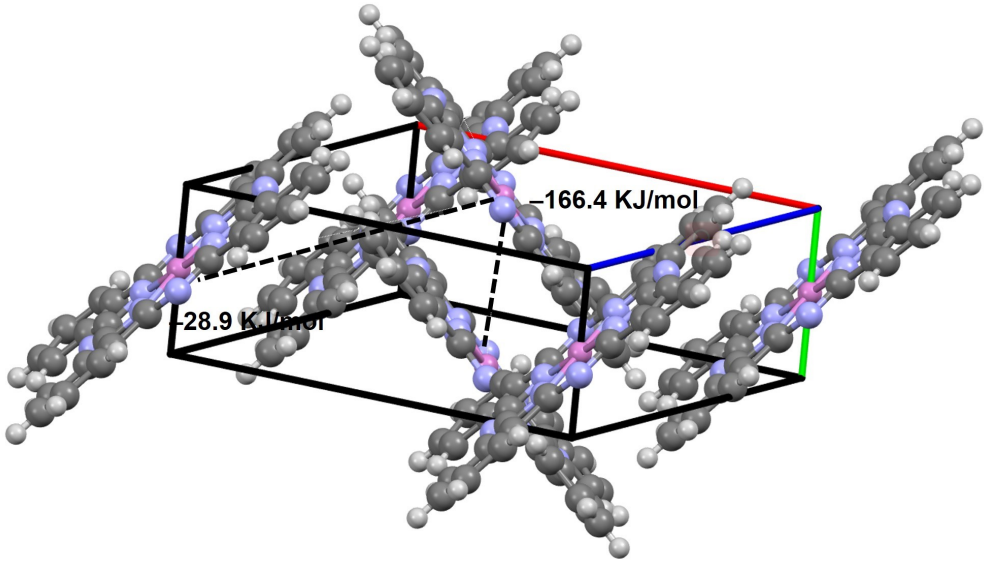

Fig. S8 The intermolecular potential energy of ZnPc.

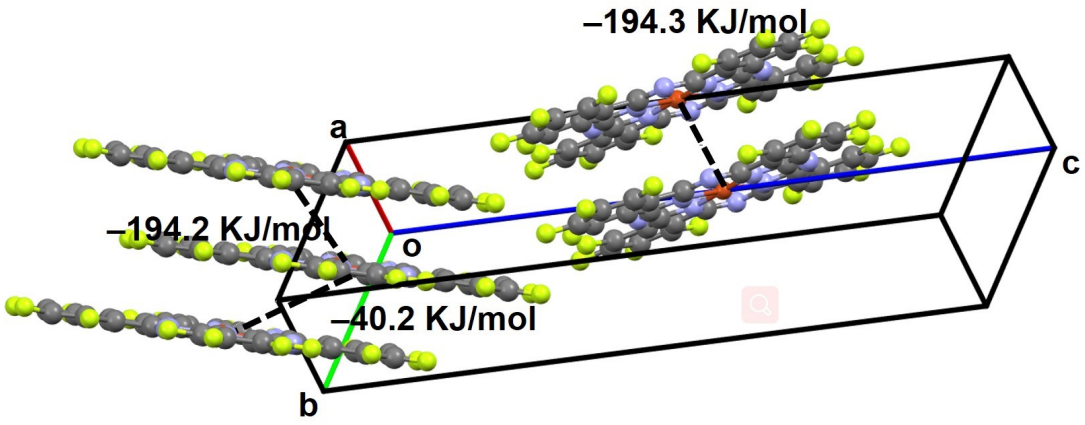

Fig. S9 The intermolecular potential energy of F_{16}CuPc.

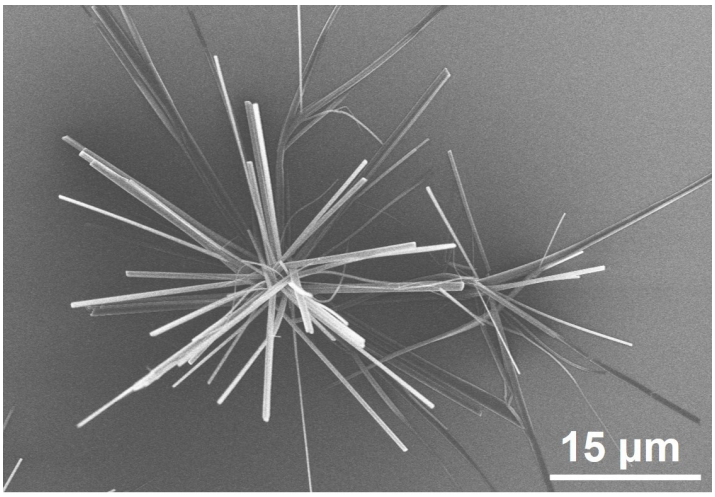

Fig. S10 The SEM image of ZnPc–F_{16}CuPc nanobelts in-situ growing onto the Si/SiO_2 substrates.

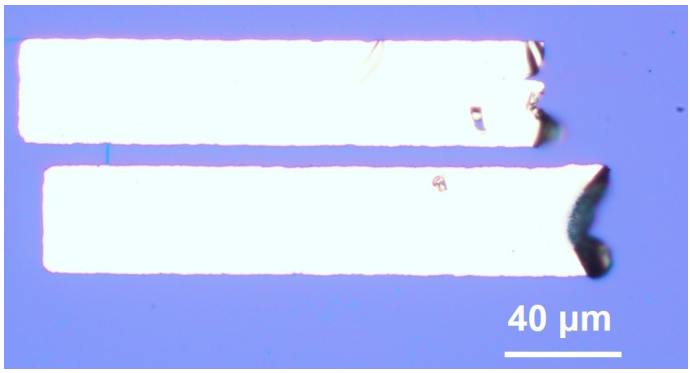

Fig. S11 Optical microscopy image of ZnPc–F_{16}CuPc nanobelt FET.

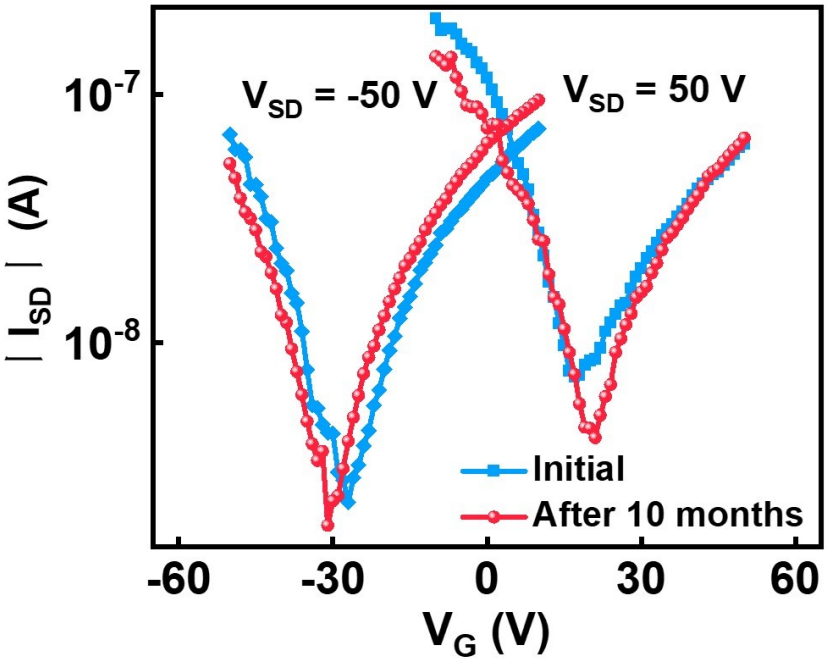

Fig. S12 The stability of the ZnPc–F_{16}CuPc cocrystal OFET after ten months of storage in air.

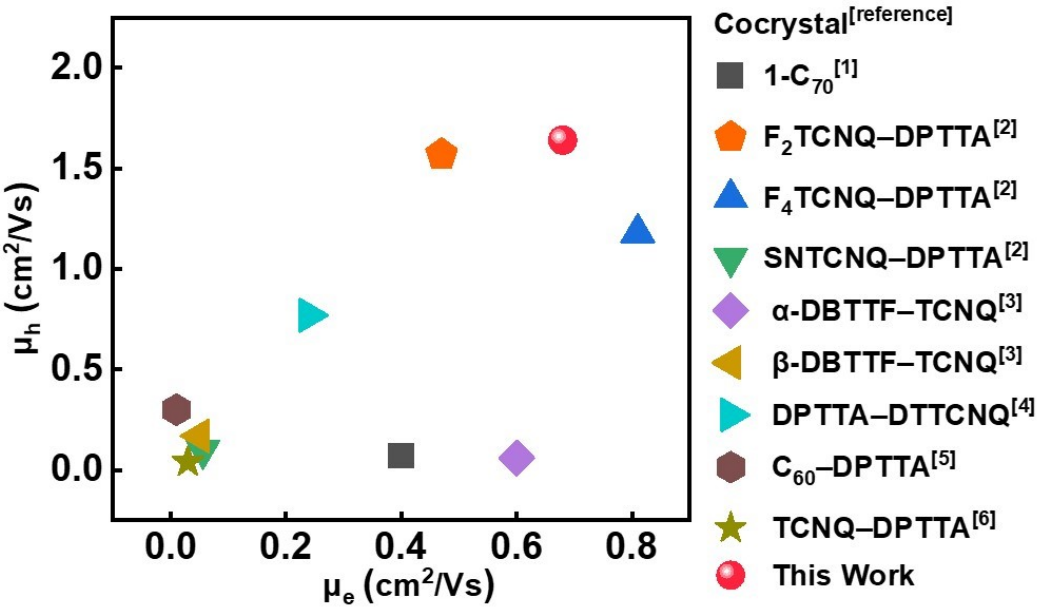

Fig. S13 Comparison of mobility based on ambipolar cocrystals with high-performance transport property for electron and hole in air.

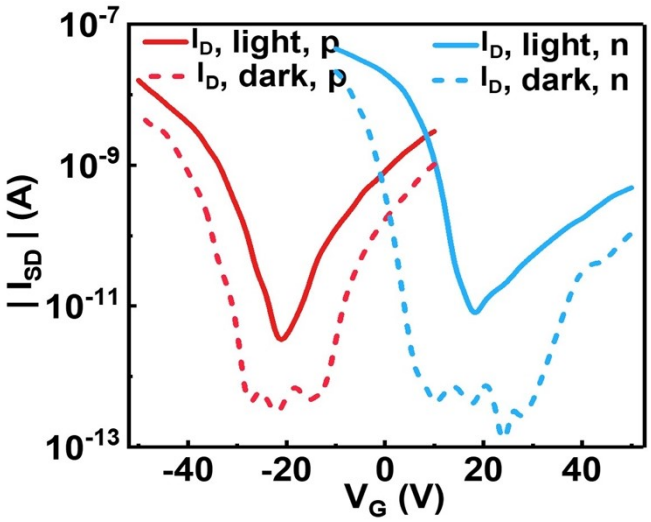

Fig. S14 The saturated transfer curves of the ZnPc–F_{16}CuPc cocrystal phototransistor operated in n-and p-channel under dark condition and 900 nm excitation pulse (160 μW cm^{-2} illumination intensity). The channel area (W×L) is 0.37 um × 17.5 um.

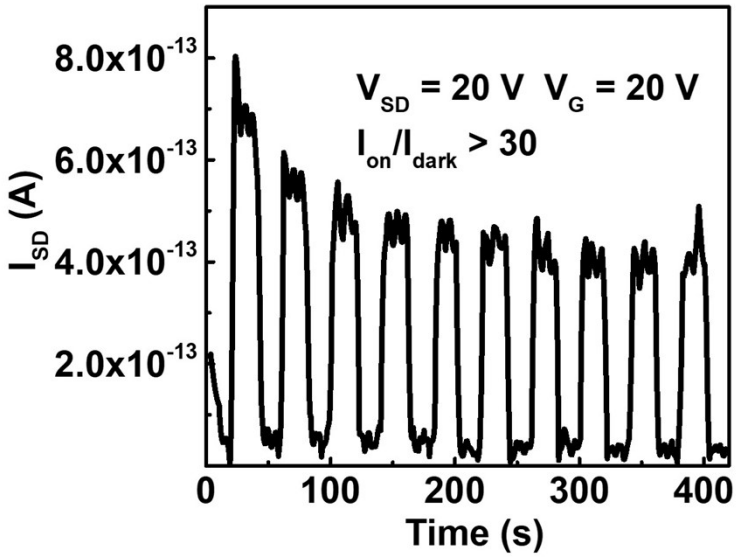

Fig. S15 Photoswitch of the cocrystal phototransistor under 900 nm excitation pulse (160 μW cm^{-2} illumination intensity).

Table S1 Single crystal structure of ZnPc–F_{16}CuPc cocrystal.

Empirical formula	C64 H16 F16 N16 Zn Cu
Formula weight	1441.84
Wavelength	1.54184 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a=7.2654(2) Å b=13.0351(3) Å c=13.6626(3) Å α= 85.043(2)° β= 89.559(2)° γ = 79.911(2)°.
Volume	1269.11 $Å^3$
Z	1
Density (calculated)	1.887 g cm^{-3}
μ	2.23 mm^{-1}
F(000)	715
Rint	0.0538
Goof	1.182
Final R indices [I>2sigma(I)]	R1=0.0708 wR2=0.2490
R indices (all date)	R1=0.0740 wR2=0.2466

Crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC): ZnPc–F_{16}CuPc (CCDC: 2039946)

References

1 G. Gao, M. Chen, J. Roberts, M. Feng, C. Xiao, G. Zhang, S. Parkin, C. Risko and L. Zhang, *J. Am. Chem. Soc.,* 2020, **142**, 2460–2470.

2 Y. Qin, C. Cheng, H. Geng, C. Wang, W. Hu, W. Xu, Z. Shuai and D. Zhu, *Phys. Chem. Chem. Phys.*, 2016, **18**, 14094–14103.

3 K. P. Goetz, J. Tsutsumi, S. Pookpanratana, J. Chen, N. S. Corbin, R. K. Behera, V. Coropceanu, C. A. Richter, C. A. Hacker, T. Hasegawa and O. D. Jurchescu, *Adv. Electron. Mater.,* 2016, **2**, 1600203.

4 Y. Qin, J. Zhang, X. Zheng, H. Geng, G. Zhao, W. Xu, W. Hu, Z. Shuai and D. Zhu, *Adv. Mater.,* 2014, **26**, 4093–4099.

5 J. Zhang, J. Tan, Z. Ma, W. Xu, G. Zhao, H. Geng, C. Di, W. Hu, Z. Shuai, K. Singh and D. Zhu, *J. Am. Chem. Soc.,* 2013, **135**, 558–561.

6 J. Zhang, H. Geng, T. S. Virk, Y. Zhao, J. Tan, C. A. Di, W. Xu, K. Singh, W. Hu, Z. Shuai, Y. Liu and D. Zhu, *Adv. Mater.,* 2012, **24**, 2603–2607.