

Supporting

Optimization of the Thermoelectric Performance of Layer-by-Layer Structured Copper-Phthalocyanine (CuPc) Thin Films Doped with Hexacyano-Trimethylene-Cyclopropane (CN6-CP)

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Table. S1. A comparison of electrical conductivity of two different structure of devices, bilayer and multilayer.

The thick of each CuPc layer/nm	The thick of each CN6-CP layer/nm	Repeat times	The total thickness/nm	σ_{\max} (S/cm)
40	8	1	48	0.002
10	2	4	48	0.12
2	0.4	20	48	0.30

Table. S2. Comparing of the electrical conductivity of CuPc films doped by CN6-CP by layer-by-layer-evaporation with the substrates treated with five different self-assembled monolayers (SAM).

SAM	σ_{\max} (S/cm)
Bare	0.30
OTS (octadecyltrichlorosilane)	0.50
((1H,1H,2H,2H-Heptadecafluorodecyl)trichlorosilane)	0.35
Octadecylphosphonic acid	0.28
HexaMethyldisilazane	0.30
poly(amic acid)	0.25

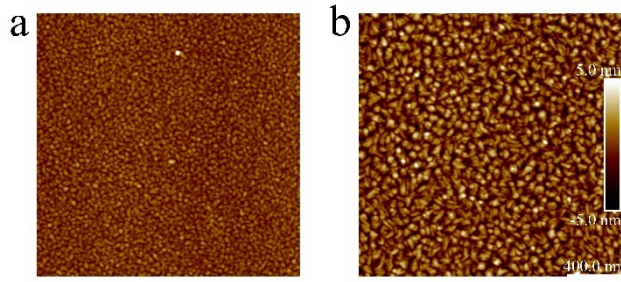


Fig. S1. The AFM images of pristine CuPc films on bare glass substrate and OTS-modified glass substrate. (a) glass substrate, (b) OTS-modified glass substrate.

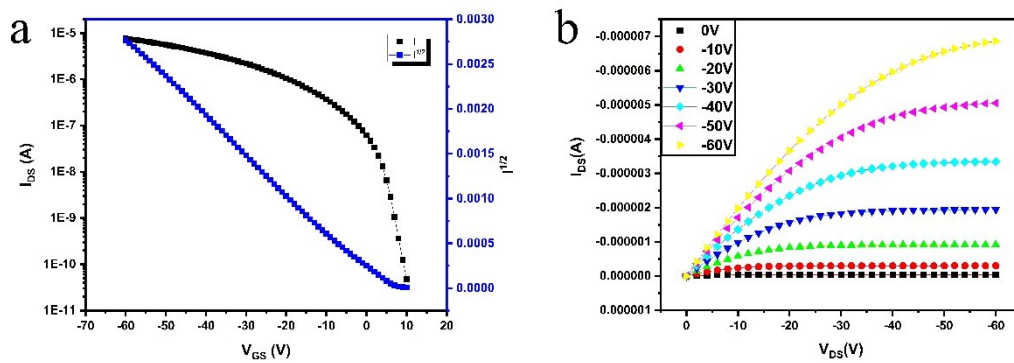


Fig. S2. The OFET performance of pristine CuPc films. (a) the transfer curves of 10nm CuPc (

$$I_{DS} = \frac{W}{2L} \mu C_i (V_{GS} - V_{th})^2$$

(c) the output curves of the same device.

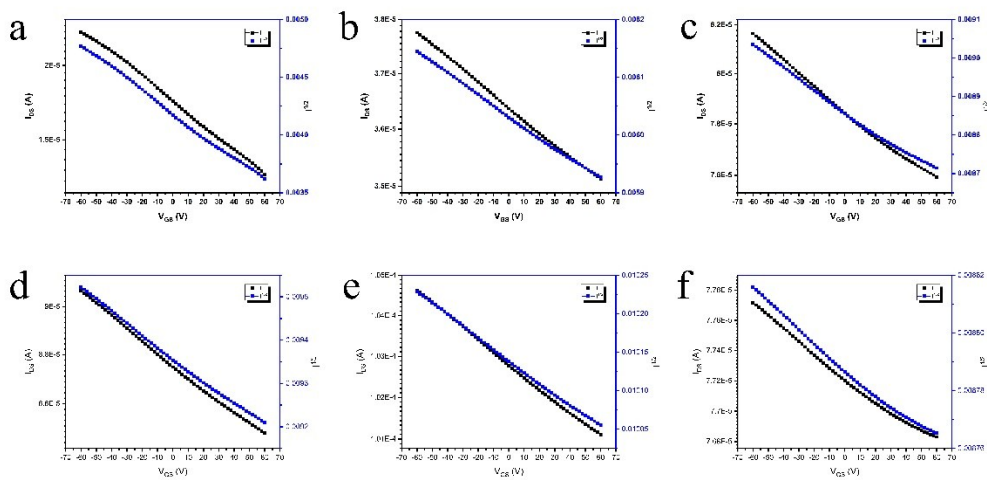


Fig. S3. The transfer curves of 10nm CuPc thin films with different doping concentration (

$I_{DS} = W/L\mu C_i(V_{GS} - V_{th})V_{DS}$. (a) MR= 14%, (b) MR=24%, (c) MR=27%, (d) MR=30%, (e) MR=34%, (f) MR=52%

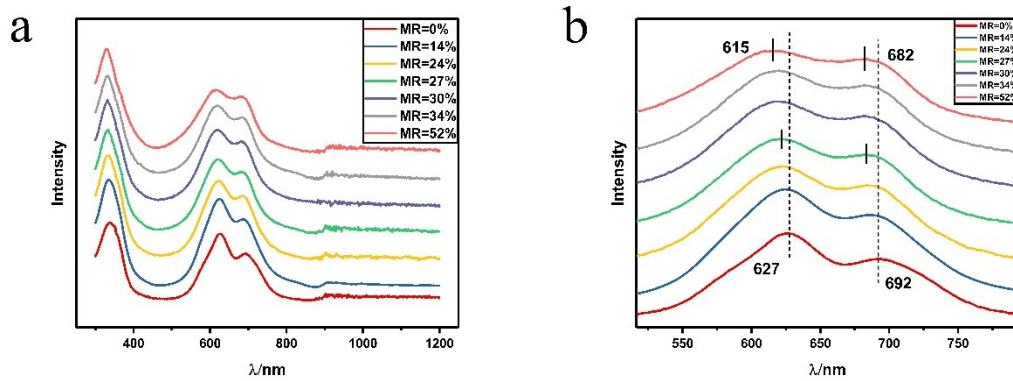


Fig. S4. UV-vis absorption of pristine and doped CuPc films in different molar ratios (a) 300-1200 nm; (b) 500-800 nm

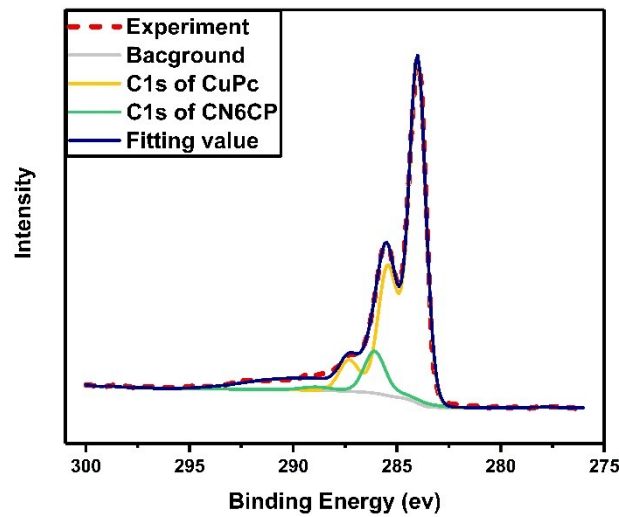


Fig. S5. The XPS spectra of C1s of CuPc/CN6-CP film. The red short dashed line represents the experimental data. The gray line represents the background. The yellow and green line represent the C1s of CuPc and CN6-CP respectively. The purple line represents the fitting curve.

Table. S3. The value of molar ratio, calculated from the Fig. S5.

Sample No.	1	2	3	4	5	6	7
Monolayer thickness of CN6-CP (T_D) (nm)	0	0.1	0.2	0.3	0.4	0.5	0.8
C1s of CuPc (%)	100	94.99	91.77	90.93	89.74	88.65	83.74
C1s of CN6-CP (%)	0	5.01	8.23	9.07	10.26	11.35	16.26
Molar ratio (MR) (%)	0	14	24	27	30	34	52

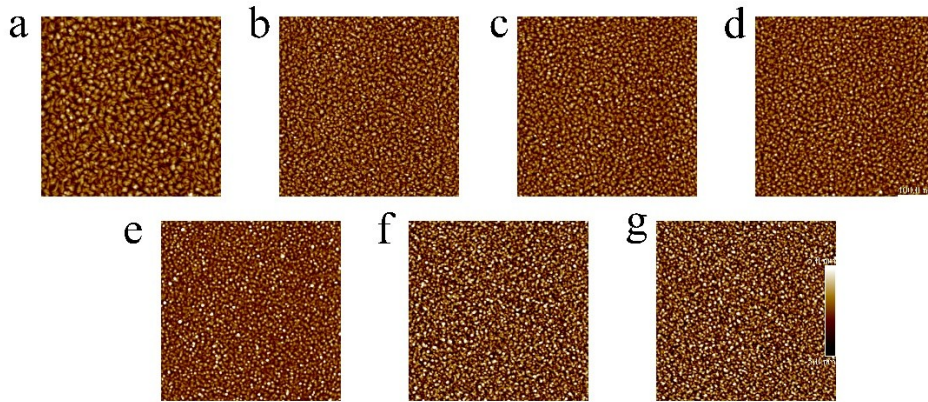


Fig. S6. The AFM images of CuPc films with different doping concentration deposited on OTS-modified substrate. (a) MR=0%, (b) MR= 14%, (c) MR=24%, (d) MR=27%, (e) MR=30%, (f) MR=34%, (g) MR=52%