

Supplementary Information

Dopant-Free Hole-Transporting Material Based on Poly(2,7-(9,9-bis(*N,N*-di-*p*-Methoxyphenylamine)-4-phenyl))Fluorene for High-Performance Air-processed Inverted Perovskite Solar Cells

Baomin Zhao ^{a,*}, Meng Tian ^a, Xingsheng Chu ^a, Peng Xu ^a, Jie Yao ^a, Pingping Hou ^b, Zhaoning Li ^a and Hongyan Huang ^{b,*}

^a State Key Laboratory for Organic Electronics and Information Displays & Jiangsu Key Laboratory for Biosensors, Institute of Advanced Materials (IAM), Nanjing University of Posts and Telecommunications, 9 Wenyuan Road, Nanjing 210023, Jiangsu, China

^b School of Electronic Information, Nanjing Vocational College of Information Technology, 99 Wenyuan Road, Nanjing 210023, Jiangsu, China
Technology, 99 Wenyuan Road, Nanjing 210023, Jiangsu, China

*Corresponding authors. E-mail addresses: provost@nwpu.edu.cn (W. Huang)

NMR and MALDI-ToF spectra

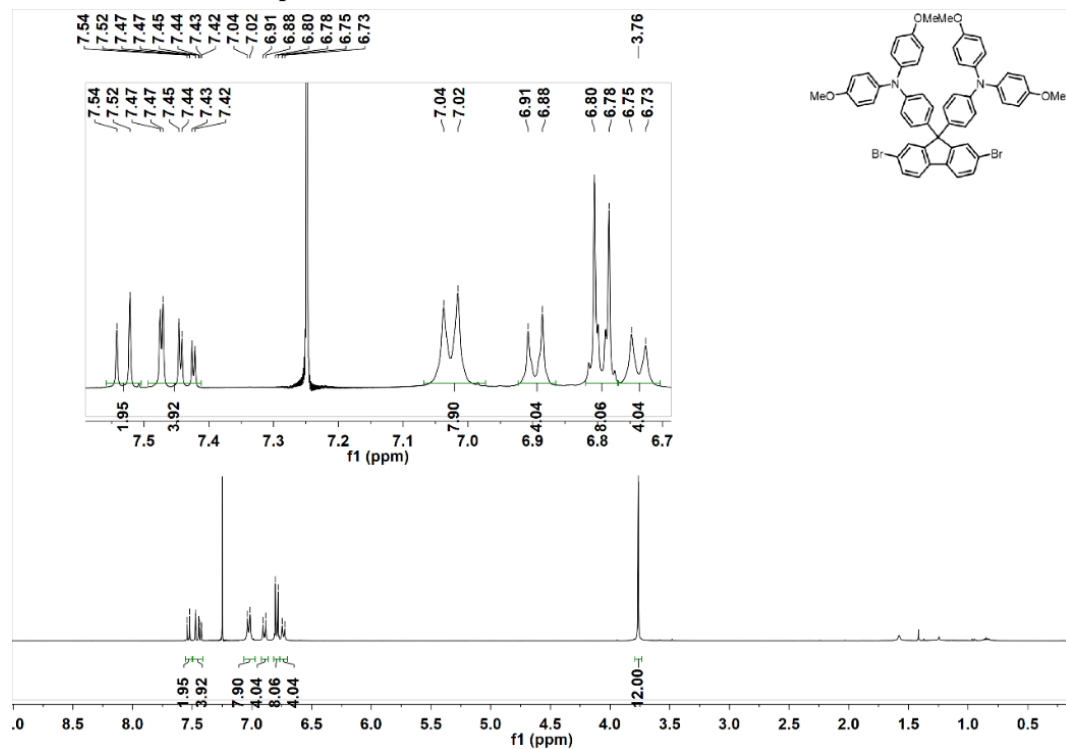


Figure S1 ¹H NMR spectrum of 2BrFTP in CDCl₃.

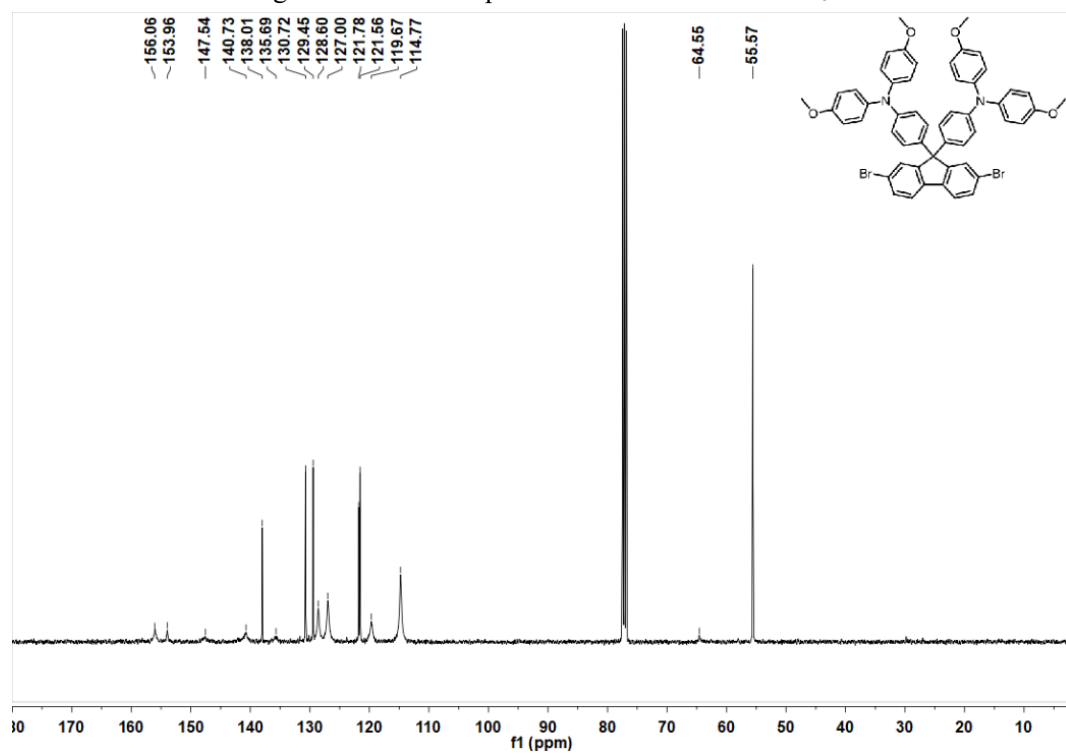


Figure S2 ¹³C NMR spectrum of 2BrFTP in CDCl₃.

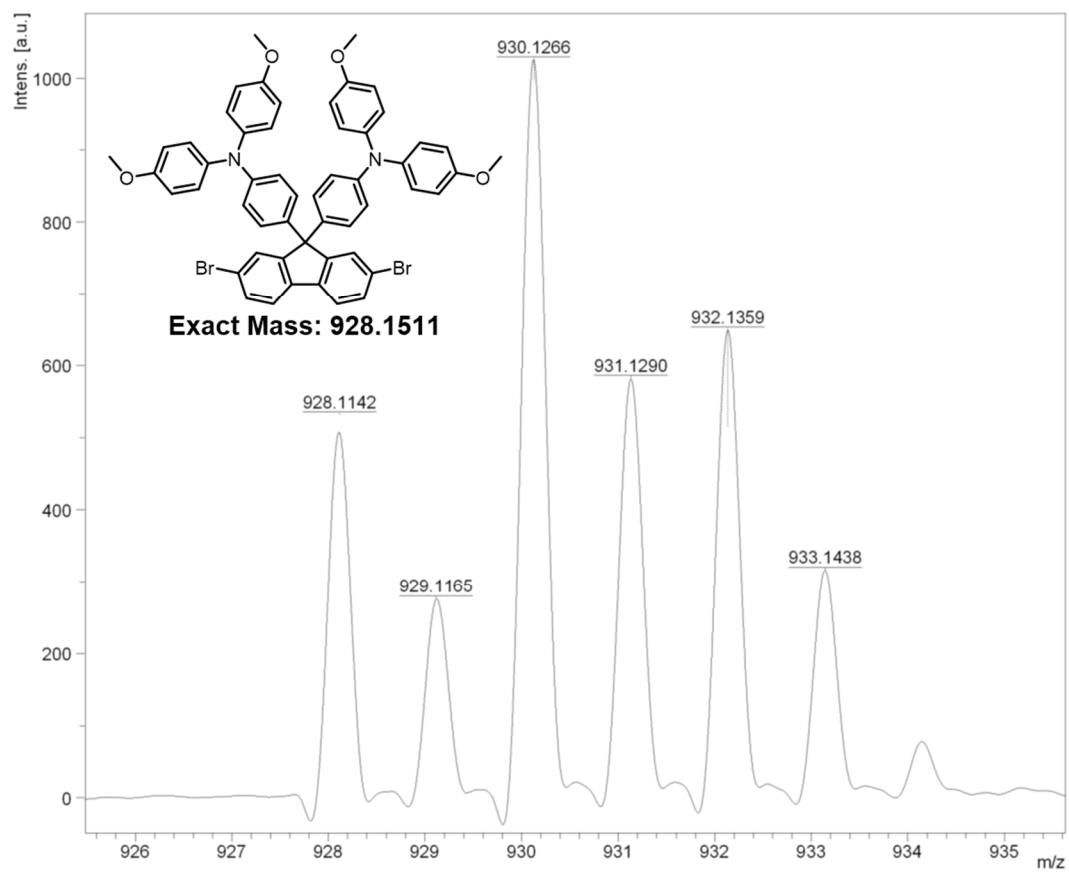


Figure S3 MALDI-TOF MS spectrum of 2BrFTP.

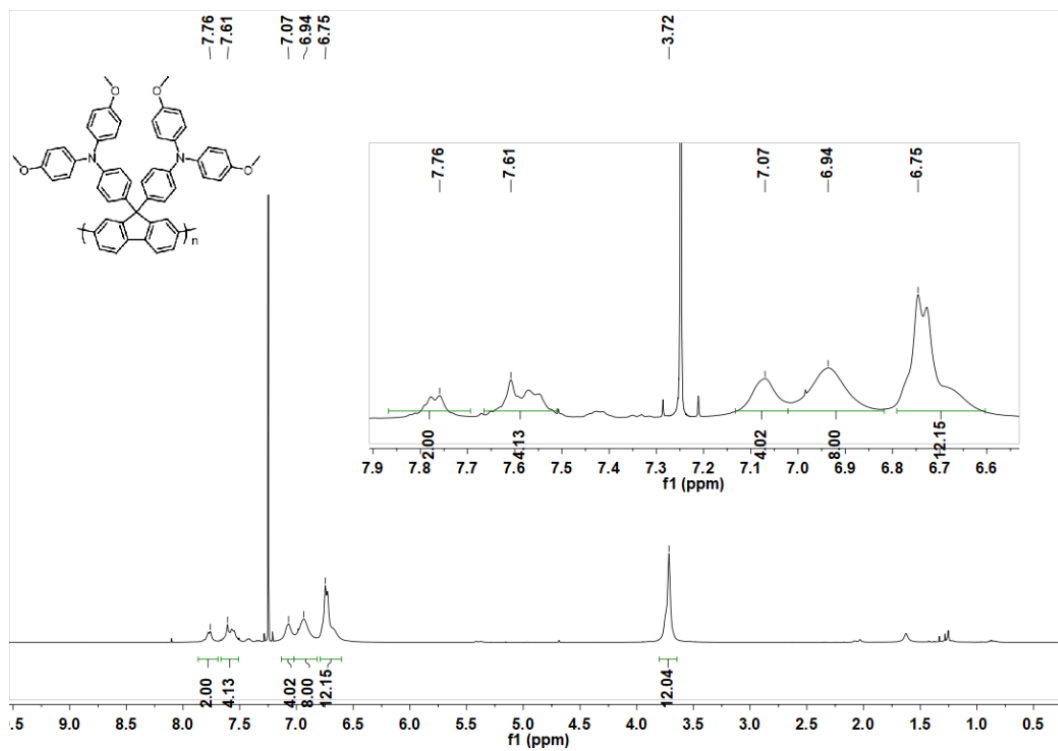


Figure S4 ^1H NMR spectrum of PFTP in CDCl_3 .

The cost of PFTPA in this study

Table S1 The synthetic cost analysis of PFTPA in this study.

	Reagent	Weight (g or L)	Price (\$/g or L) ^a	Cost (\$)	Cost (\$/g)
2BrFPA	4,4-dimethoxytriphenylamine	10.85	1.75	18.98	
	2,7-dibromo-9H-fluoren-9-one	1.5	0.36	0.54	
	Methylsulfonic acid	6.0	0.028	0.17	
	Dichloromethane	0.50	1.85	0.93	5.35
	Ethyl acetate	0.3	1.22	0.37	
	hexane	0.80	1.0	0.8	
	Na ₂ SO ₄	30	0.0035	0.105	
PFTPA	2BrFPA	0.37	5.35	1.98	
	bis-(1,5-cyclooctadiene) nickel	0.13	12.25	1.594	
	2,2-Bipyridine	0.076	0.39	0.03	
	1,5-cyclooctadiene	0.052	0.38	0.02	
	Bromobenzene	3.2	0.05	0.16	
	methanol	0.2	0.85	0.17	16.74
	HCl (3M)	0.1	0.3	0.03	
	Toluene	0.05	1.15	0.0575	
	chloroform	0.02	2.4	0.048	
	acetone	0.25	1.05	0.26	

^a The price information was obtained from Energy Chemical Technology (Shanghai) Co., Ltd and Shanghai Titan Scientific Co., Ltd.

DSC

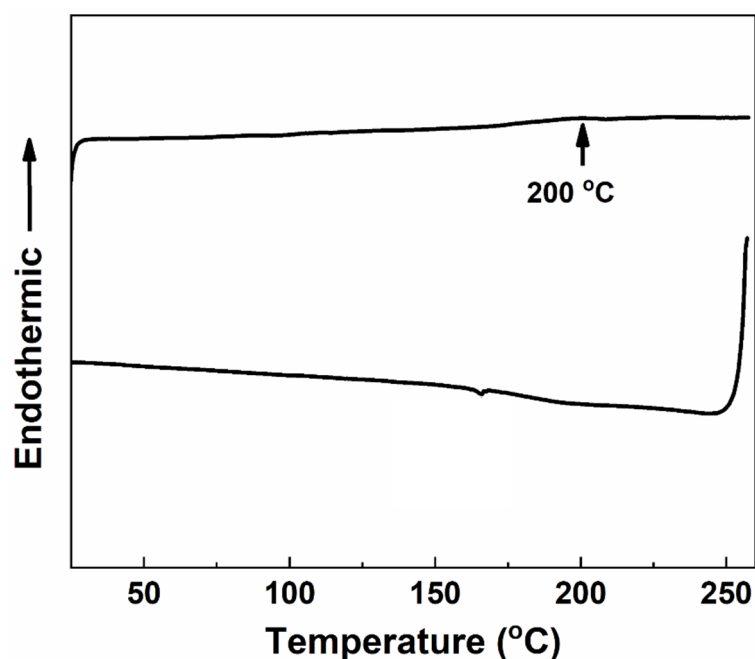


Figure S5 DSC curves of PFTPA recorded at a heating rate of 10 °C/min and a cooling rate of 20 °C/min.

CV curve for Ferrocene vs Ag/Ag⁺

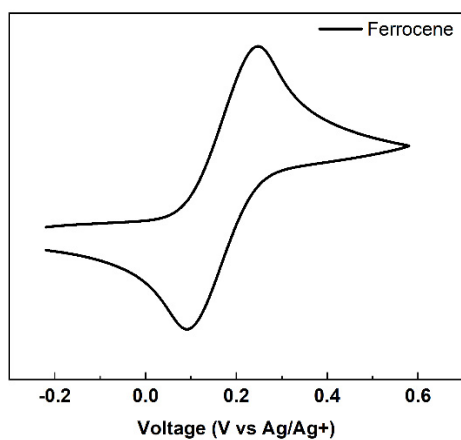


Figure S6 The cyclic voltammetry (CV) curve of Ferrocene measured with Ag/Ag⁺ as the reference electrode in acetonitrile.

DFT calculation

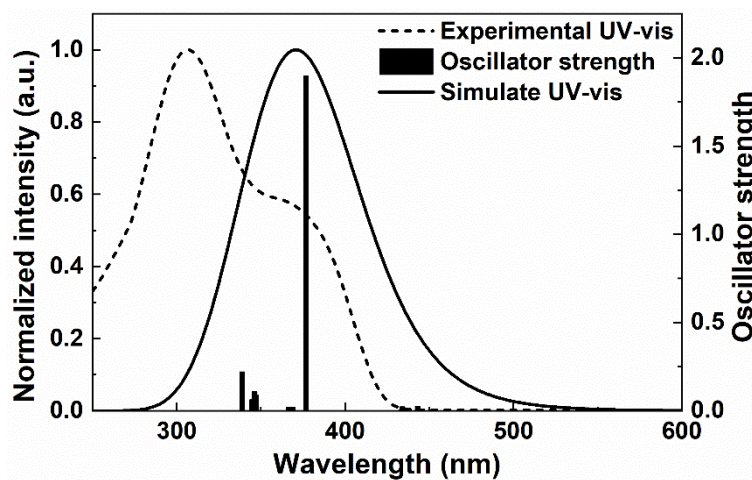


Figure S7 The overlay of TD-DFT simulation and experimental UV-vis spectra of PFTPA.

Table S2 The calculation results of TD-DFT

State	λ/nm	f	Major transitions	Character	$\lambda_{\text{exp}}/\text{nm}$
2	338	0.0270	H-3 \rightarrow L (49%)	$n\text{-}\pi^*$	310
			H-4 \rightarrow L (39%)		
5	376	0.0235	H-3 \rightarrow L (39%)	$\pi\text{-}\pi^*$	370
			H-4 \rightarrow L (37%)		

Device stability

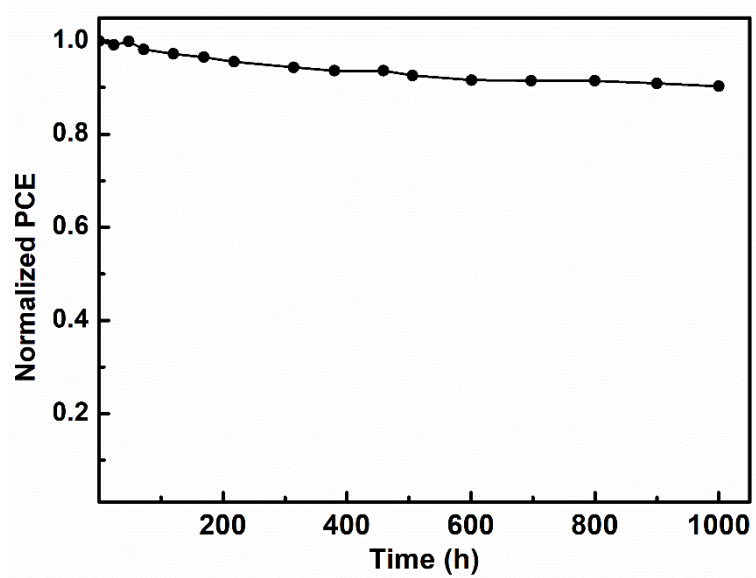


Figure S8 The longtime device stability of PFTPA-based PSC.

The contact angle between HTM and DMF.

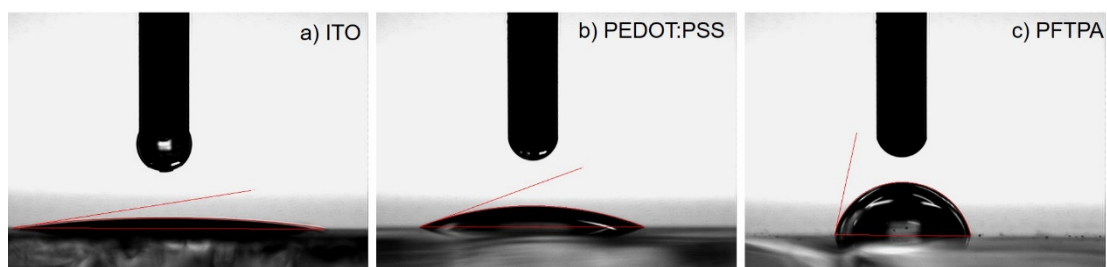


Figure S9. The measured contact angles of DMF a) on ITO substrate, b) on PEDOT:PSS substrate and on PFTPA substrate.

The perovskite crystal size distribution.

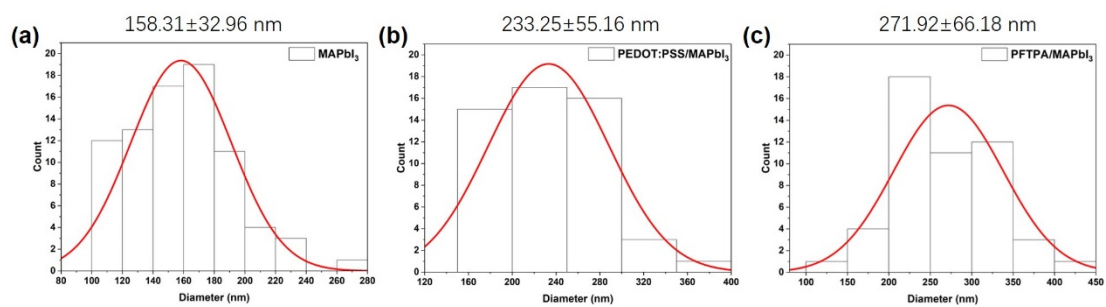


Figure S10. The perovskite crystal size distribution, a) MAPbI₃ @ bare ITO substrate, b) MAPbI₃@PEDOT:PSS/ITO substrate and c) MAPbI₃@PFTPA/ITO substrate, estimated according to the statistical data deduced from the SEM images shown in Figure 4.

AFM

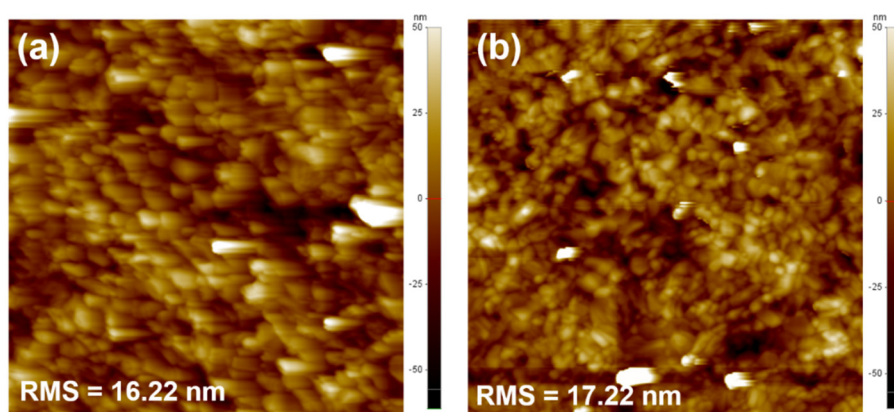


Figure S11. AFM height images (size: $5\ \mu\text{m} \times 5\ \mu\text{m}$) of perovskite on (a) PFTPA and (b) PEDOT:PSS substrates.

SCLC

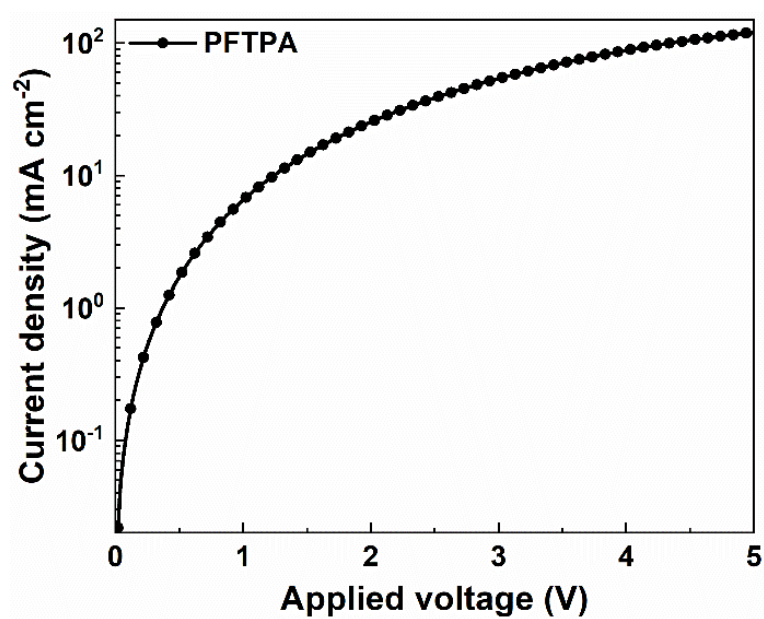


Figure S12. The J - V curve of hole-only device based on PFTP.

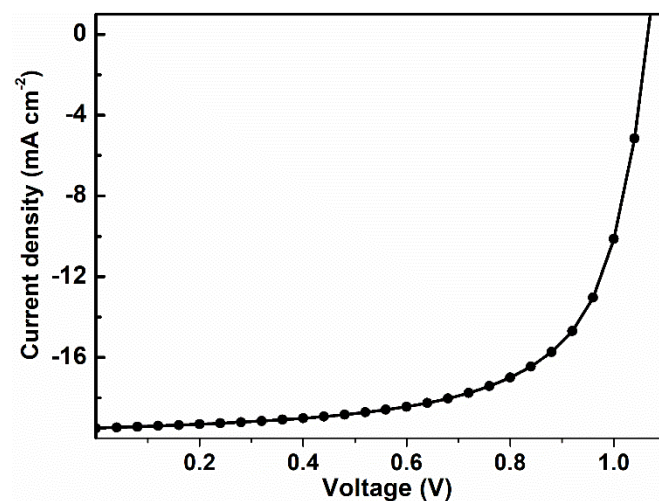


Figure S13. The J - V curve of slot-die coated perovskite device based on PFTP.