Electronic Supplementary Information

The Impact of Space Charge Polarization on Light-soaking Phenomena in Non-Fullerene Organic Solar Cells

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1. Experiment details

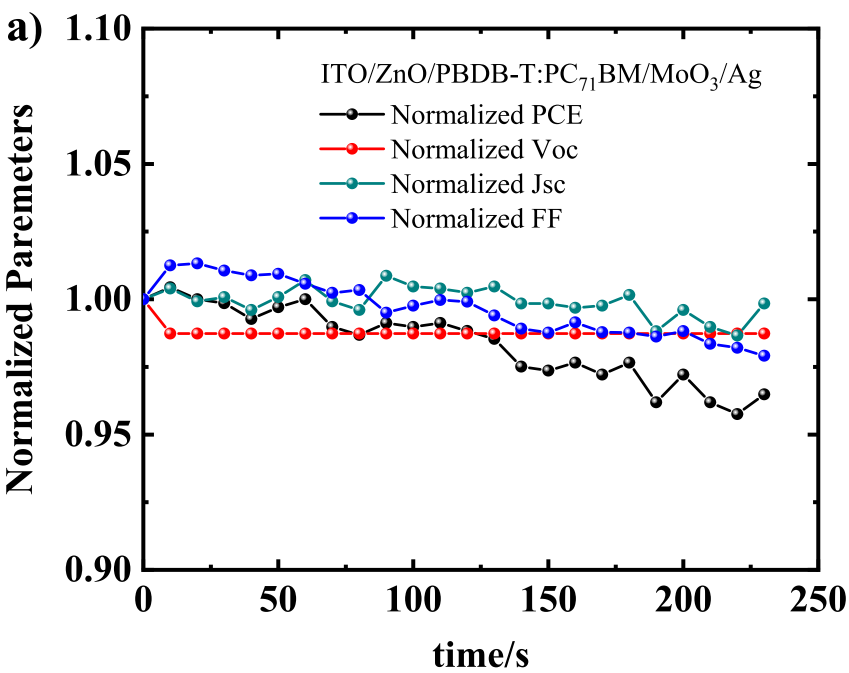
1.1 Materials

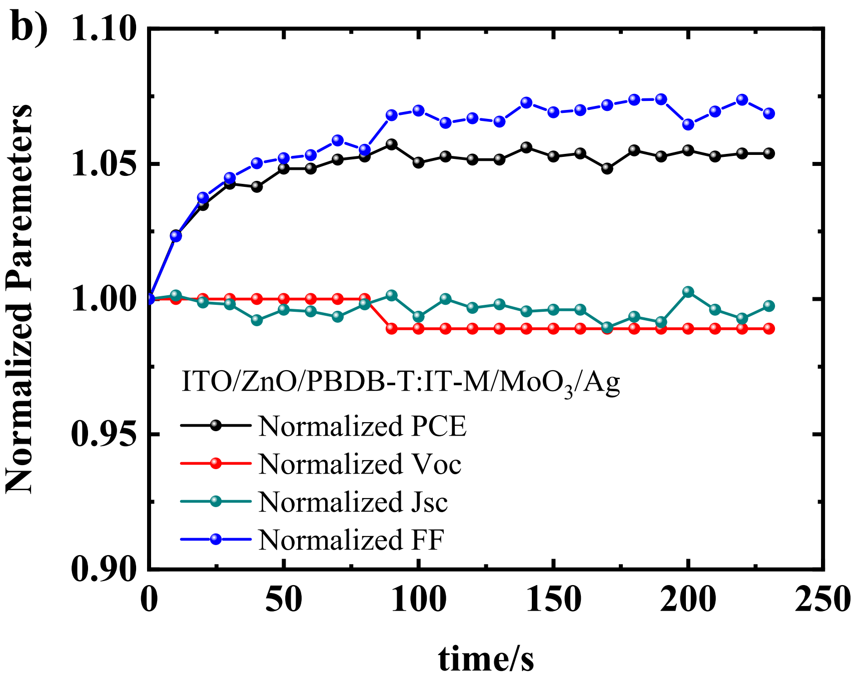
The electron donors and acceptors used in this study are poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)] (PBDB-T)[17], poly [[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b'] dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl]] (PTB7)[18], poly[(2,6-(4,8-bis(5-(2-ethylhexyl-3-fluoro)thiophen-2-yl)-benzo[1,2-b:4, 5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)] (PBDB-T-F or PM6)[19], 3,9-bis(2-methylene-((3- (1,1-dicyanomethylene)-6/7-methyl)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophen(IT-M)[17],2,2'-((2Z,2'Z)-((12,13-bis(2-ethylhexyl)-3,9-diundecyl-12,13-dihydro-[1,2,5]thiadiazolo[3,4-e]thieno[2",3'':4',5']thieno[2',3':4,5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b]indole-2,10-diyl)bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile (Y6 or BTP-4F)[20] respectively. PBDB-T and IT-M were purchased from Organ tec. $PC_{71}BM$ was purchased from Han shang. PTB7 and Y6 were obtained from 1-materials. PM6 was purchased from Solarmer. 1-Chloronaphthalene, 1,8-Diiodooctane, Zinc acetate, 2-methoxyethanol, ethanolamine and MoO_3 were purchased from Sigma-Aldrich. All of the chemicals were used as received without further purification.

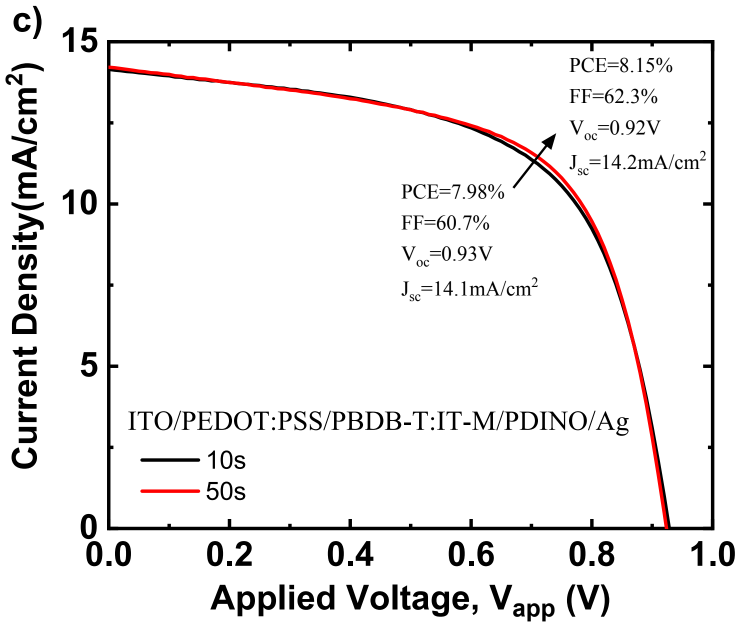
1.2 Device fabrication

The device structure was either in conventional configuration: glass/ITO/PEDOT:PSS (40 nm)/active layer (100 nm)/Ca (or PDINO)/Ag (100 nm) or an inverted type: glass/ITO/ZnO (30 nm)/active layer (100 nm)/MoO_3(10 nm)/Ag(100 nm). For dielectric measurement, a device structure of ITO/active layer (100 nm)/Ag was used. ITO glass substrates were cleaned with isopropanol, de-ionized water and isopropanol successively and ultrasonicated for 15 min, respectively. Sol-gel ZnO solution was prepared by mixing zinc acetate (1 g), 2-methoxyethanol (10 ml) and ethanolamine (280 μl) together in sequence, followed by heating at 60℃ and stirring overnight. ZnO layer was prepared on the ITO substrate following well-established procedure[21], followed by post-treatment of thermal annealing 200°C for 1h. The active blend layer was deposited by spin-coating blends of PBDB-T:IT-M (D:A=1:1, 20 mg/ml in total, 1% DIO), PBDB-T:$PC_{71}BM$ (D:A=1:1, 20mg/ml in total, 3% DIO), PTB7:$PC_{71}BM$ (D:A=1:1.5, 25 mg/ml in total, 3% DIO) chlorobenzene (CB) solution, and PM6:Y6 (D:A=1:1.2, 16 mg/ml in total, 0.3% CN) chloroform (CF) solution, respectively. The PM6:Y6 layer was thermal annealed at 110℃ for 15 min. Finally, a 10 nm MoO_3 layer and a 100 nm Ag layer were deposited on the active layer under 5×10^{-4} Pa by thermal evaporation through a shadow mask (5.7 mm^2) for the inverted devices, while a 10 nm Ca layer and a 100 nm Ag cathode were thermally evaporated for the conventional devices. All devices were encapsulated with UV-curable epoxy resin (ELC-2500, Electro-Lite Corp.) and a cover glass plate for testing in a nitrogen-filled glovebox before testing.

2. Figure




b)
1.10
1.05
1.00
0.95
0.90
Normalized Paremeters
0
50
100
150
200
250
time/s
ITO/ZnO/PBDB-T:IT-M/MoO3/Ag
Normalized PCE
Normalized Voc
Normalized Jsc
Normalized FF


c)
15
10
5
0
Current Density(mA/cm2)
0.0
0.2
0.4
0.6
0.8
1.0
Applied Voltage, Vapp (V)
PCE=8.15%
FF=62.3%
Voc=0.92V
Jsc=14.2mA/cm2
PCE=7.98%
FF=60.7%
Voc=0.93V
Jsc=14.1mA/cm2
ITO/PEDOT:PSS/PBDB-T:IT-M/PDINO/Ag
10s
50s

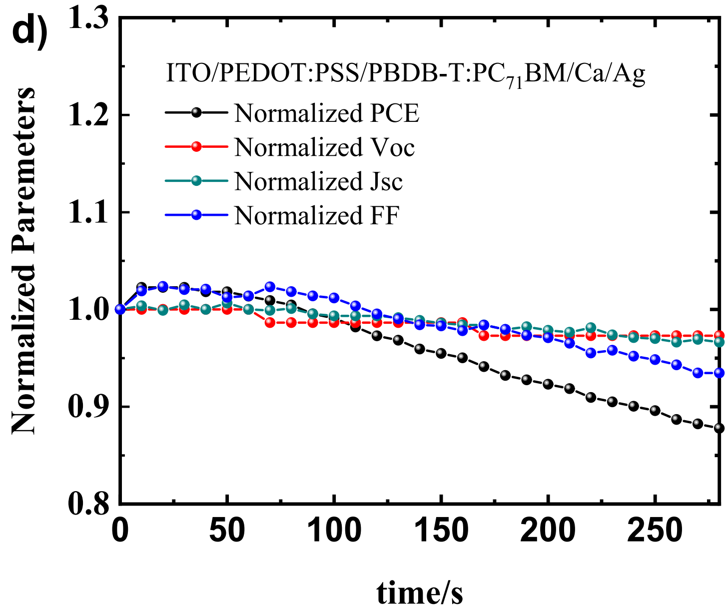
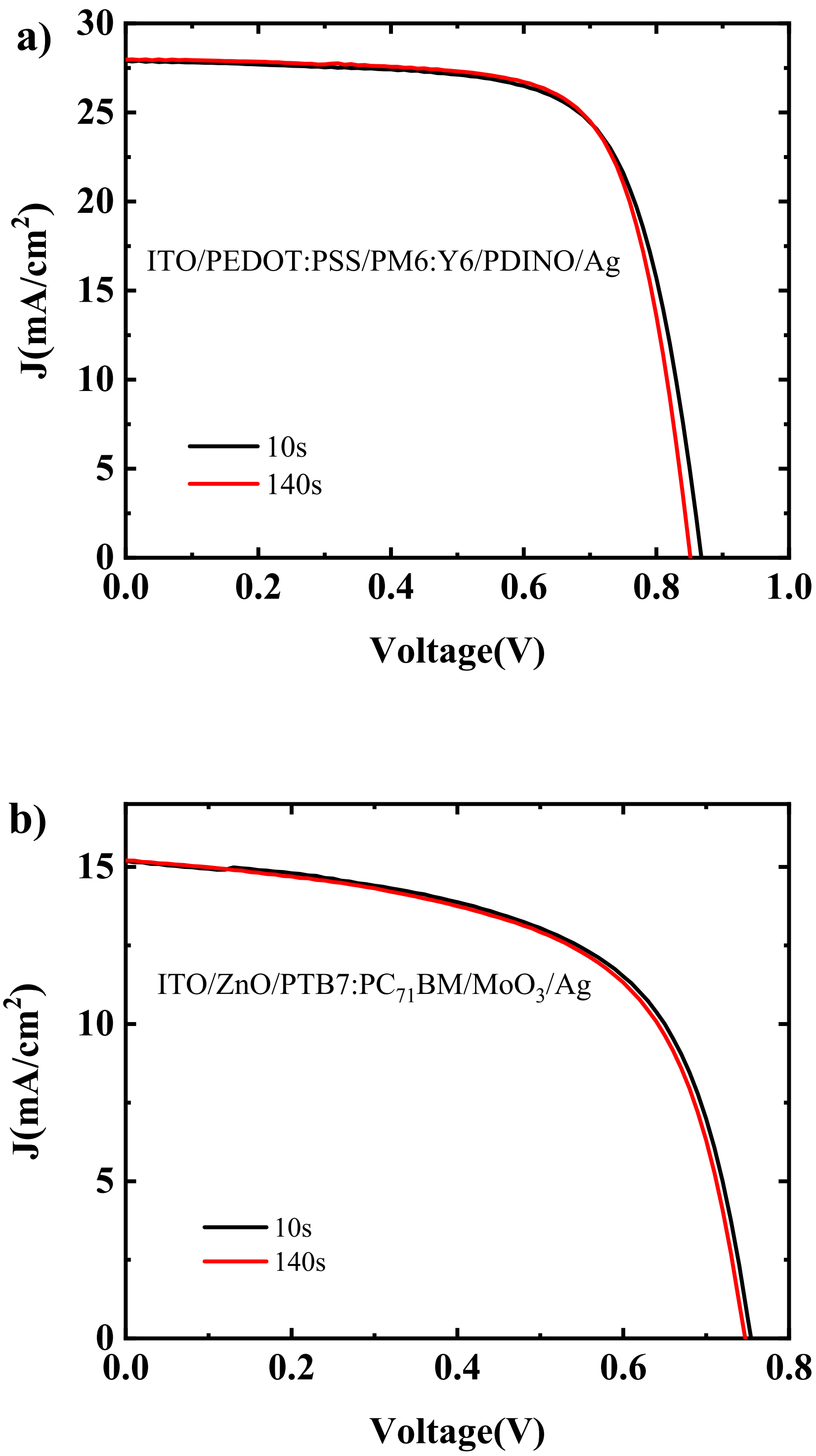


Fig. S1. The normalized device performance parameters **(a)** for the PBDB-T:$PC_{71}BM$ device and **(b)** the PBDB-T:IT-M device with inverted device structure. **(c)** *J-V* characteristics of PBDB-T:IT-M device with the conventional structure upon light-soaking for 0s and 50s. **(d)** The normalized device performance parameters for the PBDB-T:$PC_{71}BM$ device with inverted device structure.



a)
30
25
20
15
10
5
0
0.0
0.2
0.4
0.6
0.8
1.0
J(mA/cm^2)
Voltage(V)
ITO/PEDOT:PSS/PM6:Y6/PDINO/Ag
10s
140s
b)
15
10
5
0
0.0
0.2
0.4
0.6
0.8
J(mA/cm^2)
Voltage(V)
ITO/ZnO/PTB7:PC$_{71}$BM/MoO$_3$/Ag
10s
140s

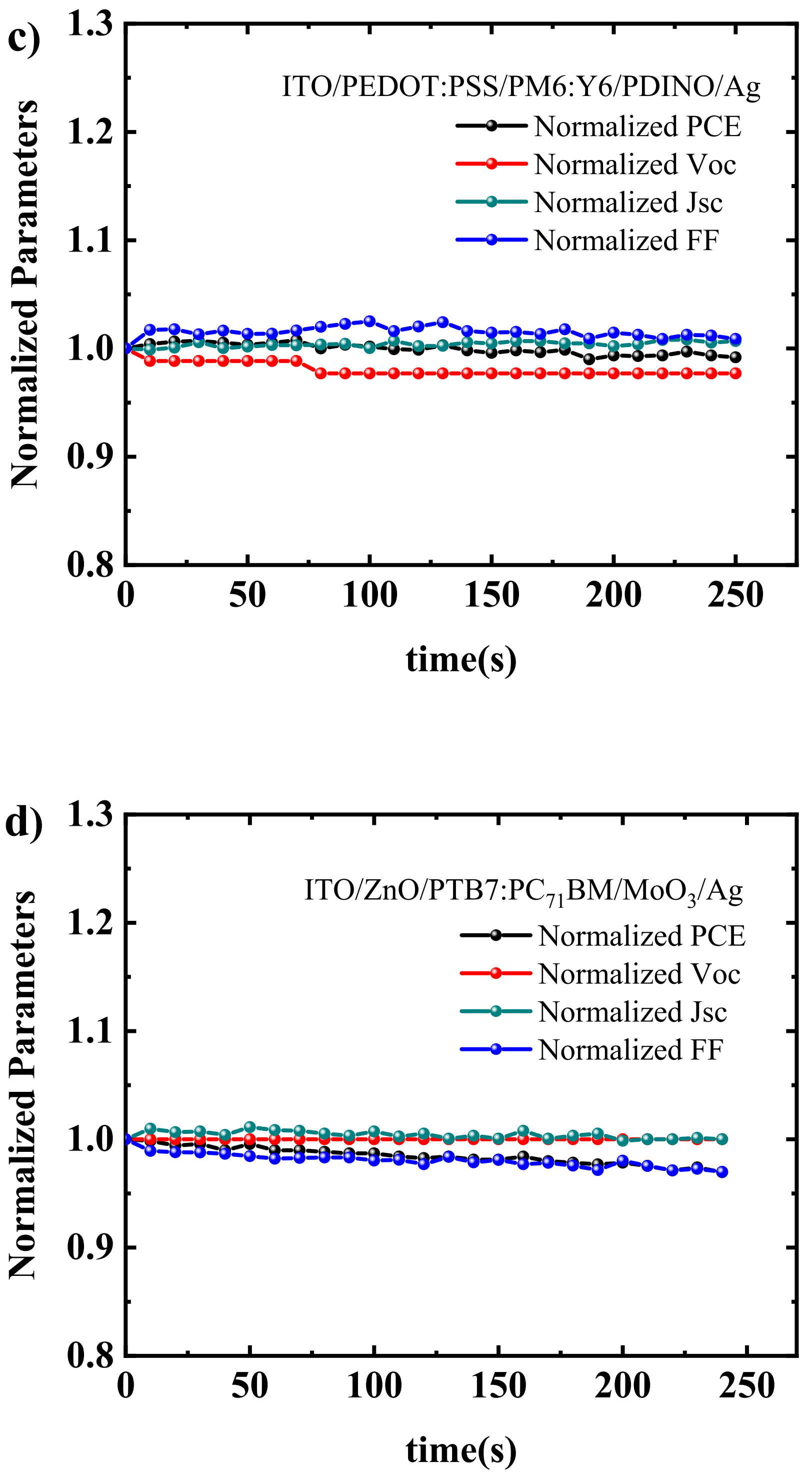
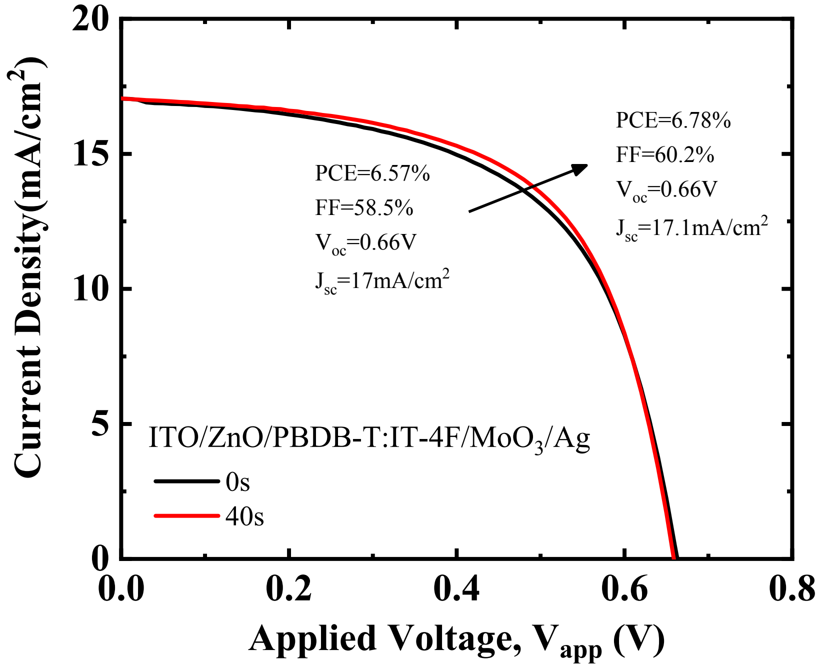


Fig.S2. The *J-V* characteristics and the normalized device performance parameters **(a,c)** for thePM6:Y6 device and **(b,d)** for the PTB7:$PC_{71}BM$ device with conventional device structure.



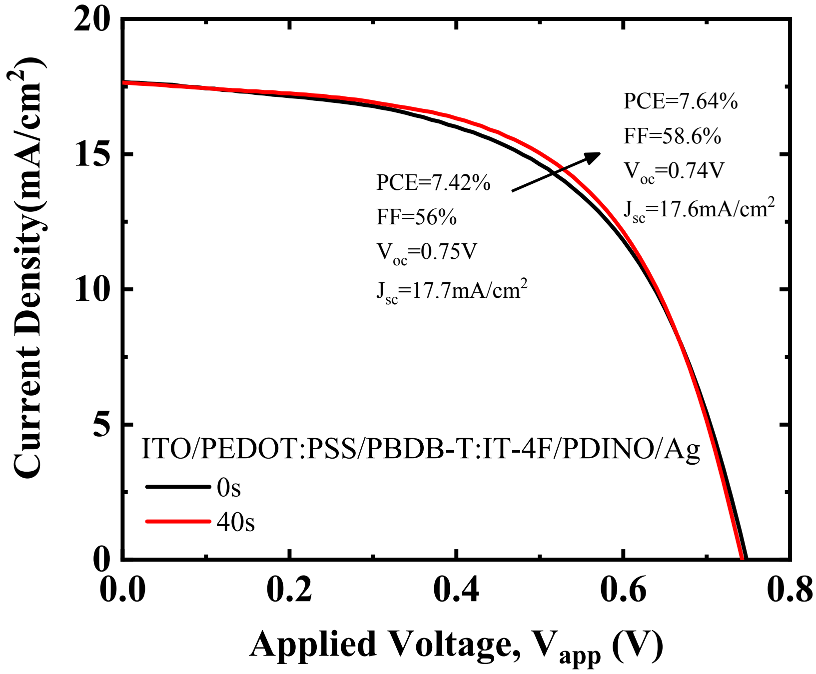


Fig. S3 *J*-*V* characteristics for the inverted **(a)** and **(b)** conventional OSCs based on PBDB-T:IT-4F upon light-soaking for 0s and 40s.

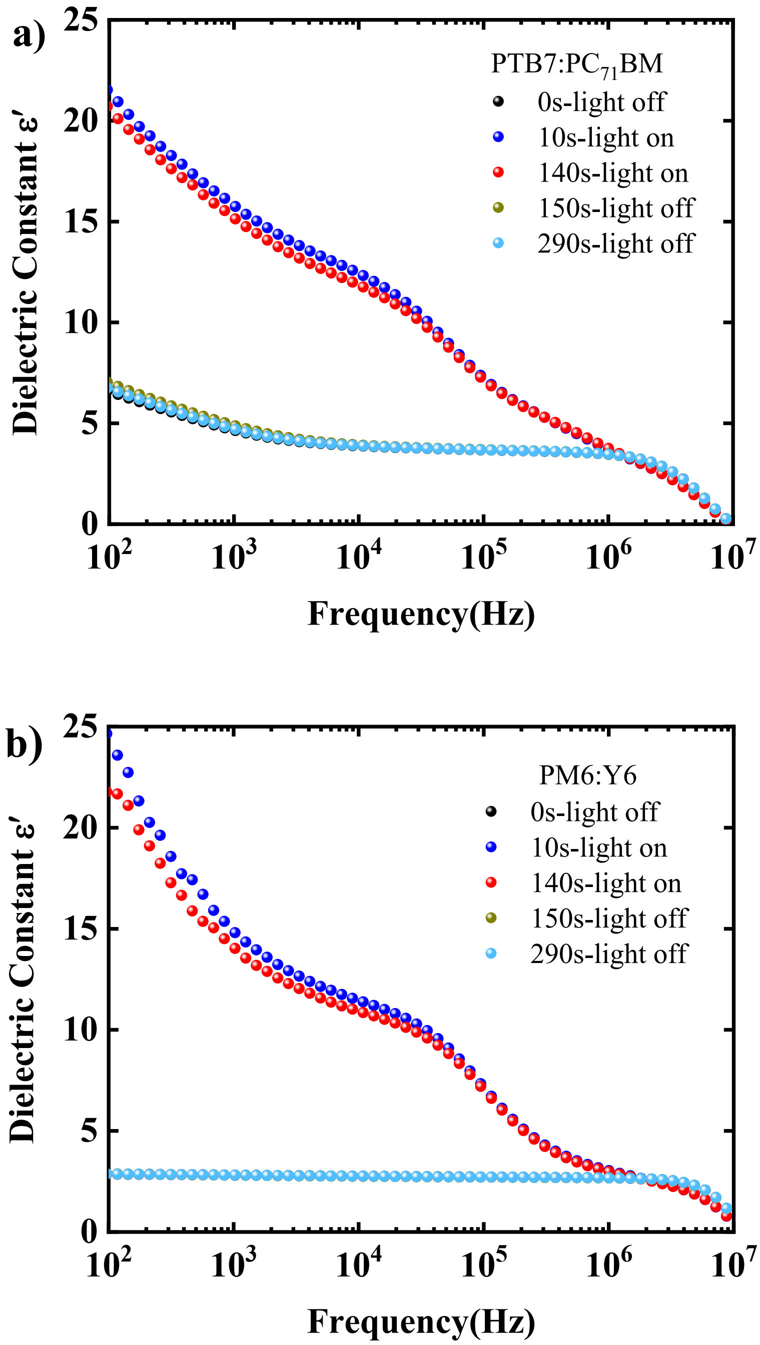
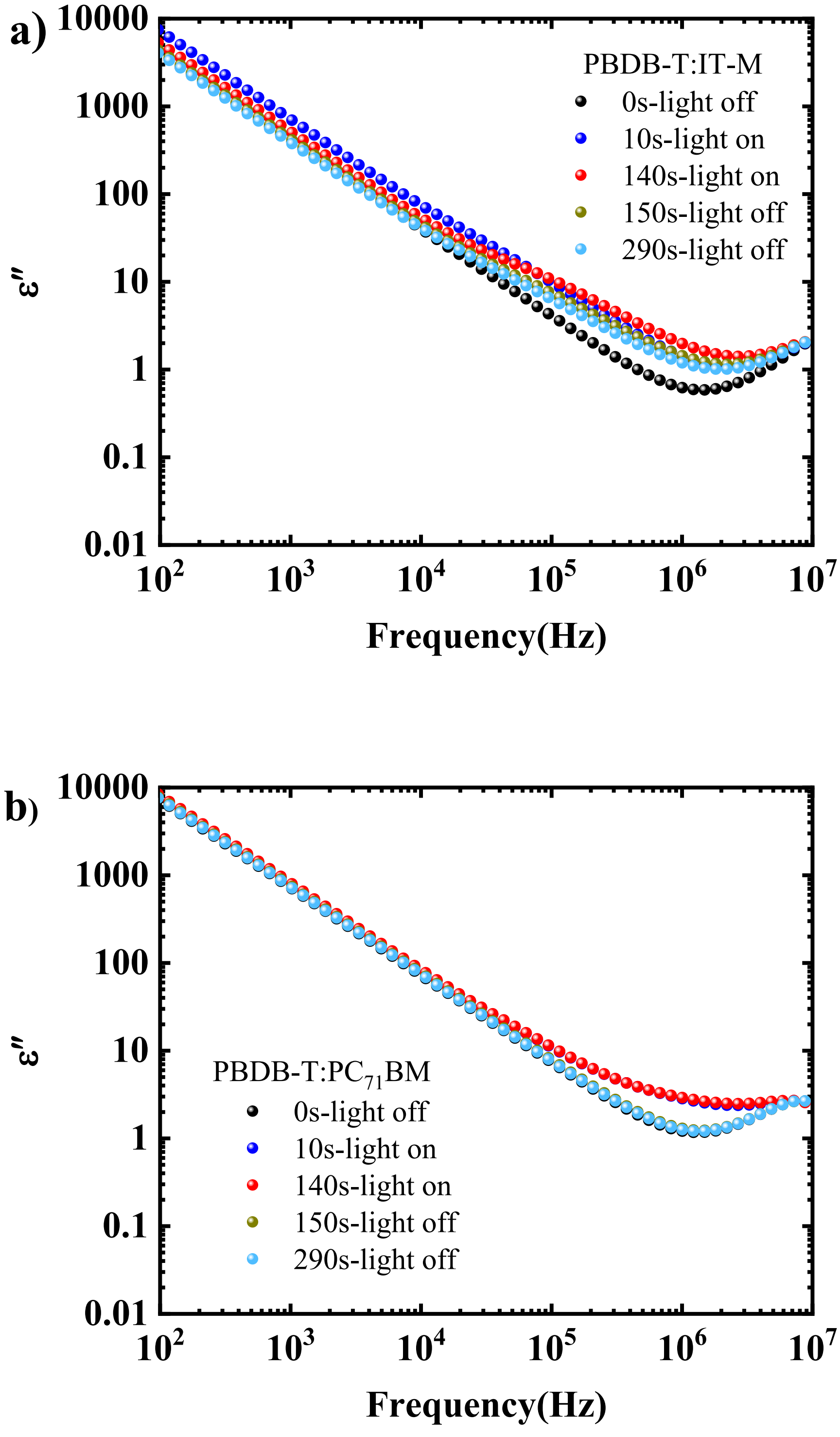
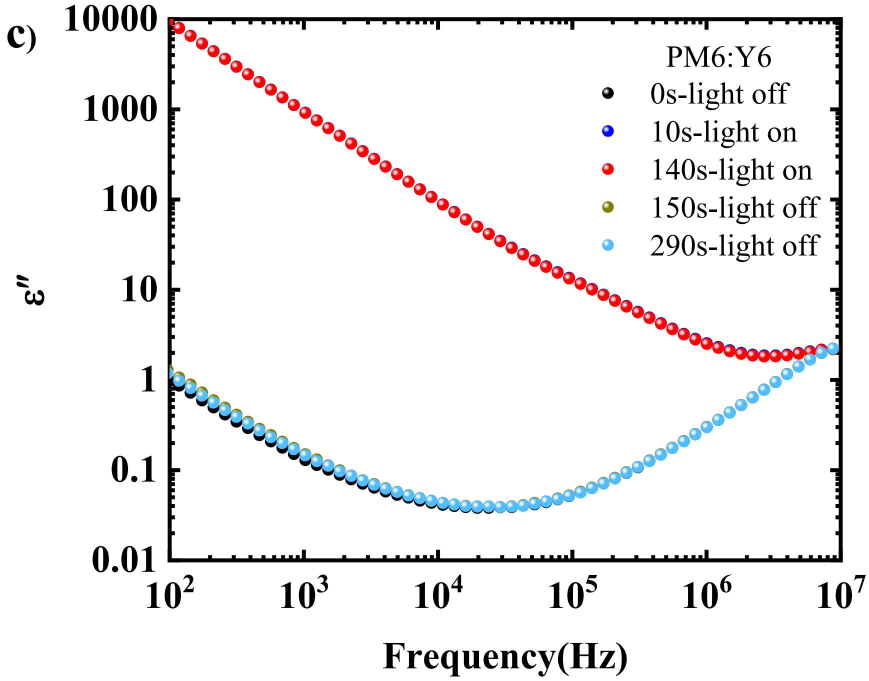


Fig. S4 The dielectric constants relaxation of PTB7:$PC_{71}BM$ **(a)** and PM6:Y6 **(b)** device as a function of A.C frequency under different illumination time *t*. When *t*=0s, device is in the dark. Turn on the light at *t*=1s, then we test at *t*=10s and *t*=140s, and then turn off the light immediately. Then we test again at when *t*=150s and *t*=290s.


a)
PBDB-T:IT-M
0s-light off
10s-light on
140s-light on
150s-light off
290s-light off
ε''
Frequency(Hz)
b)
PBDB-T:PC71BM
0s-light off
10s-light on
140s-light on
150s-light off
290s-light off
ε''
Frequency(Hz)



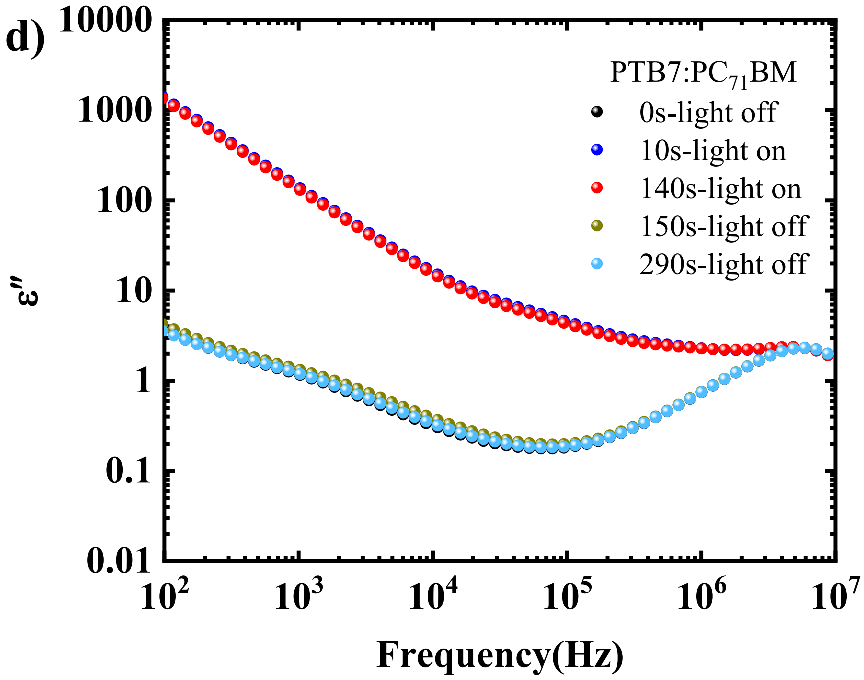


Fig. S5. The dielectric loss for the **(a)** PBDB-T:IT-M, **(b)** PBDB-T:$PC_{71}BM$, **(c)** PM6:Y6 devices and **(d)** the PTB7:$PC_{71}BM$ device.

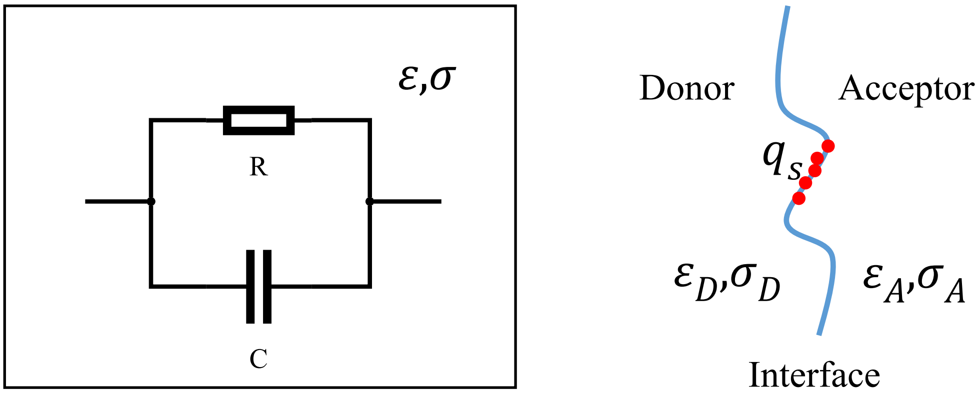


Fig. S6 (a) Equivalent circuit of the active layer in the OSCs devices and **(b)** Schematic of Maxwell-Wagner effect.

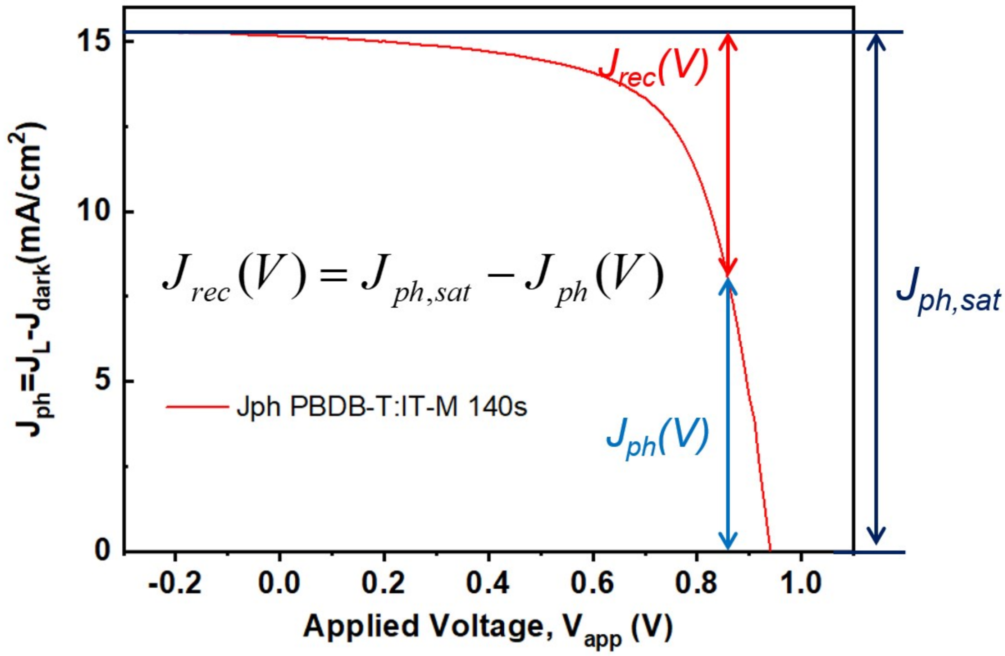


Fig. S7 Schematic diagram showing the relation about three types of current, including saturation current J_{sat}, light current J_L and recombination current J_{rec}