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Non-toxic green food additive enables efficient polymer solar cells through adjusting phase composition distribution and boosting charge transport

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Materials

PTB7-Th and $PC_{71}BM$ (99.5%) were purchased from Cal-os. MoO_3 (99.99%) and Ag (99.99%) were purchased from zhong nuo (Beijing, China). Chlorobenzene (99.8%) from Sigma–Aldrich, 1,8-diiodooctane (97%) from Alfa Aesar, diphenyl sulfide (99%) Benzyl salicylate was prepared from Aladdin.

Device fabrication and characterization

The inverted device with ITO/ZnO/PTB7-Th:$PC_{71}BM$/MoO_3/Ag was fabricated. The ITO (indium tin oxide) glass substrates were continuously cleaned with detergent, deionized water, acetone, deionized water and isopropanol in turn. After blowing dry ITO glass substrates, a thin film of ZnO was spin-casted on ITO with spin rate 3000 rpm 40s. The photoactive layer PTB7-Th:$PC_{71}BM$ (total concentration 25 mg·mL^{-1}, 1:1.5) solution was dissolved in CB. 3 vol % DIO and various concentrations BS (1 vol%~5 vol %) was added in CB, respectively. Subsequently, a 100 nm photoactive layer film were formed on PFN film by spin-coating. Finally, MoO_3 (10 nm) and Ag (100 nm) layer was prepared by thermal evaporation.

Keithley 2400 source meter instrument unit was used for measuring current density−voltage (*J-V*) curves under AM 1.5G (XEC-300 M2, San-EI Electric Co.). Incident photon to charge carrier efficiency (IPCE) setup (7-SCSpecIII, Beijing 7-star Optical Instruments Co.) was employed for external quantum efficiencies (EQE). Water contact angle was obtained from DSA100 Optical contact Angle/surface tension meter (Kruss, Germany). The surface roughness of blend film was acquired from atomic force microscopy (AFM, NanoMan VS, Veeco, USA). Transmission electron microscopy (TEM) images of thin film were characterized by a Tecnai G2 F20 (FEI, USA). The thicknesses were conducted by a surface profilometer (DektakXT, USA). The alternating current impedance spectrum (ACIS) measurements of devices were performed at an electrochemical Workstation (CHI660E, Shanghai Chenhua, China).

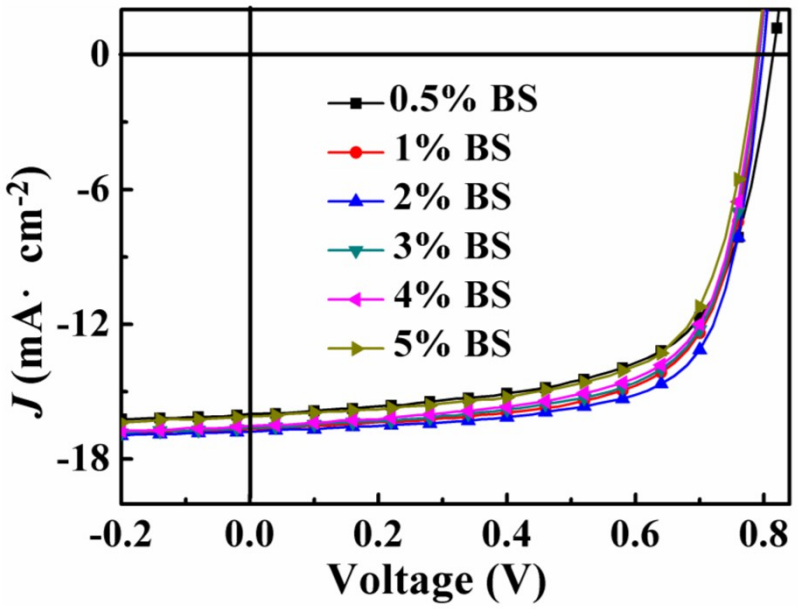

Fig. S1 *J-V* characteristics of PSCs with different BS concentrations.

Table S1 Performance parameters of PSCs based on PTB7-Th: $PC_{71}BM$ blend with different BS concentrations.

Additives	V_{oc} (V)	J_{sc} (mA·cm^{-2})	FF (%)	PCE (%)[a]	R_s (Ω·cm^2)	R_{sh} (Ω·cm^2)
BS 0.5%	0.81	15.98	65.36	8.46	4.95	630.82
BS 1%	0.80	16.65	68.02	9.06	3.79	815.16
BS 2%	0.80	16.78	70.28	9.43	3.44	1059.95
BS 3%	0.79	16.59	68.37	8.96	3.79	728.73
BS 4%	0.79	16.52	67.66	8.83	3.92	726.08
BS 5%	0.79	16.10	66.91	8.51	4.36	679.12

Table S2 WCA and PTB7-Th surface fraction of the PTB7-Th:$PC_{71}BM$ blend films processed under different conditions.

	PTB7-Th:$PC_{71}BM$ (w/o additives)	PTB7-Th:$PC_{71}BM$ (3% DIO)	PTB7-Th:$PC_{71}BM$ (2% BS)	$PC_{71}BM$	PTB7-Th
WCA	97.2°	97.7°	97.9°	91.3°	101.6°
PTB7-Th surface fraction *f*	57.5%	62.4%	64.3%	-----	-----

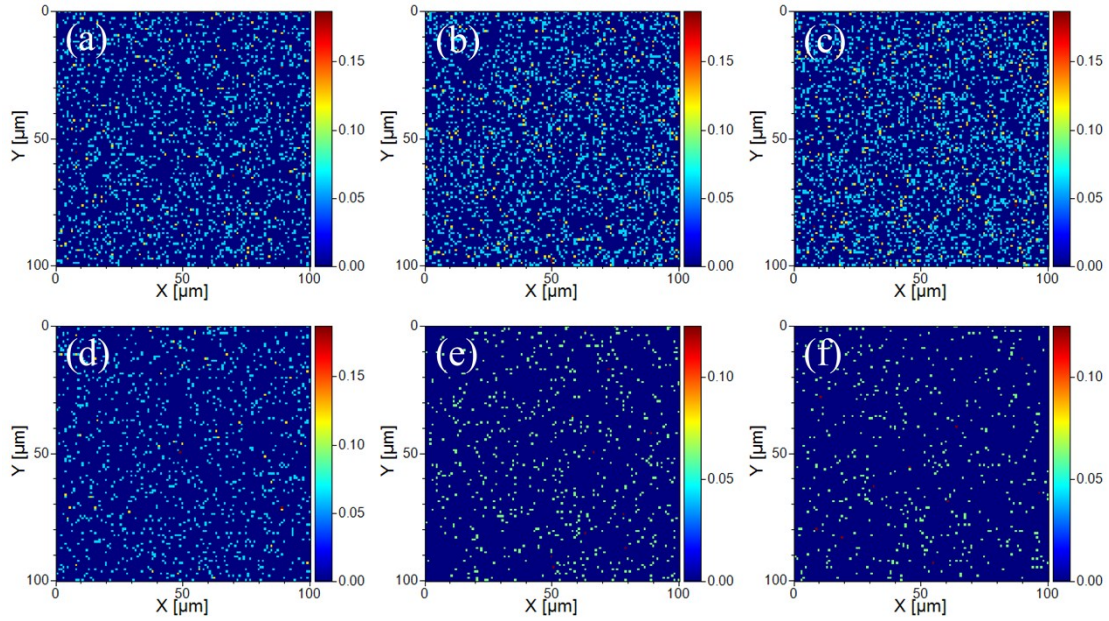

Fig. S2. Top projection images of S^- contents of blend film with additives treatment under TOF-SIMS measurement at different sputtering times, (a, b, c) 20 s and (d, e, f) 600s, (a, d) w/o additives, (b, e) 3% DIO, (c, f) 2% BS.

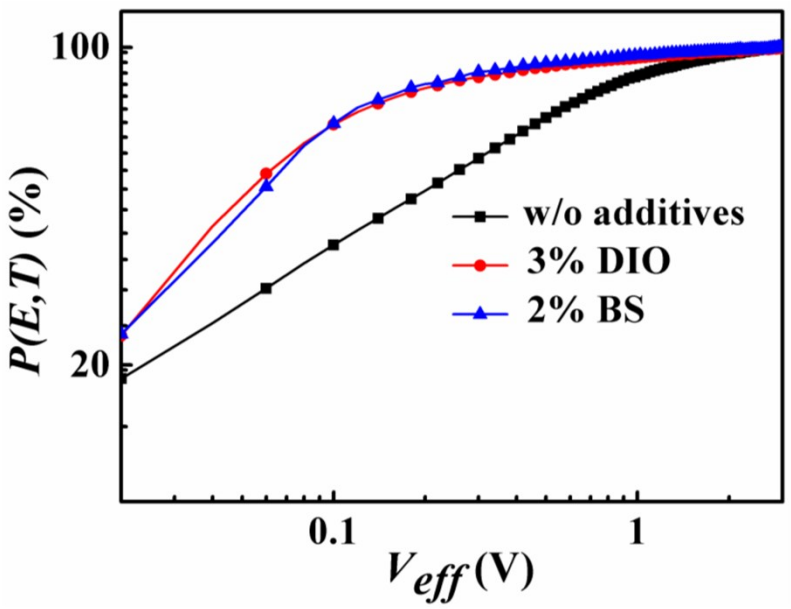

Fig. S3 Exciton dissociation rate versus effective voltage curve.

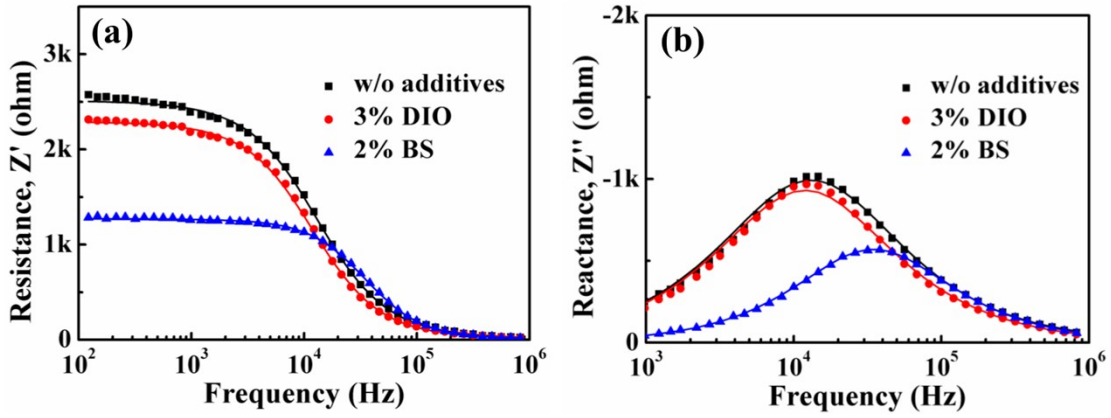

Fig. S4 (a) and (b) were the curves of resistance and reactance versus frequency, respectively.

Hole and electron mobility measurement

The hole-only device with a structure of ITO/PEDOT:PSS/active layer/MoO_3/Ag and electron-only device with a structure of ITO/ZnO/Active layer/PFN/Al. Through the J-V curves measured and the Mott-Gurney law [1, 2]

$$J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu\frac{(V_{appl}-V_{bi})^2}{L^3}$$

where J is current density, ε_r is the relative dielectric constant of the organic photoactive layer (≈3.00), ε_0 is the permittivity of the vacuum of 8.85×10-12 F/m, L is the active layer thickness（110 nm）, V_{appl} is the applied voltage, and V_{bi} is the built-in voltage since the difference in the work function of the cathode and the anode, μ is mobility. For the hole-only devices, V_{bi} is 0 V, while V_{bi} = 0.7 V in the electron-only devices.

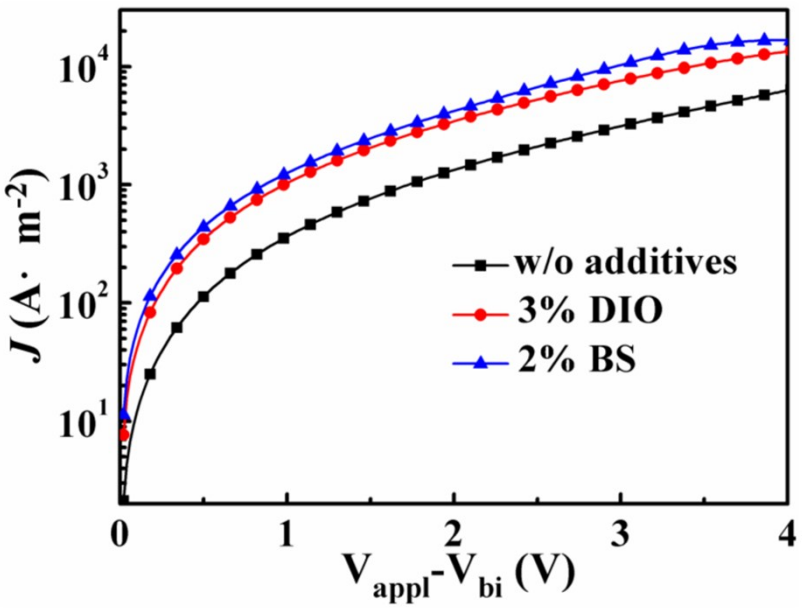

Fig. S5 *J-V* curves of electron-only photovoltaic devices with different additives.

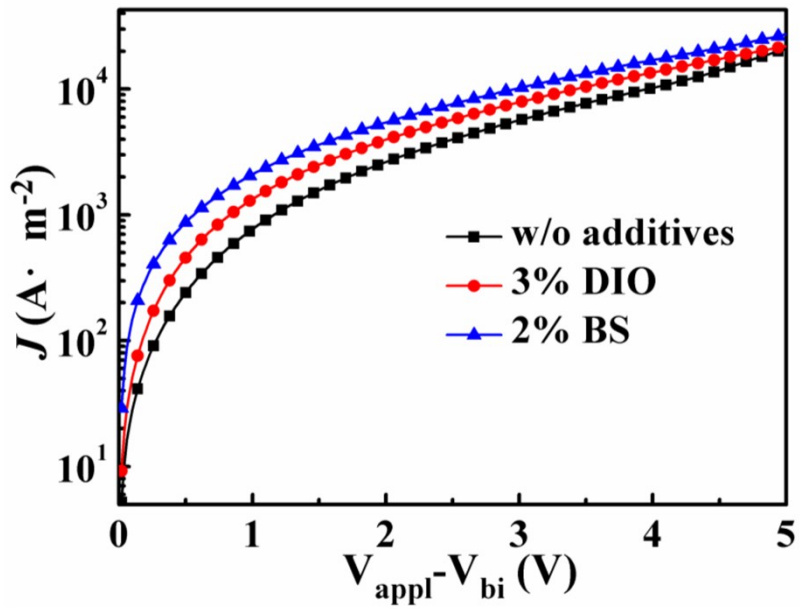

Fig. S6 *J-V* curves of hole-only photovoltaic devices with different additives.

Table S3 Hole mobility (μ_h), electron mobility (μ_e) and their ratios (μ_h/μ_e) of the PTB7-Th:$PC_{71}BM$ blend films processed with different conditions.

Additives	μ_h ($cm^2V^{-1}s^{-1}$)	μ_e ($cm^2V^{-1}s^{-1}$)	μ_h/μ_e
without	0.000218	0.000115	1.90
3% DIO	0.000275	0.000306	0.90
2% BS	0.000362	0.000361	1.00

Reference

1. C. Melzer, E. J. Koop, V. D. Mihailetchi, and P. W. M. Blom, *Adv. Funct. Mater.,* 2004, **14**, 865.
2. M. Y. Chiu, U. S. Jeng, M. S. Su, K. H. Wei, *Macromolecules.,* 2010, **43**, 428.