

High Performance All-Small-Molecule Solar Cells: Engineering the Nanomorphology via Processing Additives

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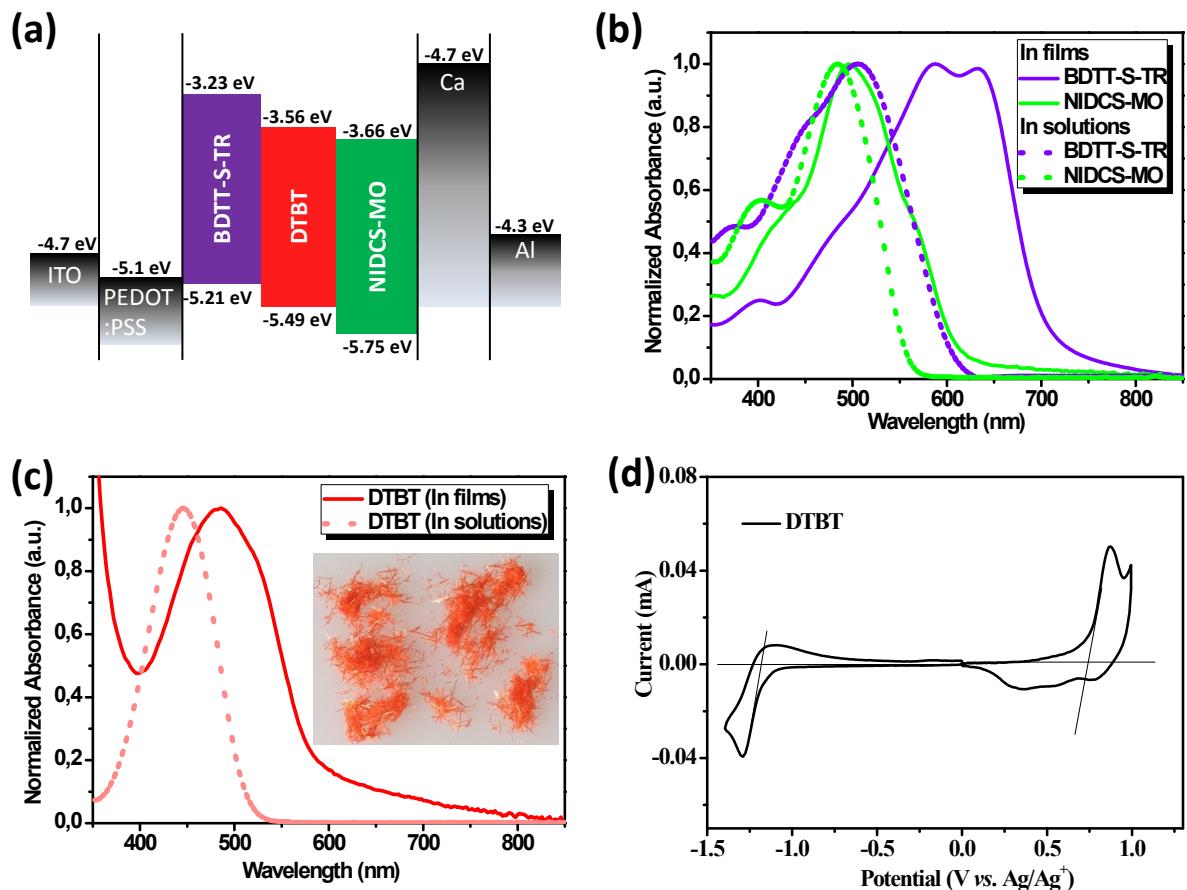


Figure S1. (a) The schematic figure of the energy level alignments; (b) The absorption spectra of BDTT-S-TR and NIDCS-MO in chloroform solutions and in thin films; (c) The absorption spectra of DTBT in chloroform solution and in thin film (Inset: one digital photograph taken through the DTBT compounds). (d) Cyclic voltammograms of DTBT dissolved in 0.1 mol L⁻¹ Bu₄NPF₆ acetonitrile solution at a scan rate of 100 mV s⁻¹.

Table S1. Optical properties of BDTT-S-TR, NIDCS-MO and DTBT molecules.

Compounds	Solution ^a			Film ^b		
	λ_{max} (nm)	λ_{onset} (nm)	E_g^{opt} (eV) ^c	λ_{max} (nm)	λ_{onset} (nm)	E_g^{opt} (eV) ^c
BDTT-S-TR	506	605	2.05	588/632	717	1.73
NIDCS-MO	484	555	2.23	496	605	2.05
DTBT	446	511	2.43	487	584	2.12

^aMeasured in chloroform solution. ^bCast from ODCB solution. ^cBandgap estimated from the onset wavelength (λ_{edge}) of the optical absorption: $E_g^{\text{opt}} = 1240/\lambda_{\text{edge}}$.

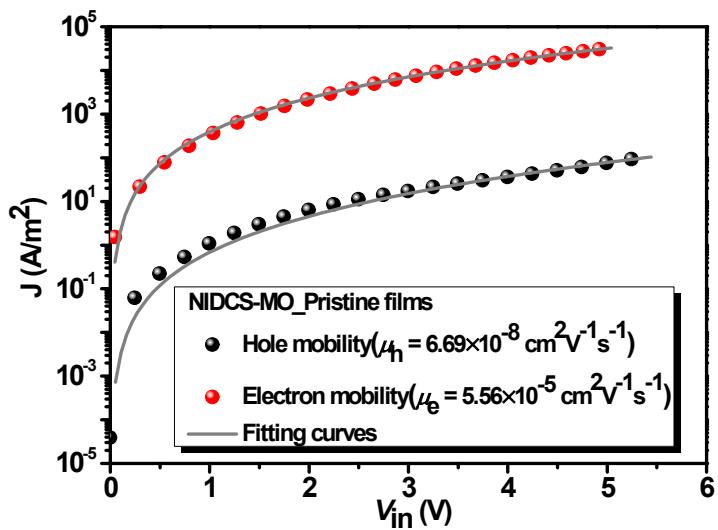


Figure S2. The dark J - V characteristics of pristine NIDCS-MO based hole-only and electron-only devices. The solid lines represent the best fitting using the SCLC model. The inset mobility data are the average mobility values obtained from six devices.

Table S2. Photovoltaic performance parameters of BDTT-TR:NIDCS-MO devices with different D/A weight ratios under the illumination of AM 1.5 G at 100 mW cm^{-2} .

D/A ratios	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE ^[a] (%)
1:0.5	1.21	2.52	28.2	0.86 [0.82]
1:0.8	1.12	3.59	27.1	1.09 [0.92]
1:1	1.12	3.10	26.2	0.91 [0.82]
1:1.5	1.10	3.03	26.6	0.89 [0.79]
1:2	1.05	3.03	27.1	0.86 [0.79]

^aThe values in square bracket are the average PCEs obtained from six devices.

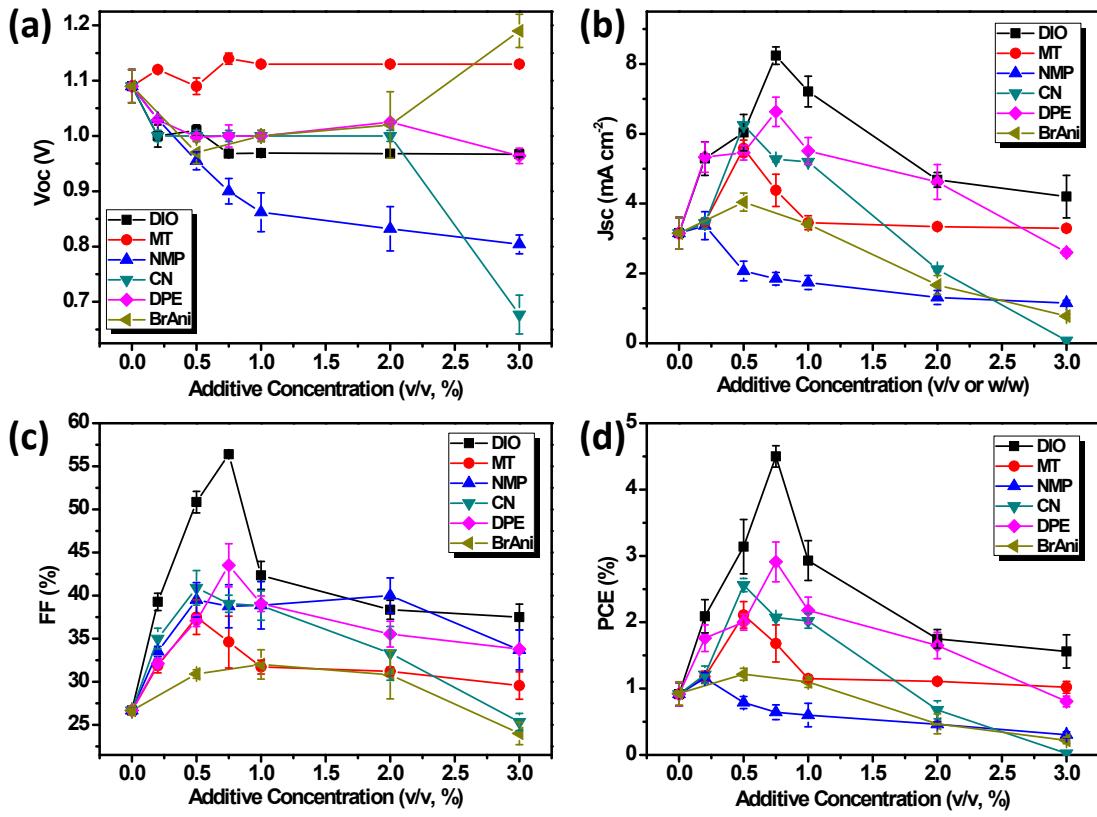


Figure S3. Changes of (a) V_{oc} , (b) J_{sc} , (c) FF and (d) PCE of BDTT-S-TR:NIDCS-MO based devices with different solvent additives as a function of concentration (vol%).

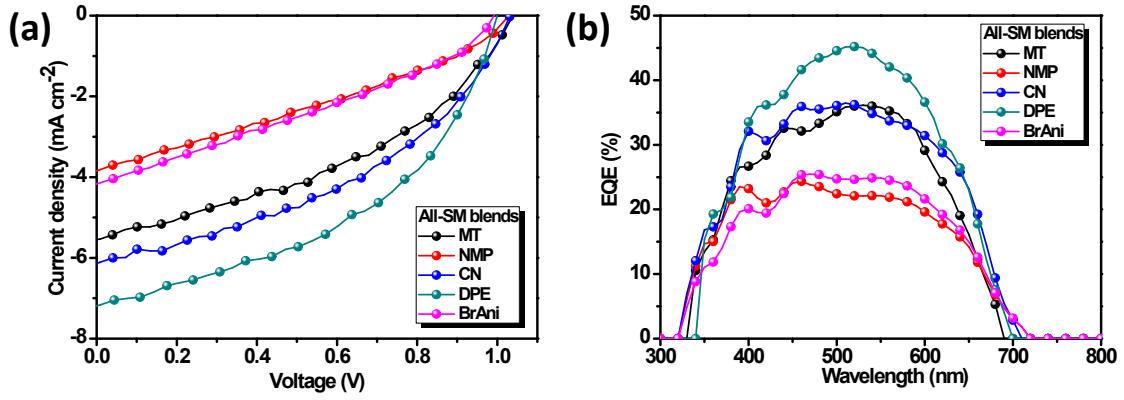


Figure S4. (a) Current density-voltage ($J-V$) characteristics and (b) EQE spectra of the OSCs with MT, NMP, CN, DPE, and BrAni additives under the illumination of an AM 1.5G solar simulator.

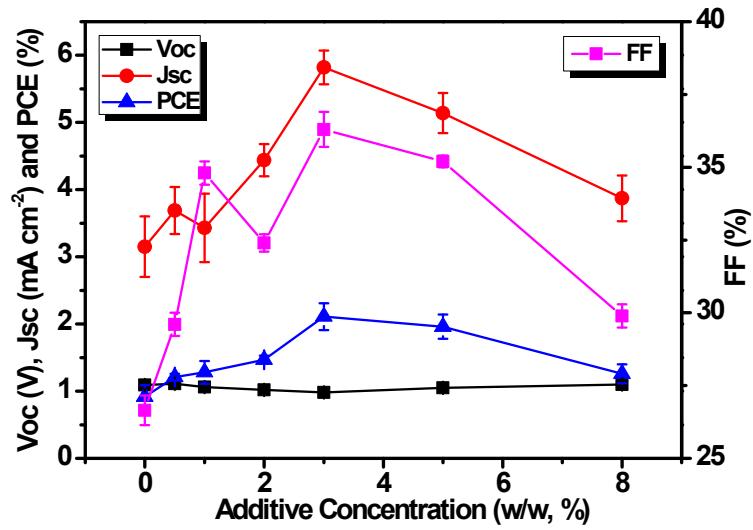


Figure S5. Changes of V_{oc} , J_{sc} , FF and PCE of BDTT-S-TR:NIDCS-MO based devices as a function of DTBT concentration (wt%).

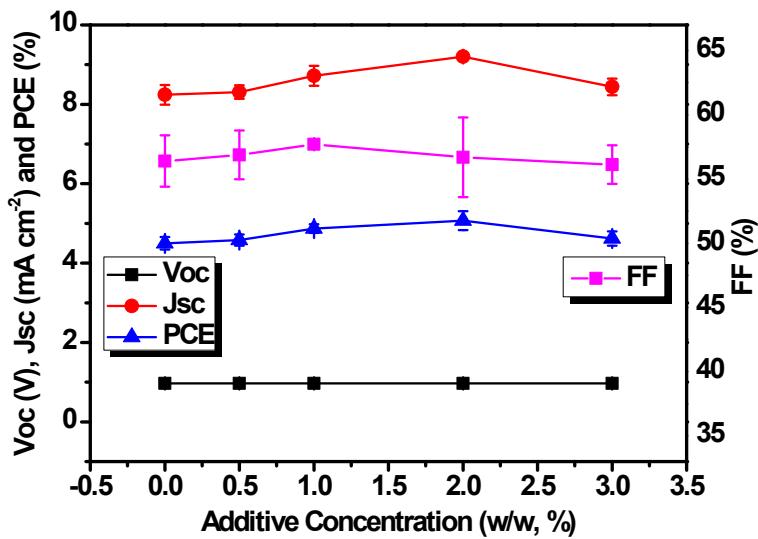


Figure S6. Changes of V_{oc} , J_{sc} , FF and PCE of BDTT-S-TR:NIDCS-MO based devices with 0.75% (vol%) DIO as a function of DTBT concentration (wt%).

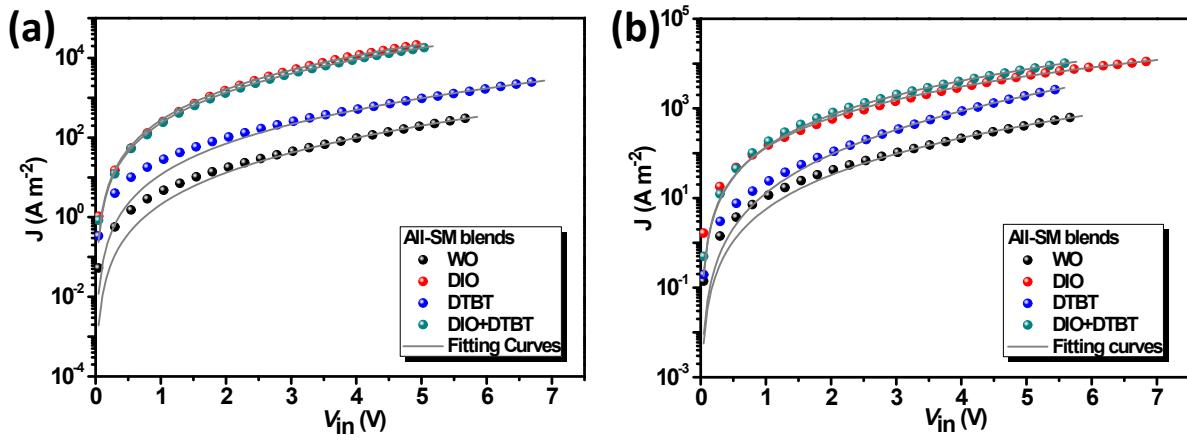


Figure S7. The dark J - V characteristics of (a) hole-only devices and (b) electron-only devices without and with additives. The solid lines represent the best fitting using the SCLC model.

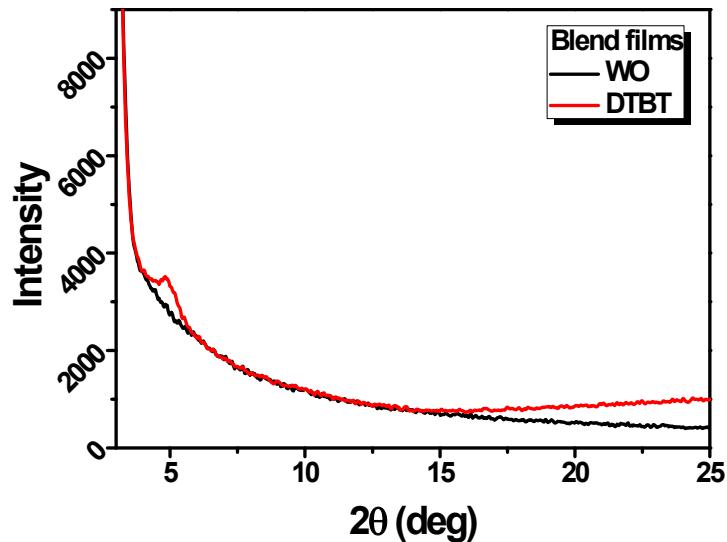


Figure S8. X-ray diffraction (XRD) patterns of BDTT-S-TR:NIDCS-MO (1:0.8, wt%) films without and with DTBT additive.