Supporting Information for

Curved BN-Embedded Nanographene in the Application of Organic Solar Cells

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1. Relative Dielectric Constant

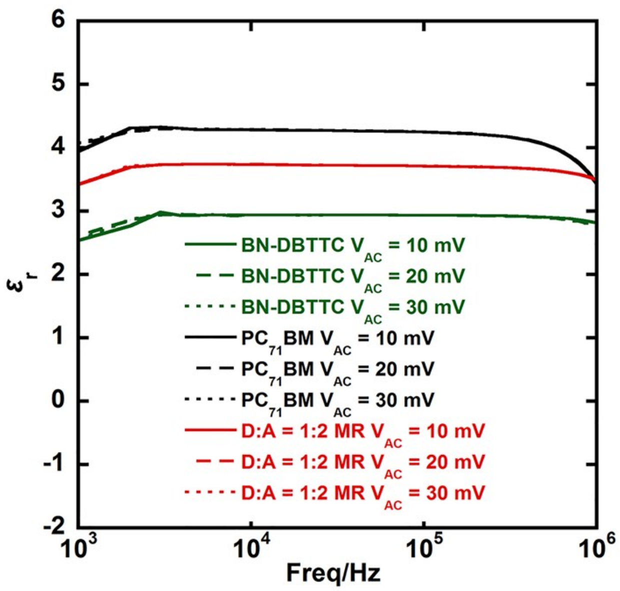

Figure S1. The frequency dependent relative dielectric constant of various films with a device structure of ITO/Active layer/Al. The DC bias is 0 V, and the AC harmonic is 10/20/30 mV.

2. PL quenching

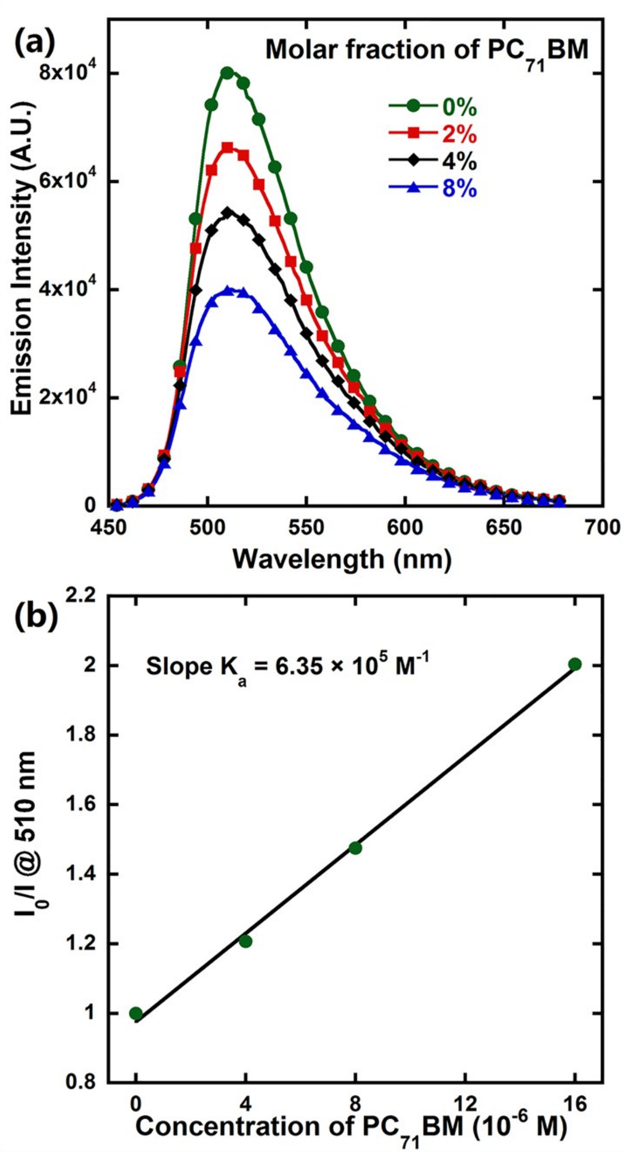

Figure S2. (a) Emission spectra of BN-DBTTC in DCB with various amount of $PC_{71}BM$ added. The BN-DBTTC's concentration is 2×10^{-4} M. (b) Stern-Volmer plot of BN-DBTTC in DCB (PL of BN-DBTTC at 2×10^{-4} M over the PL of BN-DBTTC with $PC_{71}BM$ versus the $PC_{71}BM$ concentration).

3. Toluene vs. CB Solution Device

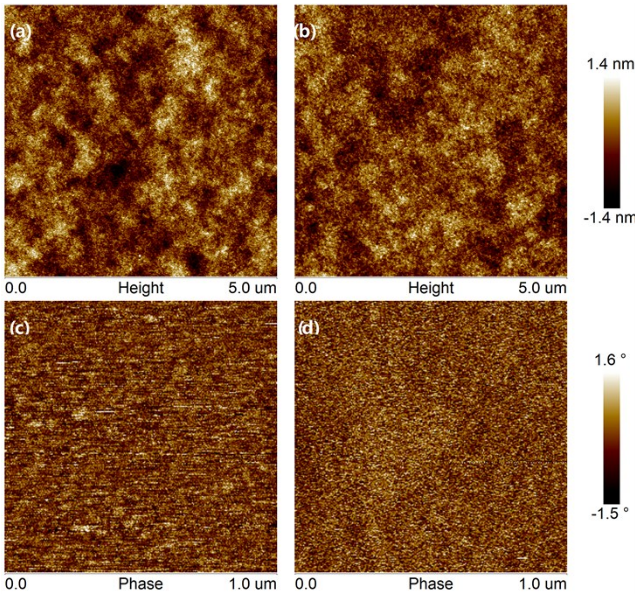

Figure S3. (a), (b) Height images, and (c), (d) phase images of the BN-DBTTC: $PC_{71}BM$ = 1: 2 MR blend films. (a) and (c) are spin-coated from CB, while (b) and (d) are spin-coated from toluene.

Table S1. Photovoltaic performance of BN-DBTTC:$PC_{71}BM$ (1:2 MR) devices with active layer cast from either chlorobenzene or toluene solution under AM1.5G irradiation. Each value is the average of 10 devices.

Solvent	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)
Chlorobenzene	7.41 ± 0.09	0.96 ± 0.01	38.82 ± 0.62	2.76 ± 0.03
Toluene	7.00 ± 0.07	0.96 ± 0.01	40.39 ± 0.32	2.74 ± 0.04

4. X-ray photoelectron spectra (XPS)

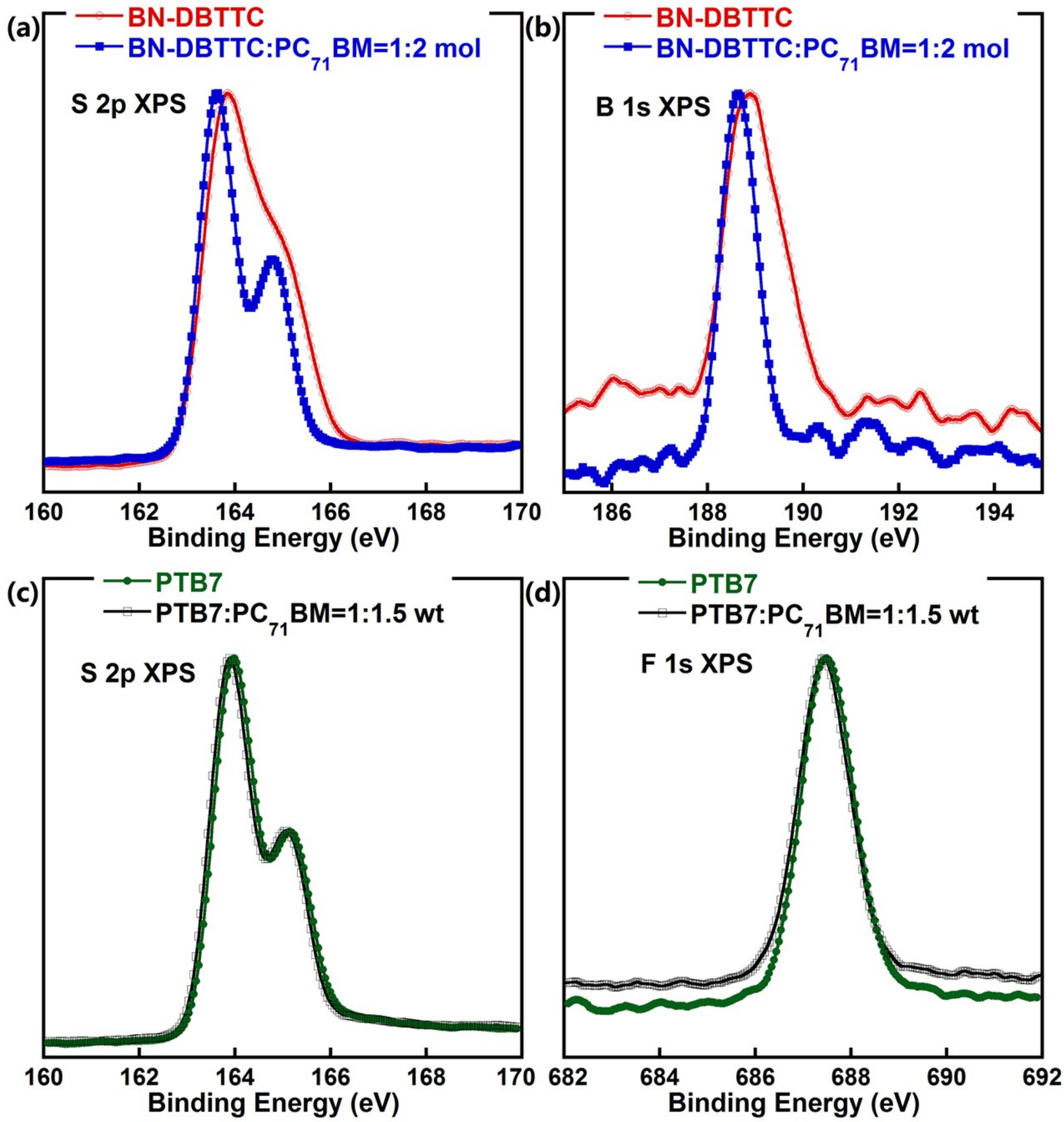

Figure S4. (a) The sulfur 2p, and (b) the boron 1s XPS of BN-DBTTC and its blend film. (c) The sulfur 2p, and (d) the fluorine 1s XPS of PTB7 and its blend film. The spectra are normalized.

5. Performance of Ternary Blend BHJ Devices

Table S2. Photovoltaic performance of PTB7:BN-DBTTC:$PC_{71}BM$ ternary blend BHJ devices with different component weight ratios under AM1.5G irradiation. Each value is the average of 10 devices.

PTB7:BN-DBTTC:$PC_{71}BM$	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)
8: 0: 12	10.60 ± 0.21	0.77 ± 0.01	48.16 ± 0.52	3.91 ± 0.17
8: 1: 12	11.90 ± 0.14	0.78 ± 0.01	44.82 ± 0.53	4.17 ± 0.07
8: 2: 12	13.11 ± 0.30	0.80 ± 0.01	44.81 ± 0.85	4.70 ± 0.12
8: 3: 12	12.96 ± 0.20	0.81 ± 0.01	45.01 ± 0.77	4.75 ± 0.09

6. Mobility Calculation

The carrier mobility could be derived from the space charge limited current (SCLC) as shown in the following equation:

$$J_{SCLC} = \frac{9}{8}\varepsilon_r\varepsilon_0\mu\frac{V^2}{d^3} \tag{S1}$$

where $\varepsilon_0 = 8.854 \times 10^{-12}$ F m^{-1} is the dielectric constant of the vacuum, and $\varepsilon_r \approx 3.7$ is the relative dielectric constant of the active layer, d is the thickness of film, and μ is field independent mobility. By fitting into Eqn. (S1), the μ_h of PTB7: $PC_{71}BM$ = 8:12 is 1.74×10^{-4} cm^2 V^{-1} s^{-1}, and the μ_h of PTB7: BN-DBTTC: $PC_{71}BM$ = 8:3:12 is only 6.21×10^{-5} cm^2 V^{-1} s^{-1}.

If the carrier's mobility is field dependent, the mobility could be derived from the following equation:

$$\frac{J}{V^2} = \frac{9}{8}\varepsilon_r\varepsilon_0\mu_0\frac{1}{d^3}e^{0.89\beta\sqrt{V}/\sqrt{d}} \tag{S2}$$

where the β is the field dependent factor, and μ_0 is the mobility at zero field. By fitting into Eqn. (S2), the μ_e of PTB7: $PC_{71}BM$ = 8:12 is 1.33×10^{-5} cm^2 V^{-1} s^{-1}, and the μ_h of PTB7: BN-DBTTC: $PC_{71}BM$ = 8:3:12 is only 8.50×10^{-6} cm^2 V^{-1} s^{-1}.

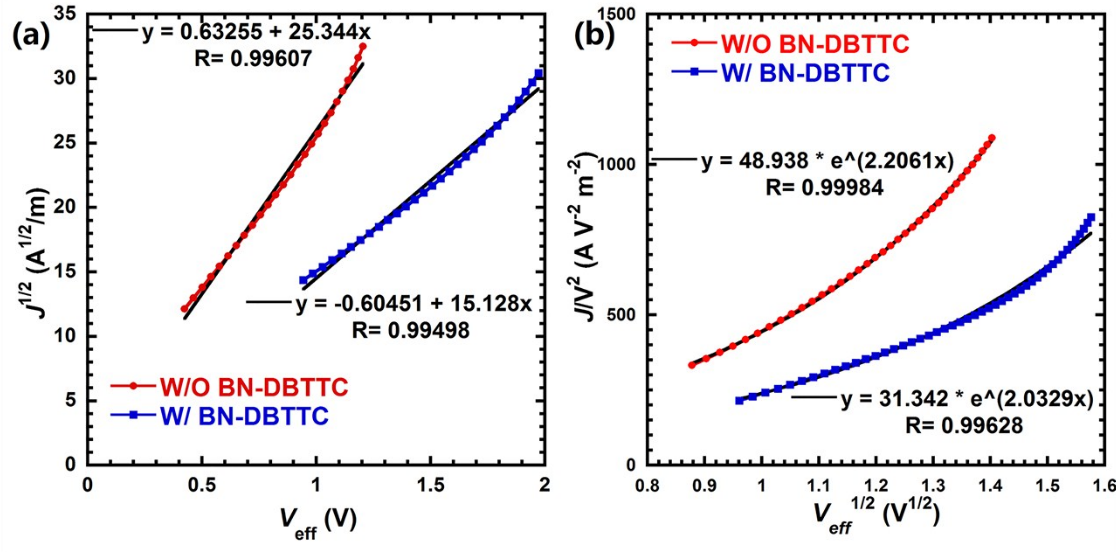

Figure S5. *J-V* characteristics of single carrier devices. a) The hole dominant devices with a configuration of ITO/PEDOT:PSS/Active Layer/(Methanol)/MoO_3/Al, and b) the electron dominant devices with a configuration of ITO/PF-NR_2/Active Layer/PF-NR_2/Al.

7. Absorption Spectra

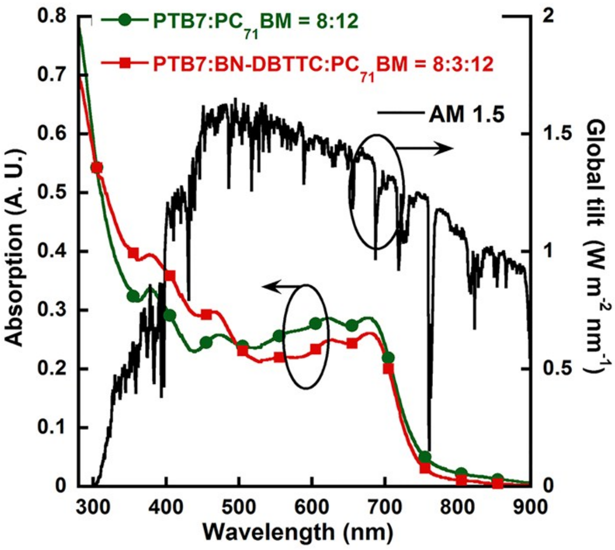

Figure S6. Absorption spectra of binary and ternary blend film with the sun's emission spectrum.

8. Stability

Table S3. Photovoltaic performance of binary and ternary blend BHJ devices under AM1.5G irradiation before and after 20 months' storage in nitrogen atmosphere at room temperature. Each value is the average of 10 devices.

PTB7:BN-DBTTC:$PC_{71}BM$	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)
8: 0: 12	10.60 ± 0.21	0.77 ± 0.01	48.16 ± 0.52	3.91 ± 0.17
after 20 months	7.64 ± 0.23 **(27.9%↓)**	0.71 ± 0.01 **(7.8%↓)**	37.49 ± 0.59 **(22.2%↓)**	2.04 ± 0.09 **(47.8%↓)**
8: 3: 12	12.96 ± 0.20	0.81 ± 0.01	45.01 ± 0.77	4.75 ± 0.09
after 20 months	10.21 ± 0.25 **(21.2%↓)**	0.79 ± 0.01 **(2.5%↓)**	43.14 ± 0.48 **(4.2%↓)**	3.48 ± 0.11 **(26.7%↓)**