Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information

High-efficiency Ternary Polymer Solar Cells with Optimized Morphology of Active Layers Enabled by Few-Layered β-InSe Nanosheets

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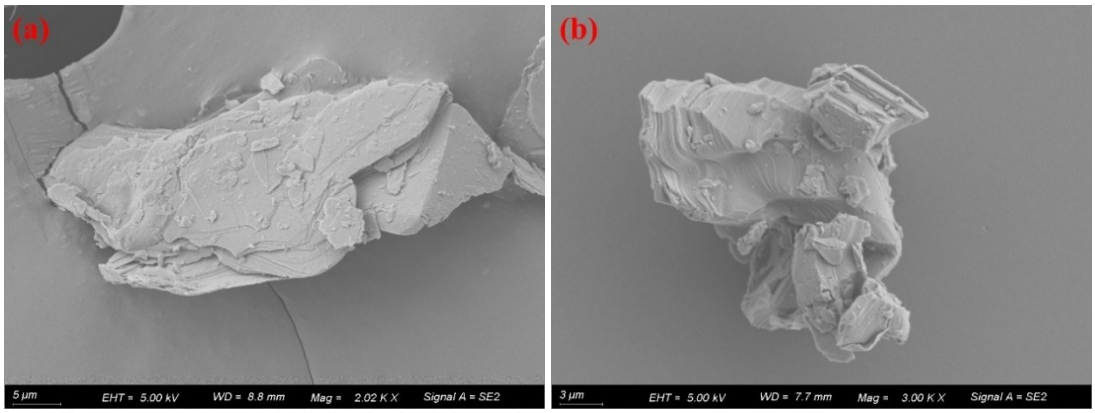

Figure S1. SEM images of bulk β-InSe.

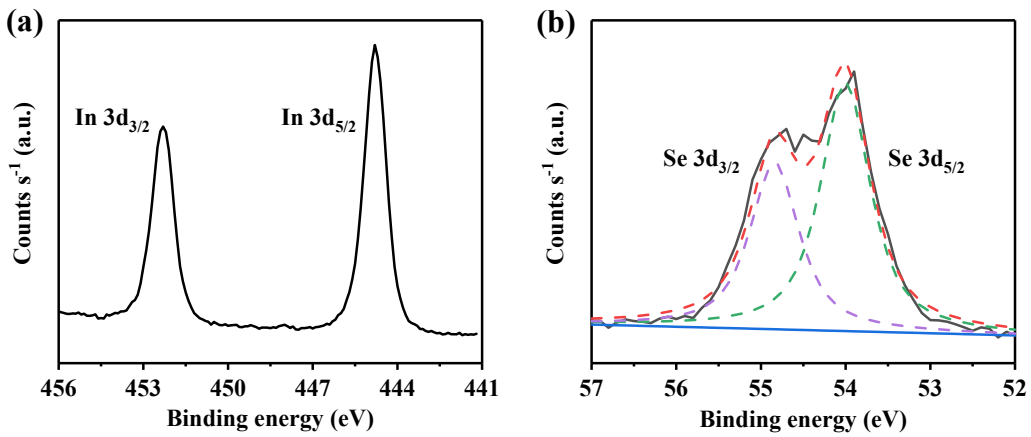

Figure S2. XPS spectra of the (a) In 3d and (b) Se 3d for the bulk β-InSe.

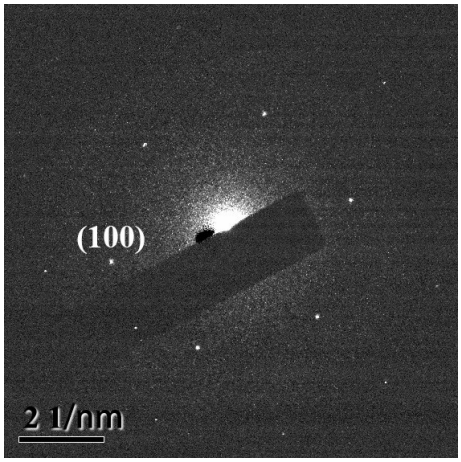

Figure S3. SAED pattern of a β-InSe nanosheet.

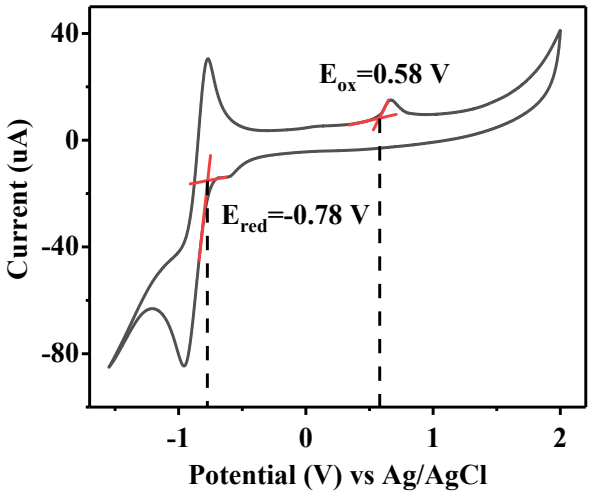

Figure S4. Cyclic voltammogram (*vs*. Ag/AgCl) of few-layered β-InSe.

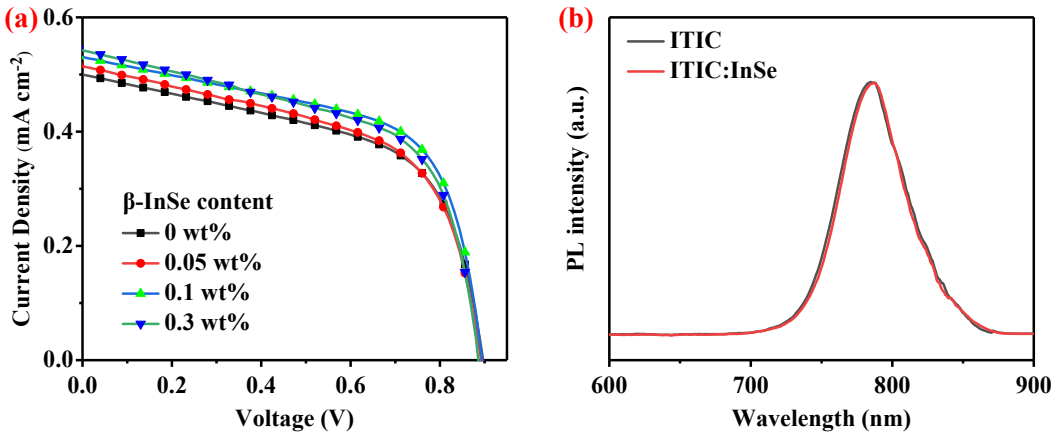

Figure S5. (a) *J-V* curves of cells with PBDB-T:β-InSe (0, 0.05 wt%, 0.1 wt% and 0.3 wt%) as active layers. (b) PL spectra of ITIC and ITIC:β-InSe.

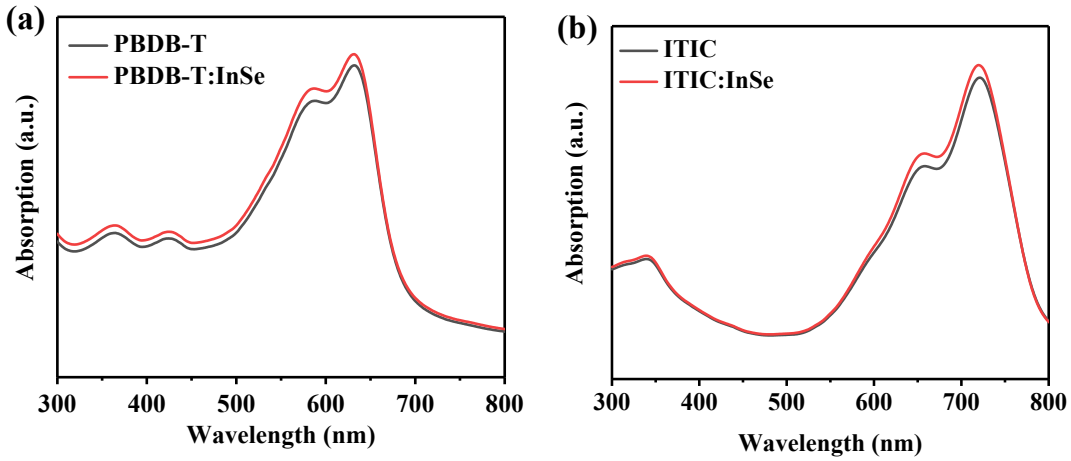

Figure S6. (a) Optical absorption spectra of PBDB-T and PBDB-T:β-InSe. (b) Optical absorption spectra of ITIC and ITIC:β-InSe.

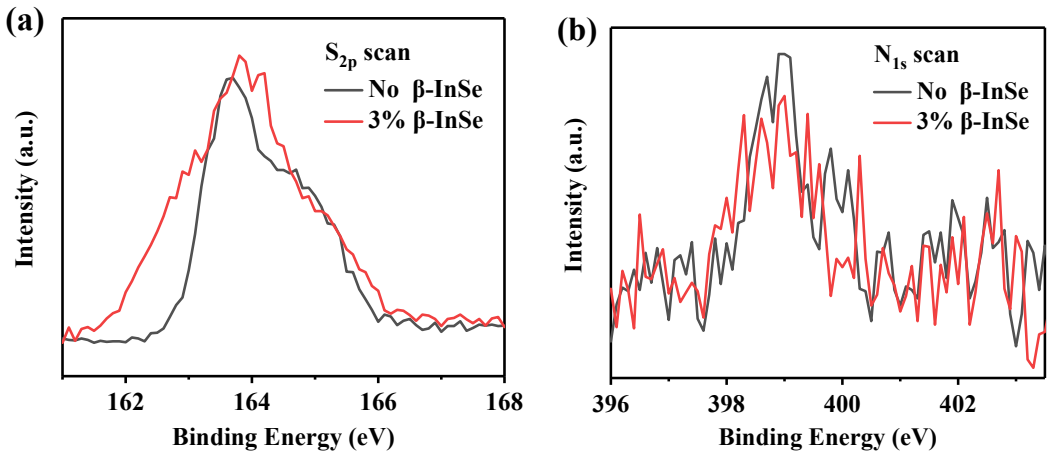

Figure S7. XPS spectra of the (a) S 2p region and (b) N 1s region obtained from PBDB-T:ITIC films with 0 and 0.3 wt% β-InSe.

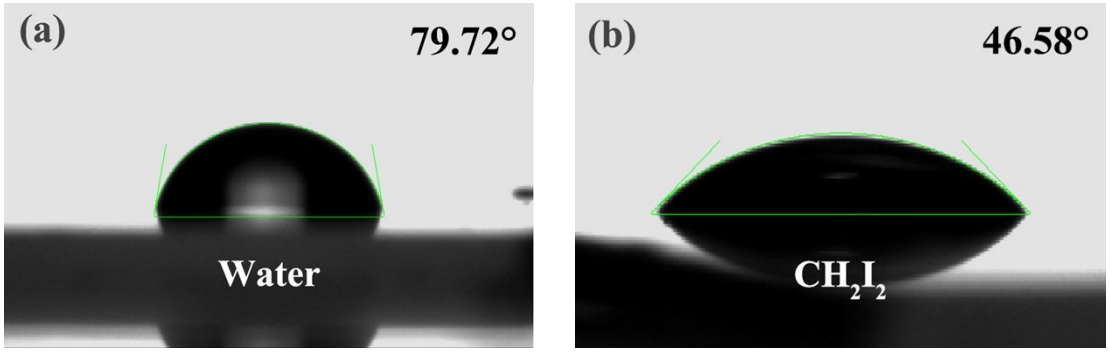

Figure S8. Contacts angles of (a) water and (b) CH_2I_2 on few-layered β-InSe film.

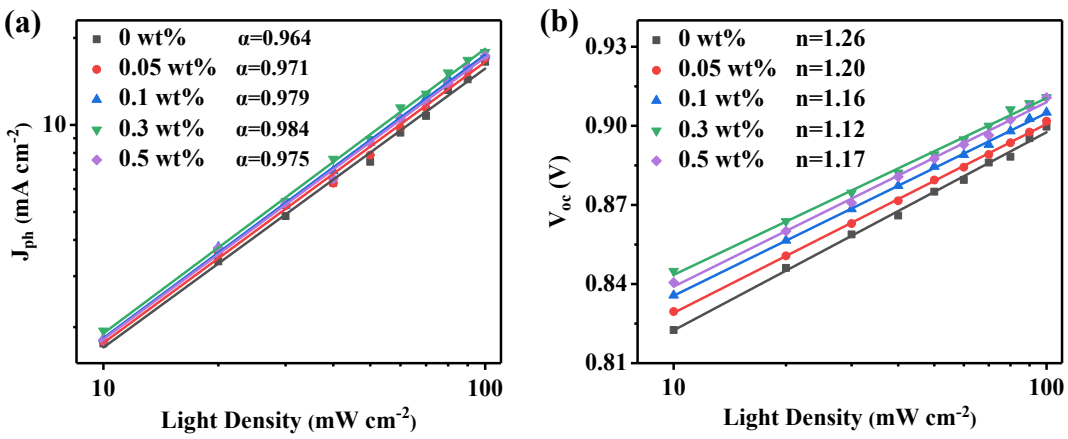

Figure S9. (a) J_{sc} and (b) V_{oc} versus light intensity characteristics of PBDB-T:ITIC:β-InSe-based PSCs with different additive ratio of β-InSe.

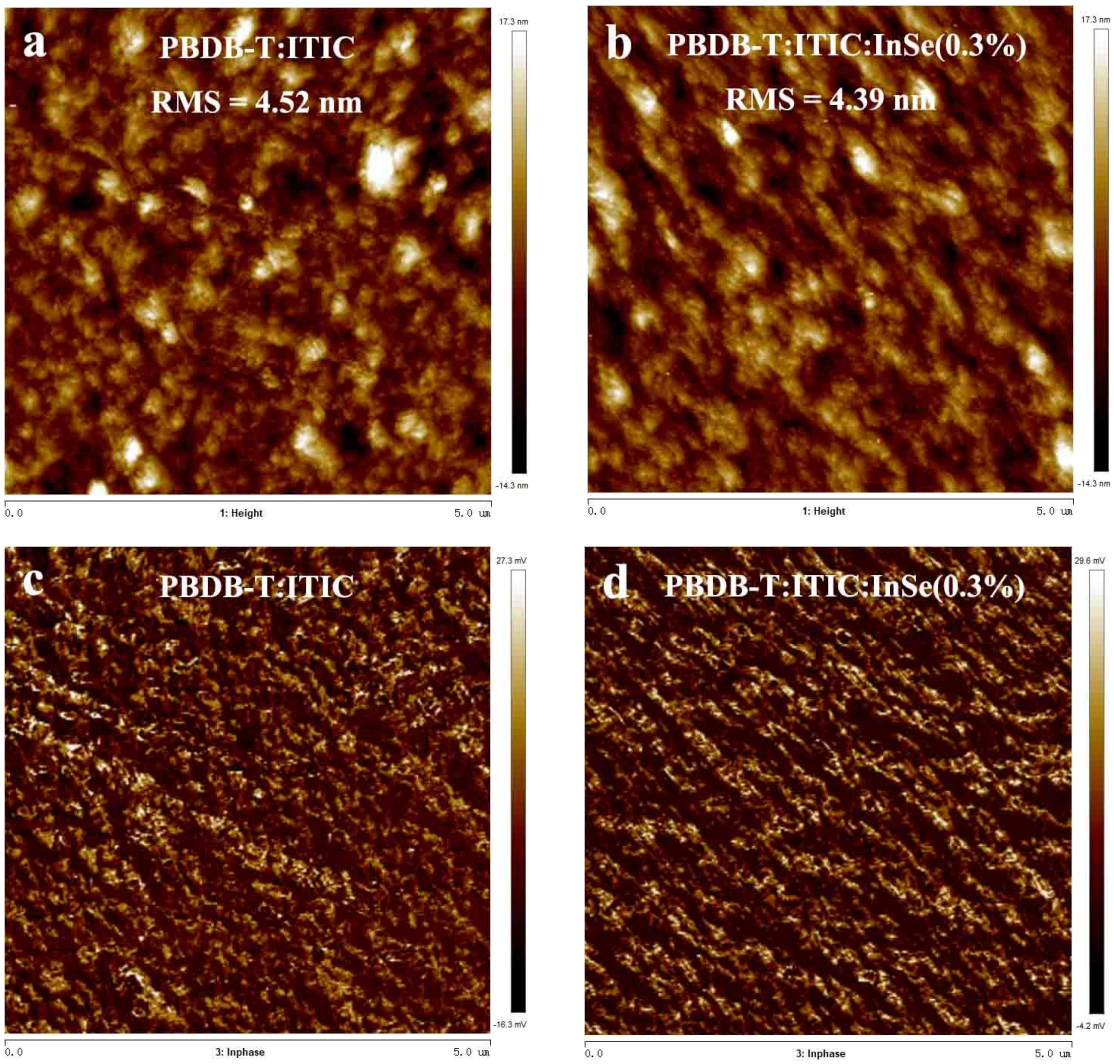

Figure S10. AFM (a) height images and (c) phase image of PBDB-T:ITIC film after storing 183 days; AFM (b) height images and (d) phase image of PBDB-T:ITIC:β-InSe (0.3 wt%) film after storing 183 days.

Table S1. Detailed photovoltaic parameters of the PM6:Y6:β-InSe-based PSCs with different additive ratios of β-InSe.

Active layer	Concentration	J_{sc} (mA cm^{-2})	Calculated J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)
PM6:Y6:β-InSe	0	24.71	23.86	0.83	73.35	15.02±0.20
	0.05 wt%	25.19	24.15	0.83	74.63	15.60±0.19
	0.1 wt%	25.56	24.62	0.83	75.42	16.01±0.17
	0.3 wt%	25.96	25.03	0.83	76.53	16.55±0.17
	0.5 wt%	25.45	24.50	0.83	75.31	15.92±0.18

Table S2. The diffraction vector values and crystal correlation lengths of the diffraction peaks in blend films.

Blend film	Diffraction vector ($Å^{-1}$)		CCL (nm)	
	OOP (010)	IP (100)	OOP (010)	IP (100)
PBDB-T:ITIC	1.66	0.30	2.27	8.89
PBDB-T:ITIC:β-InSe (0.3 wt%)	1.67	0.30	2.39	10.26
PBDB-T:ITIC:β-InSe (0.5 wt%)	1.68	0.30	2.56	12.38

Table S3. XPS results of the surface of the PBDB-T:ITIC:β-InSe (0 and 0.3 wt%) films.

Active layer	Atomic concentration (%)		S/N Ratio
PBDB-T:ITIC	S_{2p}	6.54	5.74
	N_{1s}	1.14	
	C_{1s}	89.62	
	O_{1s}	2.70	
PBDB-T:ITIC:β-InSe (0.3 wt%)	S_{2p}	3.50	10.61
	N_{1s}	0.33	
	C_{1s}	93.41	
	O_{1s}	2.75	

Table S4. Calculated surface .energy components of β-InSe film.

Contact angle				
θ_{water} (°)	$\theta_{CHI_2I_2}$ (°)	γ_s^d (mN m^{-1})	γ_s^p (mN m^{-1})	γ_s (mN m^{-1})
79.72	46.58	31.93	5.35	37.28

Table S5. Summary of J_{sat}, J_{max}, J_{sc}, G_{max}, J_{max}/J_{sat} and J_{sc}/J_{sat} values obtained from the PBDB-T:ITIC-based devices and the ternary devices with different concentrations of β-InSe.

Doping concentration	J_{sat} (mA cm^{-2})	J_{max} (mA cm^{-2})	J_{sc} (mA cm^{-2})	G_{max} (m^{-3} s^{-1})	J_{max}/J_{sat}	J_{sc}/J_{sat}
0	18.94	14.19	16.53	1.184×10^{28}	74.95%	87.28%
0.05 wt%	19.16	14.75	17.02	1.198×10^{28}	76.98%	88.83%
0.1 wt%	19.32	15.10	17.43	1.208×10^{28}	78.17%	90.22%
0.3 wt%	19.51	16.00	17.85	1.219×10^{28}	82.01%	91.49%
0.5 wt%	19.28	15.03	17.34	1.205×10^{28}	77.95%	89.94%

Table S6. Electron and hole mobility of the PBDB-T:ITIC:β-InSe devices with different concentrations of β-InSe.

Doping concentration	μ_e (cm^2 V^{-1} s^{-1})	μ_h (cm^2 V^{-1} s^{-1})	μ_e/μ_h
0	1.87×10^{-4}	3.07×10^{-4}	0.61
0.05 wt%	2.60×10^{-4}	3.69×10^{-4}	0.70
0.1 wt%	3.78×10^{-4}	4.95×10^{-4}	0.76
0.3 wt%	4.52×10^{-4}	5.60×10^{-4}	0.81
0.5 wt%	3.63×10^{-4}	4.73×10^{-4}	0.76