Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Quantitative correlation of the effects of crystallinity and additive on nanomorphology and solar cell performance of isoindigo-based copolymers

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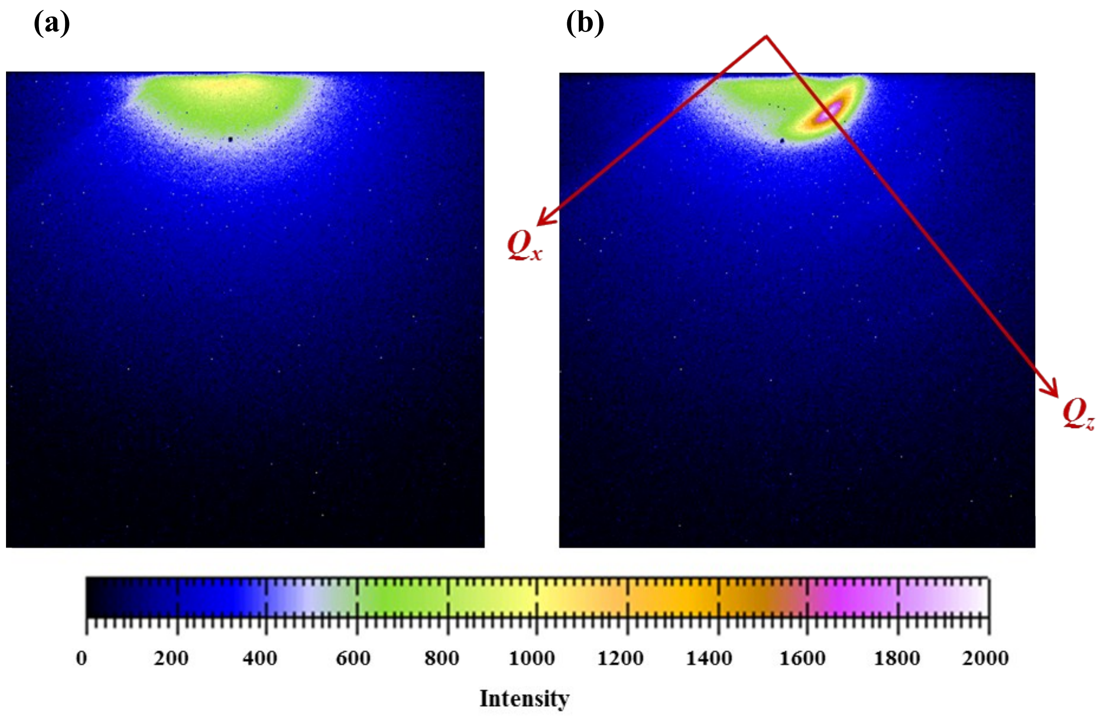

Fig. S1 Two-dimensional GIWAXS patterns of (a) P3TI and (b) P6TI.

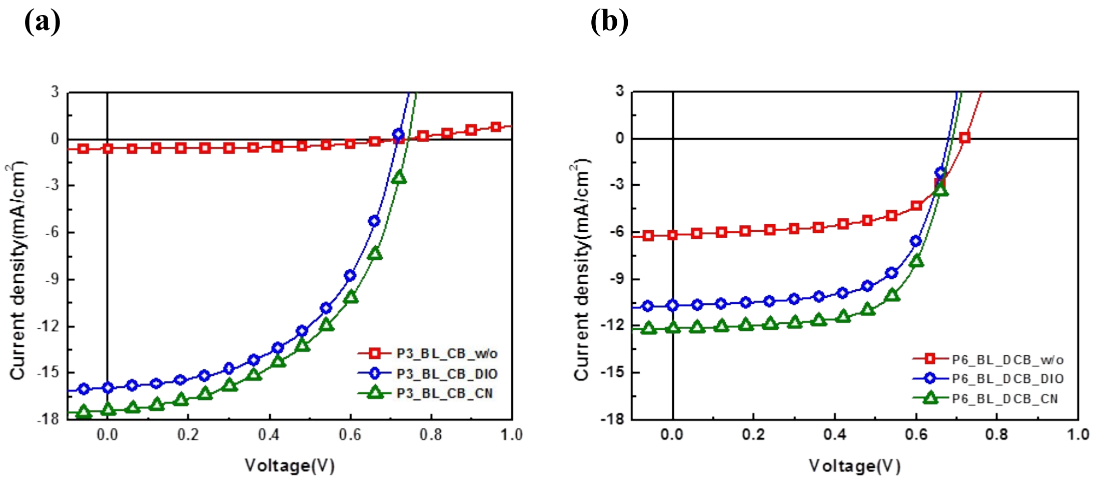

Fig. S2 Current density-voltage curves of the devices processed with CB and DCB as host solvent, respectively, (a) P3TI:$PC_{71}BM$ and (b) P6TI:$PC_{71}BM$.

Table S1 Characteristics of P3TI:$PC_{71}BM$ and P6TI:$PC_{71}BM$ devices processed with CB and DCB as host solvent, respectively.

Sample	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)	PCE $_{max}$ (%)
P3_BL_CB_w/o	0.70±0.02	0.61±0.07	50.01±0.96	0.22±0.02	0.24
P3_BL_CB_DIO	0.71±0.01	16.78±0.91	48.81±4.10	5.81±0.15	5.93
P3_BL_CB_CN	0.74±0.01	16.96±0.31	48.27±1.33	6.09±0.27	6.45
P6_BL_DCB_w/o	0.73±0.01	6.00±0.22	59.63±0.83	2.60±0.06	2.67
P6_BL_DCB_DIO	0.68±0.01	10.53±0.15	63.90±0.27	4.55±0.08	4.66
P6_BL_DCB_CN	0.70±0.01	12.01±0.29	64.67±1.31	5.41±0.02	5.43

The GIWAXS profiles show that the crystallinites of P3TI polymers processed with CB and DCB are low. The Table S1 shows that the role of additive is more pronounced for P3TI (PCE enhancement from ~0.2% to ~6%) than that of P6TI. The effect of solvent additives on the morphology of devices based on P3TI:$PC_{71}BM$ in DCB and CB as host solvent are measured by atomic force microscopy (AFM), as shown in Fig. S3. From the AFM images, the serious phase separation was shown in the pristine P3TI:$PC_{71}BM$ films without solvent additives; especially when the CB was used as host solvent. The poor PCE (0.24%) of the devices is resulted from the lack of bi-continuous transport network path for the charges. The extent of phase separation can be effectively reduced by either DIO or CN. As shown in the AFM images, the addition of DIO and CN shows the similar morphology with well-dispersed small domains, and the devices with DIO and CN also exhibits similar enhanced PCE of 5.93% and 6.45%, respectively. Fig. S4 shows the AFM images of devices based on P6TI:$PC_{71}BM$ in DCB and CB. The morphology of the printing P6TI:$PC_{71}BM$ film is similar to that of the pristine P3TI:$PC_{71}BM$ film. In addition, we can find the morphologies of P6TI:$PC_{71}BM$ devices processed with CB or DCB as host solvent are strongly influenced by the use of DIO or CN toward fine phase separation. These results imply that the solvent additives are indispensable for either P3TI or P6TI because the DCB or CB cannot be used independently to form a well-mixing phase separation, especially in CB. Our study focused on the effect of various solvent additives on the PnTI with different crystallinity. The trends of PCE variation are similar regardless of using DCB or CB. Therefore, for the optimal PCE, we adopted P3TI- and P6TI-based processed with the host solvents of DCB and CB, respectively.

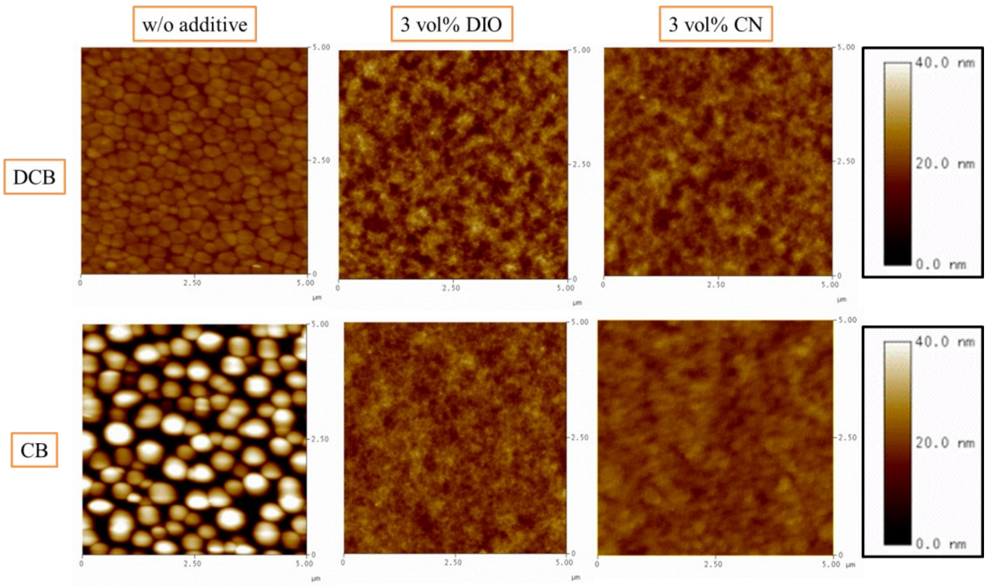

Fig. S3 AFM images of active layers based on P3TI:$PC_{71}BM$ in DCB and CB.

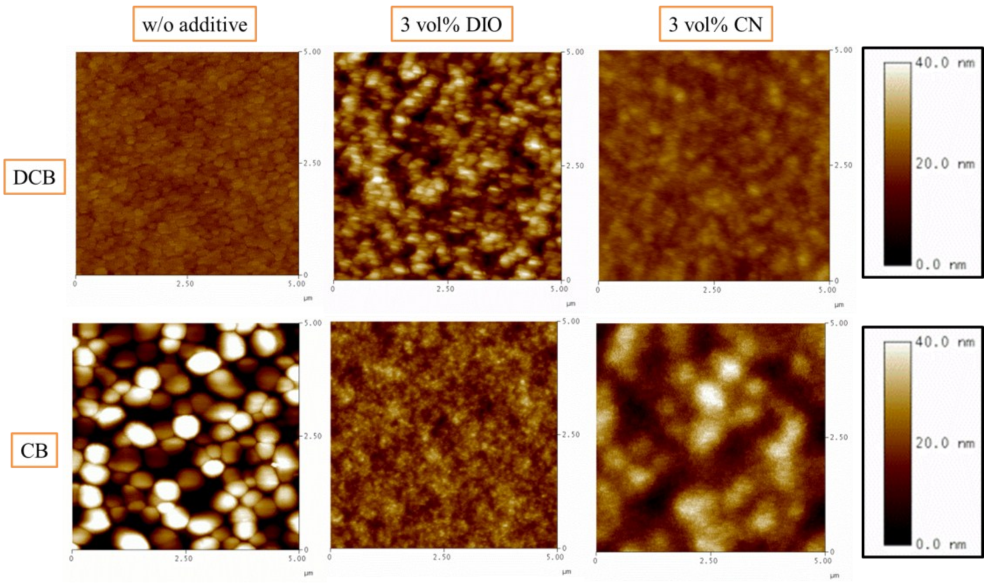

Fig. S4 AFM images of active layers based on P6TI:$PC_{71}BM$ in DCB and CB.