

Supporting information for:

Reducing the confinement of PBDB-T to ITIC to improve the crystallinity of PBDB-T/ITIC blends

Qiuju Liang,^{1,2} Jie Han,³ Chunpeng Song,³ Xinhong Yu,¹ Detlef-M. Smilgies,⁴ Kui Zhao,^{4,5*} Jiangang Liu^{1,*} and Yanchun Han^{1,*}

¹ State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

² University of the Chinese Academy of Sciences, Beijing 100049, P. R. China

³ State Key Laboratory of High Power Semiconductor Lasers, Changchun University of Science and Technology, Changchun 130022, P. R. China

⁴ Cornell High Energy Synchrotron Source, Cornell University, Ithaca, NY 14850, USA.

⁵ Key Laboratory of Applied Surface and Colloid Chemistry, National Ministry of Education, Shaanxi Key Laboratory for Advanced Energy Devices, Shaanxi Engineering Lab for Advanced Energy Technology, School of Materials Science and Engineering, Shaanxi Normal University, Xi'an 710119, China

* To whom correspondence should be addressed,

E-mail: E-mail: zhaok@snnu.edu.cn; (Kui Zhao) niitawh@ciac.ac.cn (Jiangang Liu), ychan@ciac.ac.cn (Yanchun Han)

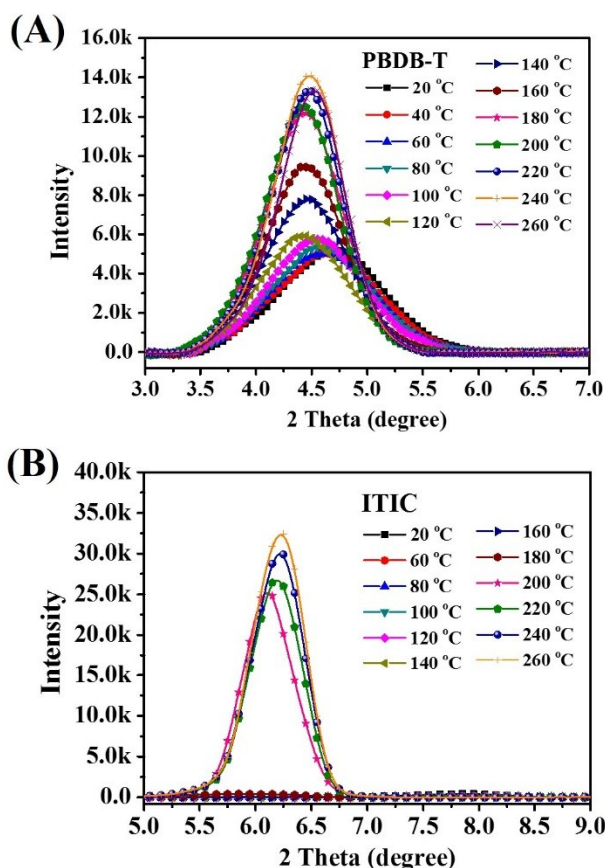


Figure S1 The XRD diffraction profiles of neat PBDB-T film (A) and neat ITIC film (B) thermal annealed at different temperature.

In order to determine the crystallization temperatures for both PBDB-T and ITIC, we investigated the XRD diffraction intensity of ITIC film and PBDB-T film thermal annealed at different temperature (Figure S1). The diffraction peaks located at around 22.5° and around 4.5° corresponds to the (010) plane of ITIC and the (100) plane of PBDB-T, respectively.

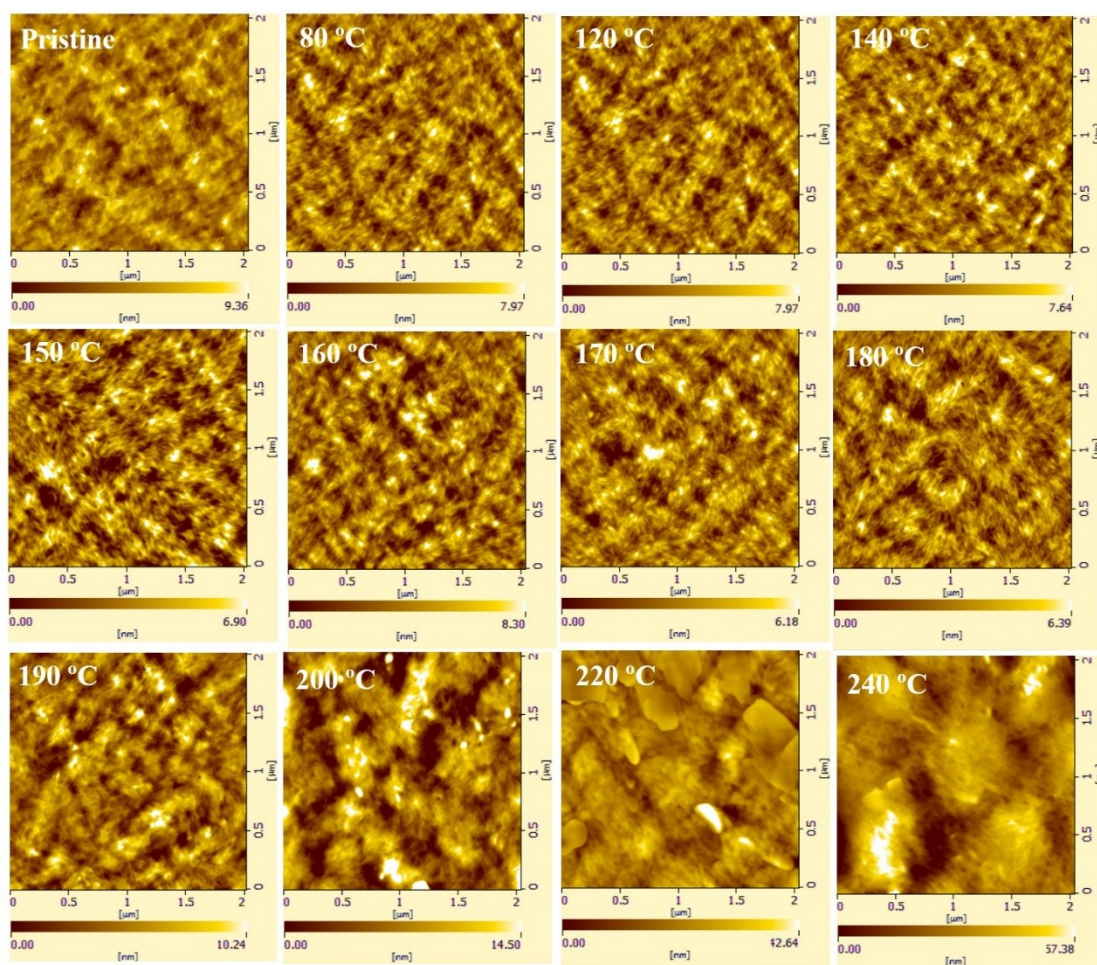


Figure S2 The AFM images of PBDB-T/ITIC blend films TA treated at different temperature for 30 min.

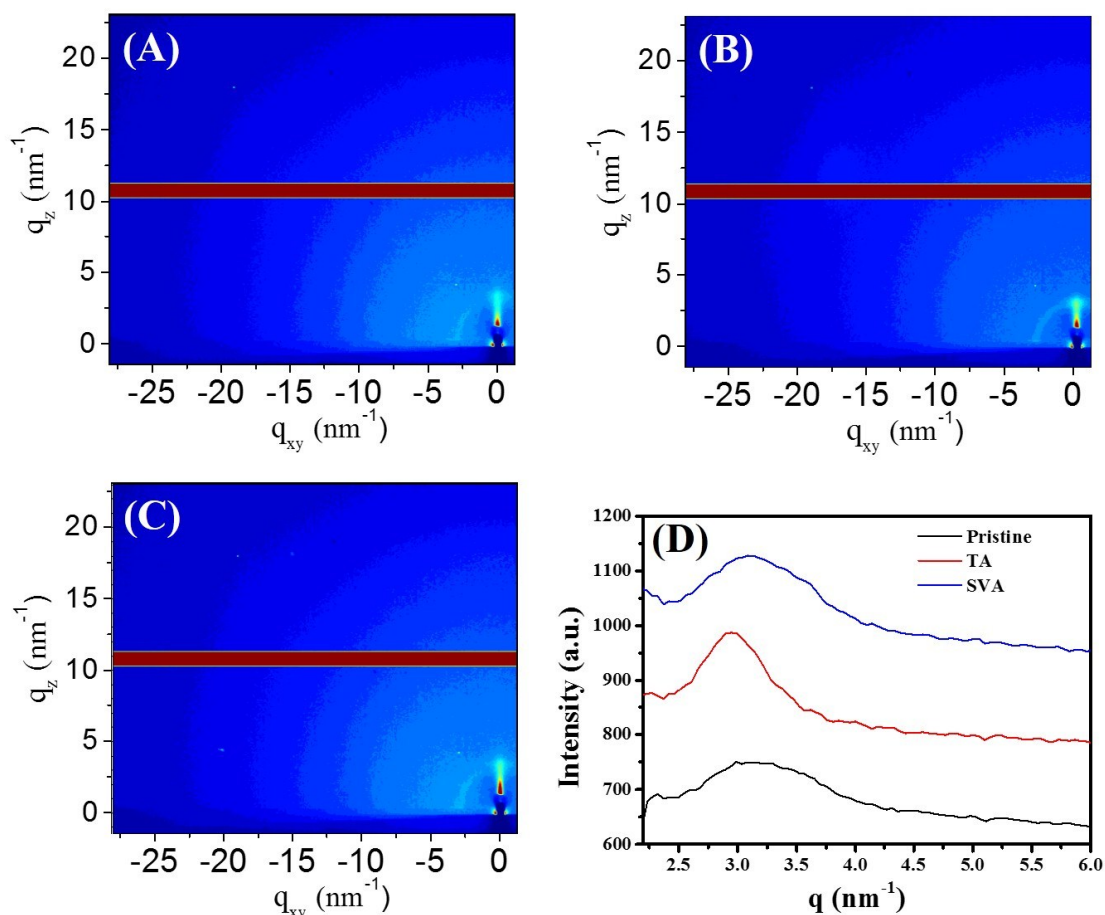


Figure S3 The GIWAXS diffraction profiles of PBDB-T/ITIC blend film without annealing (A), with TA treatment under 150 °C for 30 min (B) and with THF SVA for 30 s (C), The intensity vs. q for the diffraction features of PBDB-T/ITIC blend films without and with different annealing (D).

The selectively controlling crystallinity of PBDB-T also works in the PBDB-T/ITIC blend system. As shown in Figure S3(B) and (D), in which the diffraction intensity of PBDB-T increased after TA, while it had almost no influence on the crystallinity of ITIC. This SVA treatment also works in PBDB-T/ITIC blend system as shown in Figure S3 (C) and (D). After SVA, only the crystallinity of ITIC got enhanced, and it had almost no influence on the crystallinity of PBDB-T.

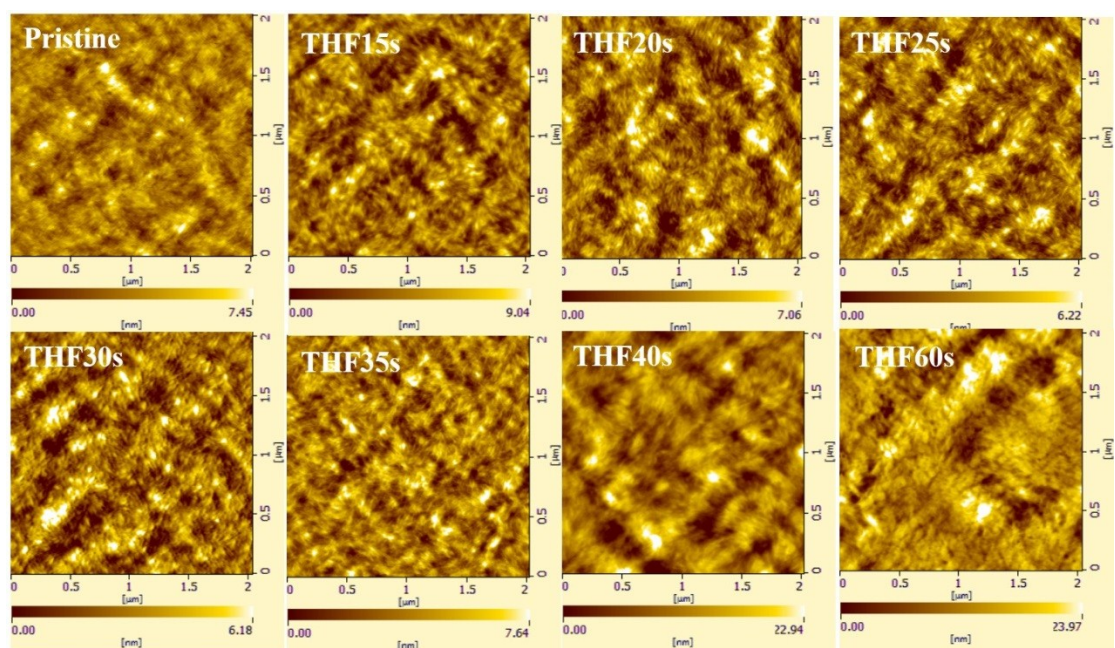


Figure S4 The AFM images of PBDB-T/ITIC blend films treated by THF SVA for different time.

For the shorter SVA time, the film morphology is similar to the film without SVA. For the longer SVA time, the ITIC dissolves out too much, which destroy the film the phase separation structure. Hence, we chose 30 s as the SVA time. Because the morphology of the film shows proper domain size and obvious fibers as shown in Figure S4.

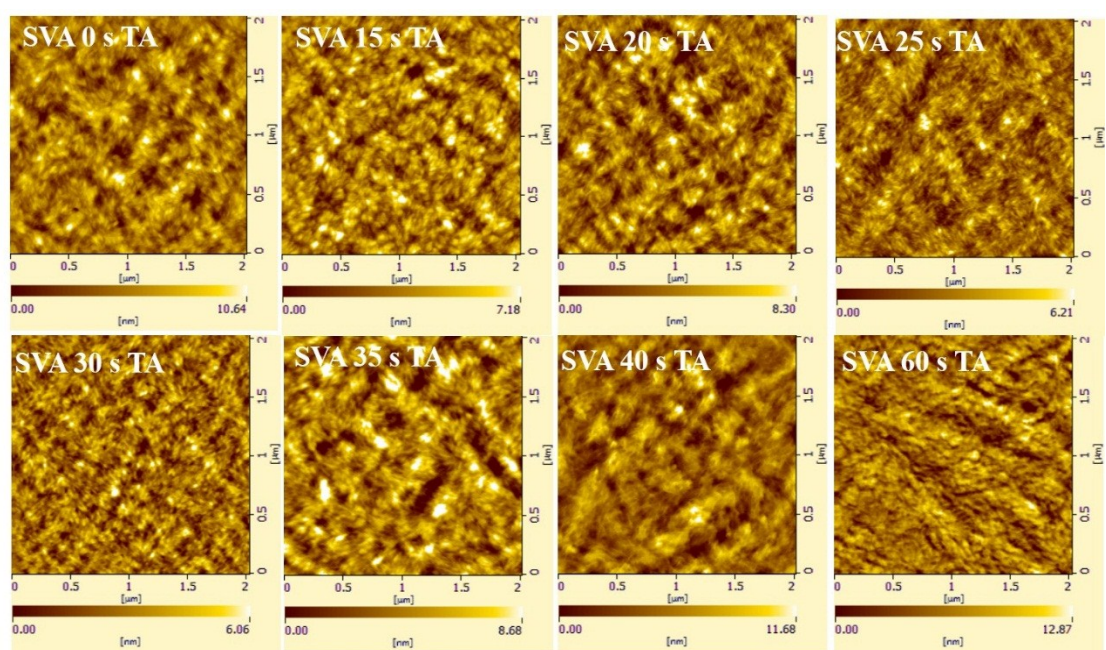


Figure S5 The AFM images of PBDB-T/ITIC blend films treated by THF SVA for different time and then TA treated for 30 min under 150 °C.

Combining Figure S4 and S5, we can conclude that the film morphology is dominated by the SVA process, because the morphology of films first treated by SVA and then TA is similar to that of the films SVA treated for the same time.

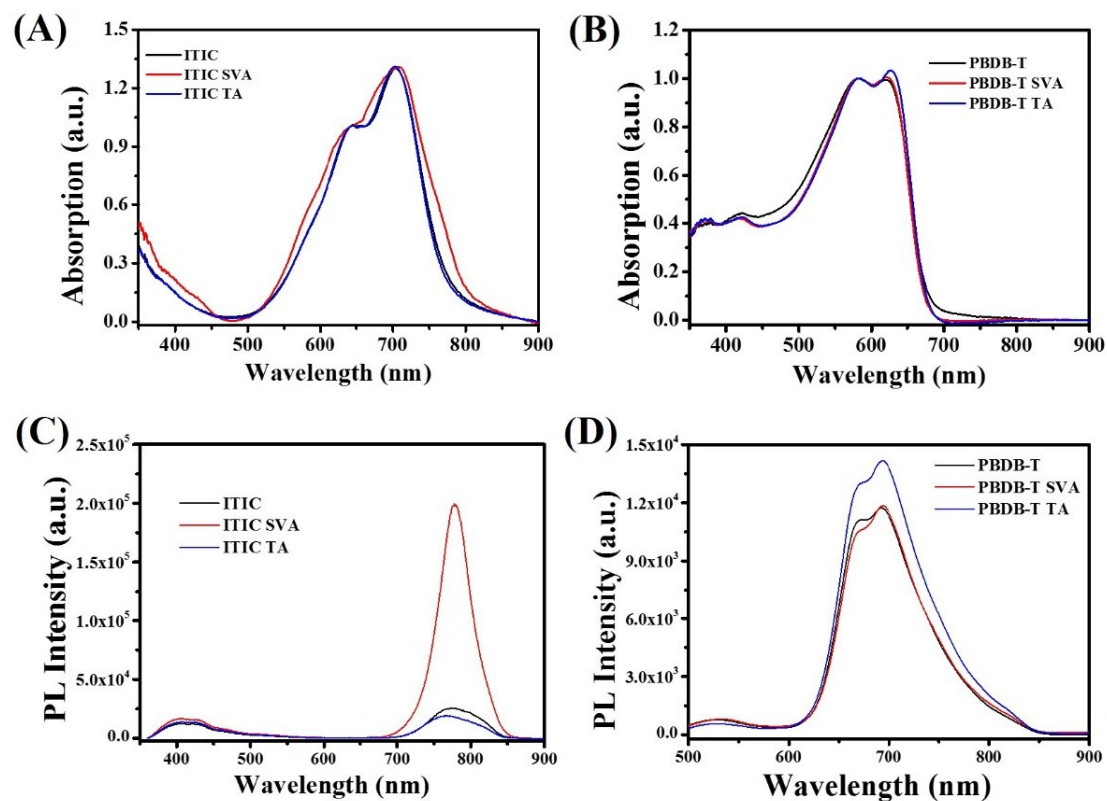


Figure S6 The UV-vis spectra of films without and with SVA, TA treatment of ITIC (A) and PBDB-T (B). The PL spectra of films without and with SVA, TA treatment of ITIC (A) and PBDB-T (B).

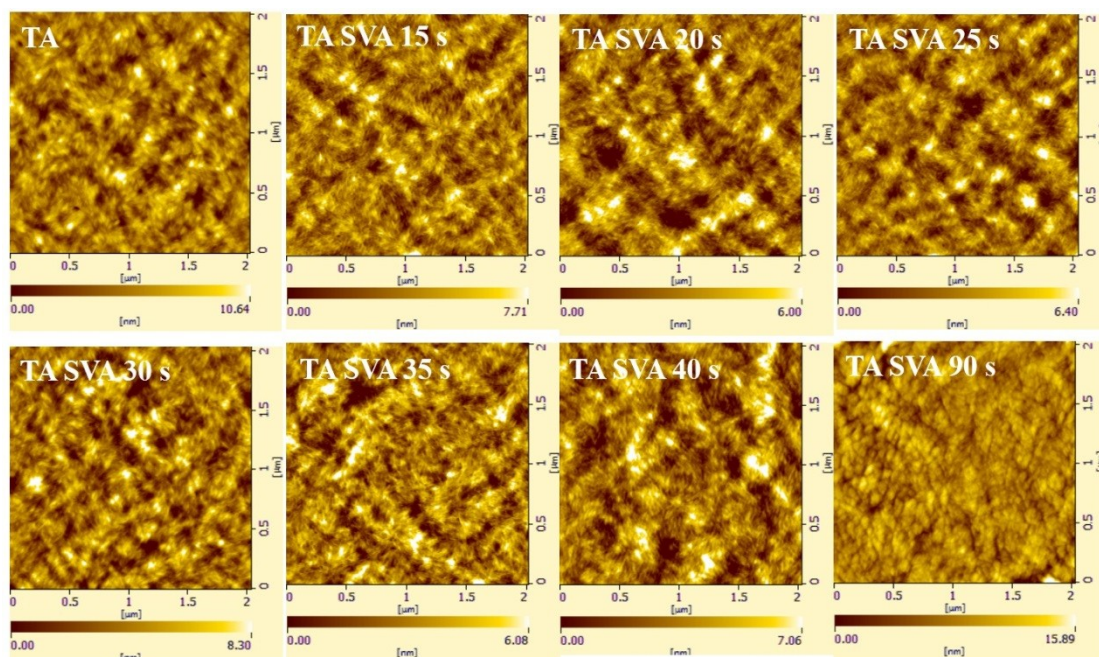


Figure S7 The AFM images of PBDB-T/ITIC blend films TA treated for 30 min under 150 °C and then THF SVA treated for different time.

We can see ITIC is difficult to diffuse out from the crystallized PBDB-T network due to the confinement. However, when the SVA time is long enough, the ITIC can diffuse out from the crystallized PBDB-T network. Once the ITIC diffuse out, the phase separation structure is out of control as shown in Figure S7.

	V_{OC} (V)	J_{SC} (mA/cm ²)	FF	PCE (%)
Pristine	0.89	14.75	0.62	8.14
SVA 15 s	0.89	14.81	0.64	8.43
SVA 30 s	0.89	15.27	0.68	9.24
SVA 40 s	0.82	8.31	0.45	3.06
SVA 60 s	0.17	0.35	0.27	0.02

Table S8 The photovoltaic parameters of the PBDB-T/ITIC blend film SVA treated for different time.

	V_{oc} (V)	J_{sc} (mA/cm ²)	FF	PCE (%)
TA	0.89	16.11	0.69	9.89
TA & SVA 15 s	0.89	16.22	0.69	9.96
TA & SVA 30 s	0.89	16.31	0.69	10.01
TA & SVA 40 s	0.88	15.79	0.63	8.75
TA & SVA 90 s	0.12	2.31	0.27	0.07

Table S9 The photovoltaic parameters of the PBDB-T/ITIC blend film TA at 150 °C for 30 min and then SVA treated for different time.

Compare the device performance listed in Table S8 and S9, taking SVA for 40 s and first TA at 150 °C for 30 min and then SVA treated for 40 s as examples, the device performance decreased in different levels. For the only SVA treated device, the device performance dropped from 8.14 to 3.06%, which is caused by the diffusion of ITIC destroying the phase separation structure of the blend film. However, the performance of the blend film TA at 150 °C for 30 min and then SVA for 40 s drops from initial 9.89 to 8.75, which means the phase separation is not destroyed very much. This phenomenon further confirm that the crystallized PBDB-T network confine the diffusion of the ITIC molecules.