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Toward High Performance Photovoltaic Cells based on Conjugated Polymers

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14. ABSTRACT

In the pursuit of high photon-to-electron conversion efficiency of organics photovoltaics, different approaches have been used, such as designing and synthesizing organic molecules with different energy band gap and good packing order for the active layers or constructing tandem devices. In the present study, we adopted a simple concept involving ternary blends that comprises a small amount of a high band-gap small molecule with a molecular structure that was structured to have energy transfer, a low band-gap polymer with good packing order as the active layer for a single-junction photovoltaic device. The light absorptions for the small molecule and the polymer are complementary for enhancing the absorption of the solar spectrum while their energy bands are offset structure for facilitating charge separation. We synthesize the SM-4OMe small molecule and chose the PTB7-Th polymer and blend them with fullerene for being used as active layers to demonstrate our approach. We found that the power conversion efficiency of the device that incorporates a ternary blend of PTB7-Th:SM-4OMe:PC71BM (0.9:0.1:1.5 by weight) as the active layer that was processed with 2 vol% di-iodine octane (DIO) with chlorobenzene (CB) increased to 10.4% from 8% for the device incorporating PTB7-th:PC71BM (1/1.5 weight) active layer that was processed in a similar way, an increase of 30%. This enhancement can be reasonably attributed to the energy transfer from the high band-gap small molecule SM-4OMe to the low band-gap polymer and optimum phase-separated morphology that is owing to a partial mixing of PTB7-th with SM-4OMe because of pi-pi stacking interaction between them since both of them were constructed with the same donor units, BDT.

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Abstract:

In the pursuit of high photon-to-electron conversion efficiency of organics photovoltaics, different approaches have been used, such as designing and synthesizing organic molecules with different energy band gap and good packing order for the active layers or constructing tandem devices. In the present study, we adopted a simple concept involving ternary blends that comprises a small amount of a high band-gap small molecule with a molecular structure that was structured to have energy transfer, a low band-gap polymer with good packing order as the active layer for a single-junction photovoltaic device. The light absorptions for the small molecule and the polymer are complementary for enhancing the absorption of the solar spectrum while their energy bands are offset structure for facilitating charge separation. We synthesize the SM-4OMe small molecule and chose the PTB7-Th polymer and blend them with fullerene for being used as active layers to demonstrate our approach. We found that the power conversion efficiency of the device that incorporates a ternary blend of PTB7-Th:SM-4OMe:PC71BM (0.9:0.1:1.5 by weight) as the active layer that was processed with 2 vol% di-iodine octane (DIO) with chlorobenzene (CB) increased to 10.4% from 8% for the device incorporating PTB7-th:PC71BN (1/1.5 weight) active layer that was processed in a similar way, an increase of 30%. This enhancement can be reasonably attributed to the energy transfer from the high band-gap small molecule SM-4OMe to the low band-gap polymer and optimum phase-separated morphology that is owing to a partial mixing of PTB7-th with SM-4OMe because of pi-pi stacking interaction between them since both were constructed with the same donor units, BDT.

Introduction:

In the pursuit of high photon-to-electron conversion efficiency of organics photovoltaics, different approaches have been used, such as designing and synthesizing organic molecules with different energy band gap and good packing order for the active layers or constructing tandem devices. We adopted a simple concept of ternary blends that comprise a high band-gap small molecule that was designed to have energy transfer, a low band-gap conjugated polymer along with fullerene as the active layer for the photovoltaic devices. The small molecule and the polymer thus have complementary light absorptions for the solar spectrum, and the energy band alignment between that of the small molecule and that of the polymer is designed to have an off-set energy band structure such that charge separation and energy transfer can occur between them. In order to have better interaction between the small molecules and the polymers; the small molecule used, SM-4OMe, has a structure that was constructed from a weak donor, benzodithiophene (BDT) units with π-conjugated spacer on the BDT units in conjugation with electron-deficient moieties on the ends. On the other hand, the conjugated polymer PTB7-th that was used in this study also comprises BDT donor units, and thus it is expected that π-π stacking between the two molecules can take place, which can facilitate the energy transfer between them when they are in close proximity. We synthesized SM-4OMe small molecules and purchased PTB7-th polymers for our study.

Results and Discussion:

Figure 1 shows (a) the chemical structure of the small molecule, SM-4OMe, $PC_{71}BM$ and PTB7-th that were used in the active layer of the photovoltaic devices (b) the UV-Vis absorption spectra of solution and film of SM-4OMe, indicating an band gap of 1.79eV from the onset of absorption (c) the energy bands of PTB7-th, SM-4OMe and $PC_{71}BM$, respectively. The energy band gap of PTB7-th is 1.58 eV as determined in the previous reports.

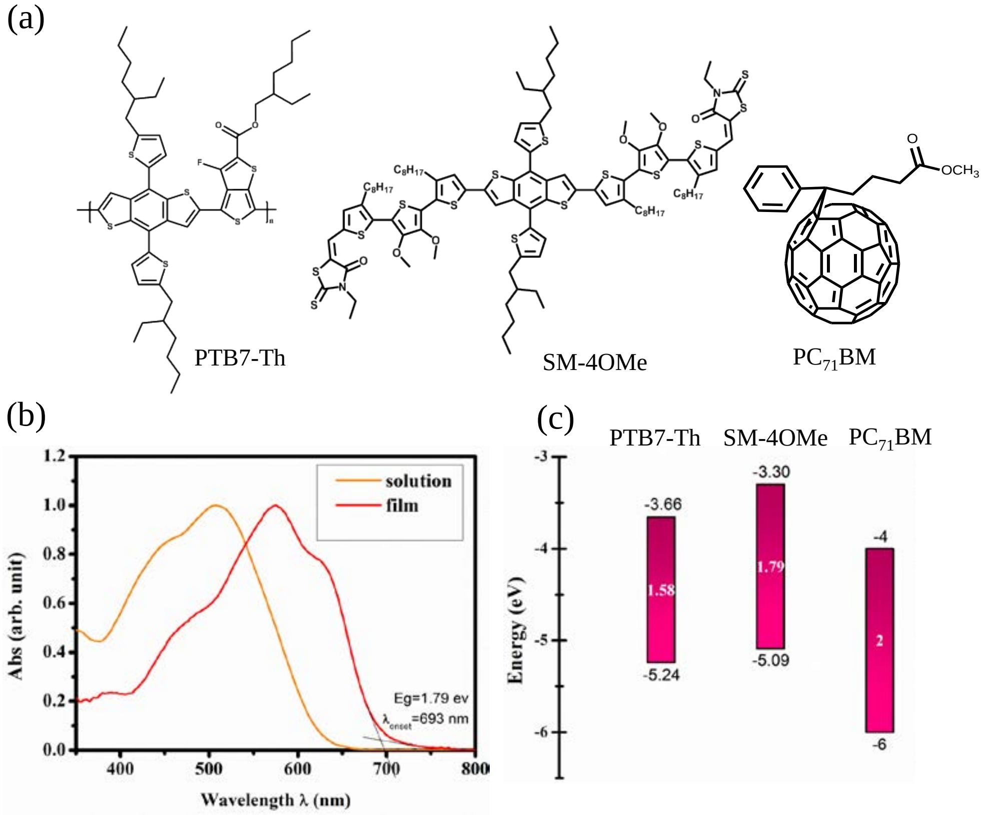
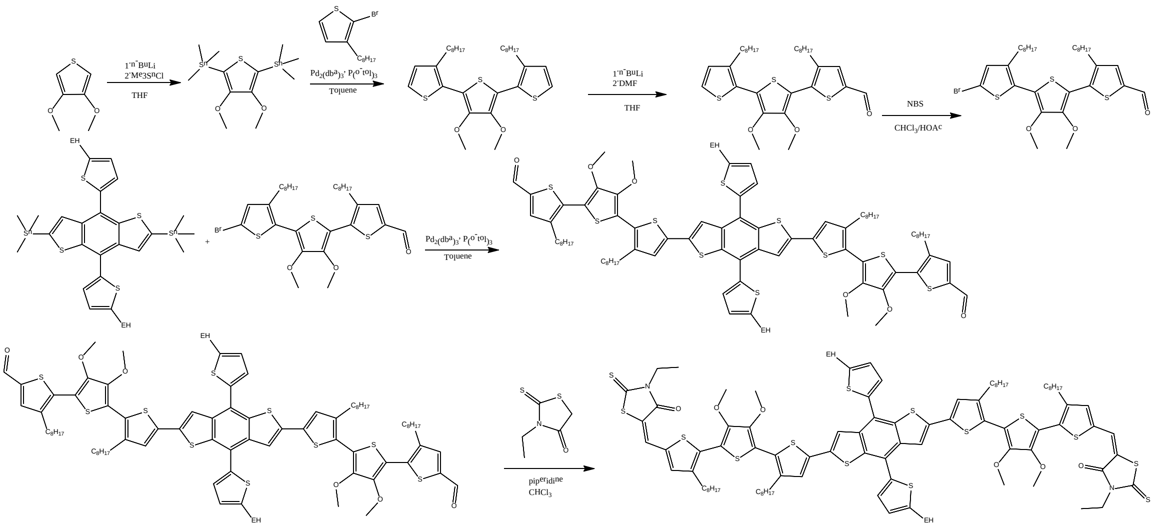


Figure 1: (a) Chemical structures of PTB7-Th, SM-4OMe and $PC_{71}BM$; (b) UV-Vis absorption spectra of SM-4OMe in solution and film states. The onset of absorption indicates a band gap of 1.79 eV; (c) energy level diagram of PTB7-Th, SM-4OMe and $PC_{71}BM$.



Scheme 1: Synthesis and Structures of SM-4OMe

Figure 2 displays (a) the UV-Vis absorption spectra of SM-4OMe, $PC_{71}BM$ and PTB7-th (b) inverted device structures that were used in this study, involving ZnO and MoO_3 layer as electron and hole transport layer, respectively. The peaks at 630 and 725nm are owing to the absorption and aggregated-state absorption, respectively, of PTB7-th while the peak at 560 and 660nm resulted from the absorption and aggregated-state absorption, respectively, for SM-4OMe.

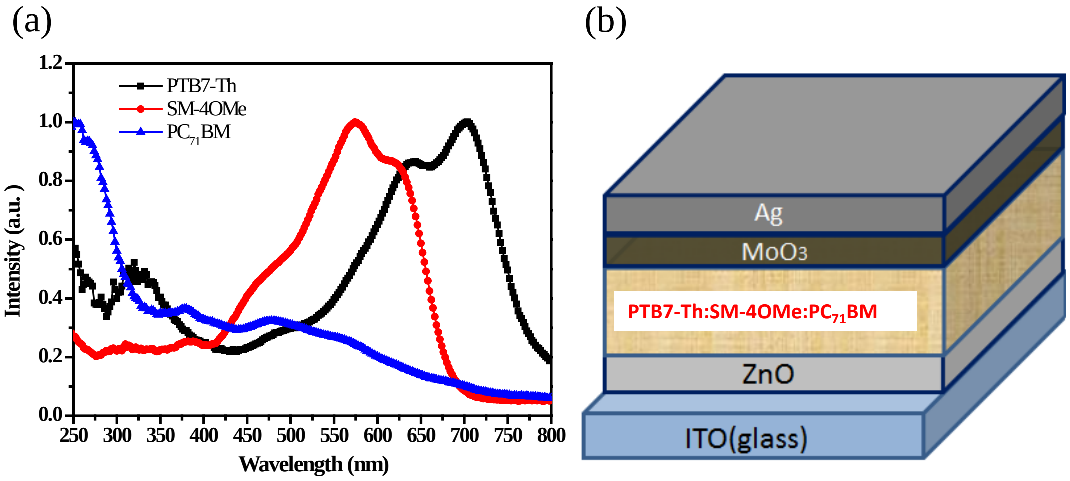


Figure 2: (a) UV-Vis absorption spectra of SM-4OMe, $PC_{71}BM$ and PTB7-Th thin films; (b) inverted device structures that were used in this study, involving ZnO and MoO_3 layer as electron and hole transport layer, respectively.

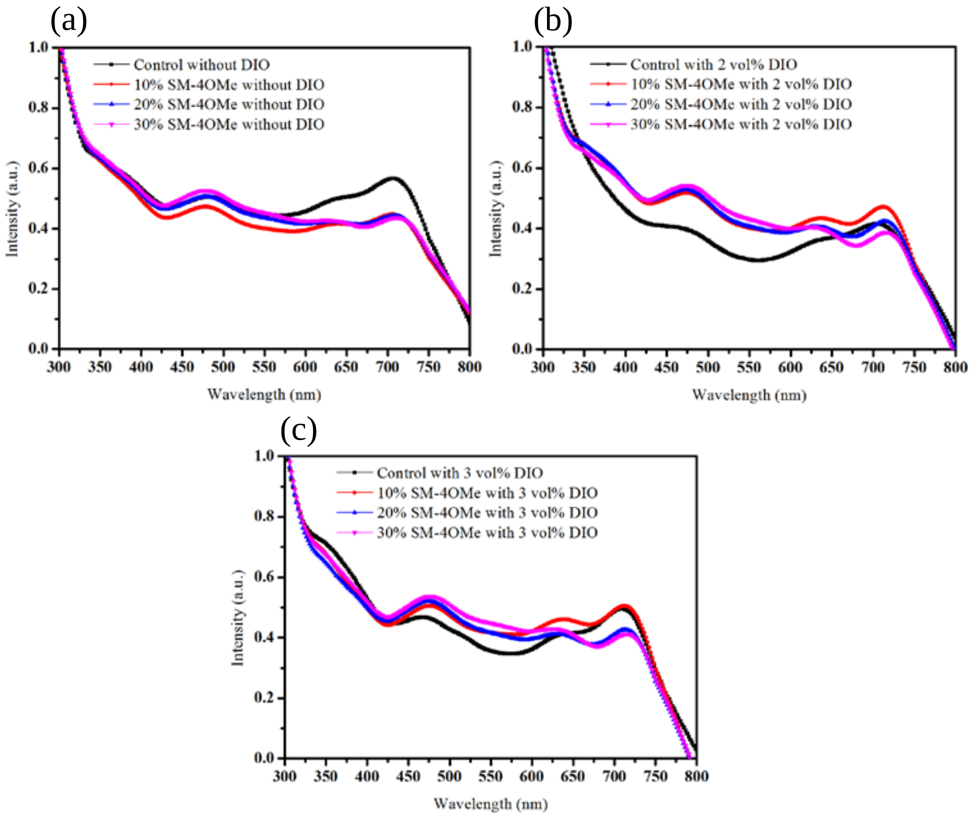


Figure 3. UV-vis absorption spectra of PTB7-Th:SM-4OMe:$PC_{71}BM$ films processed by (a) w/o, (b) 2 vol%, (c) 3 vol% DIO.

Table 1 shows the photovoltaic properties of the devices incorporating active layers comprising PTB7-Th:SM-4OMe:$PC_{71}BM$ with different weight ratio that were processed with 0, 2 and 3 vol% solvent additive DIO.

PTB7-Th:SM-4OMe: $PC_{71}BM$		PCE (%) (best value)	V_{oc} (V)	J_{sc} (mA/cm^2) (best value)	FF (%) (best value)
1-0-1.5	w/o DIO	5.7	0.81	14.9	47.2
	2 vol% DIO	8.0	0.77	15.8	65.6
	3 vol% DIO	9.5	0.79	17.9	66.7
0.9-0.1-1.5	w/o DIO	6.7	0.80	14.8	56.7
	2 vol% DIO	10.4	0.78	18.2	73.0
	3vol% DIO	9.2	0.79	17.6	65.7
0.8-0.2-1.5	w/o DIO	6.4	0.81	13.8	57.0
	2 vol% DIO	9.0	0.78	16.9	68.6
	3 vol% DIO	9.1	0.78	16.6	70.3

0.7-0.3-1.5	w/o DIO	6.5	0.82	13.4	59.1
	2 vol% DIO	7.9	0.79	14.8	67.1
	3 vol% DIO	7.9	0.79	14.9	67.3
0-1-1.5	w/o DIO	0.6	0.7	2.78	31.8
	2 vol% DIO	0.8	0.82	2.28	44.6

The device that incorporates an active layer of PTB7-th:SM-4OMe:$PC_{71}BM$ with a weight ratio of (0.9/0.1/1.5) gives the best power conversion efficiency (PCE) of 6.7% as compared to 5.7% for the case of PTB7:$PC_{71}BM$ (1.0/1.5) device without any solvent additive DIO, as increase of 16%. Because the SM-4OMe:$PC_{71}BM$ (1/1.5) device has only a PCE of 0.6%, owing to low short current density and fill factor, this reflects that either the exciton dissociation in the interfaces between SM-4OMe and $PC_{71}BM$ is not so efficient or the carrier transport in the SM-4OMe and $PC_{71}BM$ phase is not effective, possibly owing to their poor morphology. When a moderate amount of SM-4OMe was added into PTB7:$PC_{71}BM$ that induces energy transfer from SM-4OMe to PTB7-th, the device of PTB7-th:SM-4OMe:$PC_{71}BM$ with weight ratio of (0.9/0.1/1.5) become much more efficient. The device incorporated an active layer of PTB7-th:$PC_{71}BM$(1/1.5) that was processed with 2 vol% DIO in CB give a PCE of 8% as compared to 5.7% for the device with an active layer that was processed without DIO, an increase of 40%, owing to much better molecule packing for PTB7-th and proper fullerene aggregation size. When the small molecules were included in the active for these photovoltaic devices, the power conversion efficiency of the devices increased substantially; for instance, the PCE of the device incorporates an active layer of PTB7-th:SM-4OMe:$PC_{71}BM$ with weight ratio of (0.9/0.1/1.5) increased to 10.4% from a PCE of 8%. This can be explained from the UV-Visible absorption spectra for SM-4OMe and PTB7-th that have its maximum peak at 630 and 750 nm, respectively, indicating not only complementary absorption but also possible energy transfer between them.

Figure 4 shows the X-ray data that indicate crystallinity of the polymers and small molecules increased substantially when a small amount of solvent additive DIO is involved in the processing. It appears that the crystallinity of PTB7-th decreases slightly upon the incorporation of a low concentration (10%) of SM-4OMe, indicating some degree of mixing might have taken place that could result in some degree of energy transfer, but the extent of decrease increase sharply when the concentration of SM-4OMe reaches 20% in case of without DIO. In case of processing with solvent additive DIO with CB, the extent of decrease in the crystallinity becomes moderate.

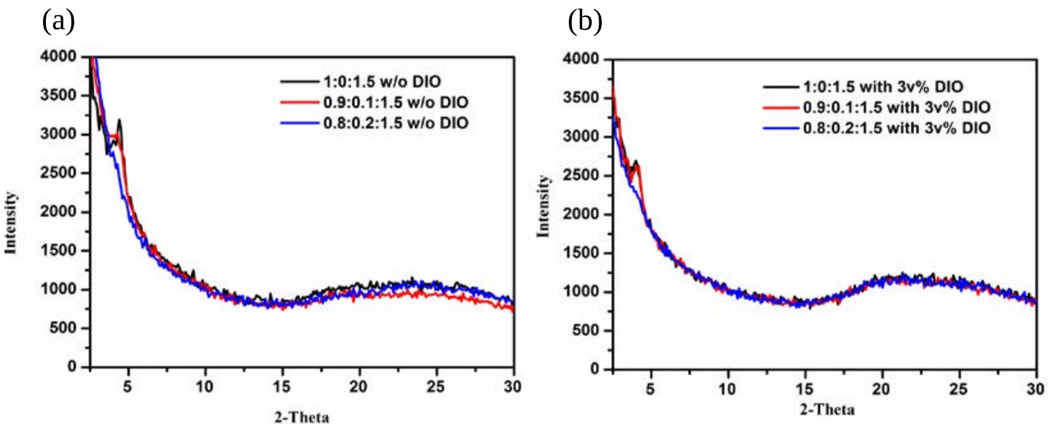
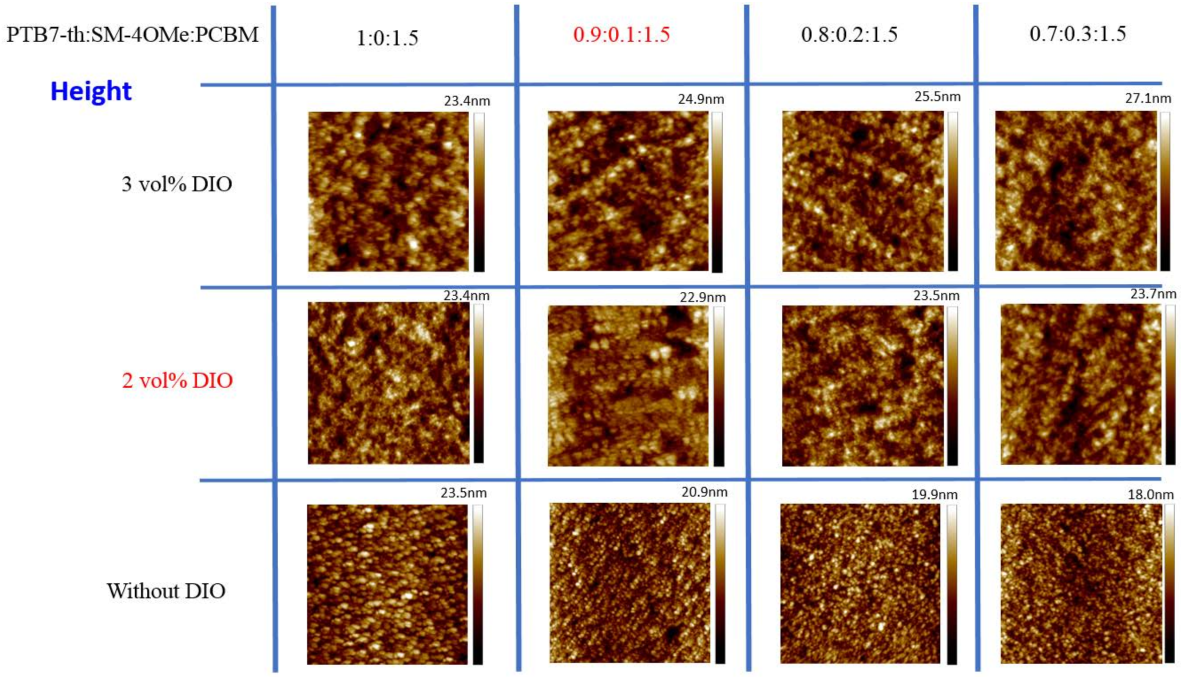


Figure 4: X-ray diffraction profiles of the pristine films with different weight ratios of SM-4OMe.



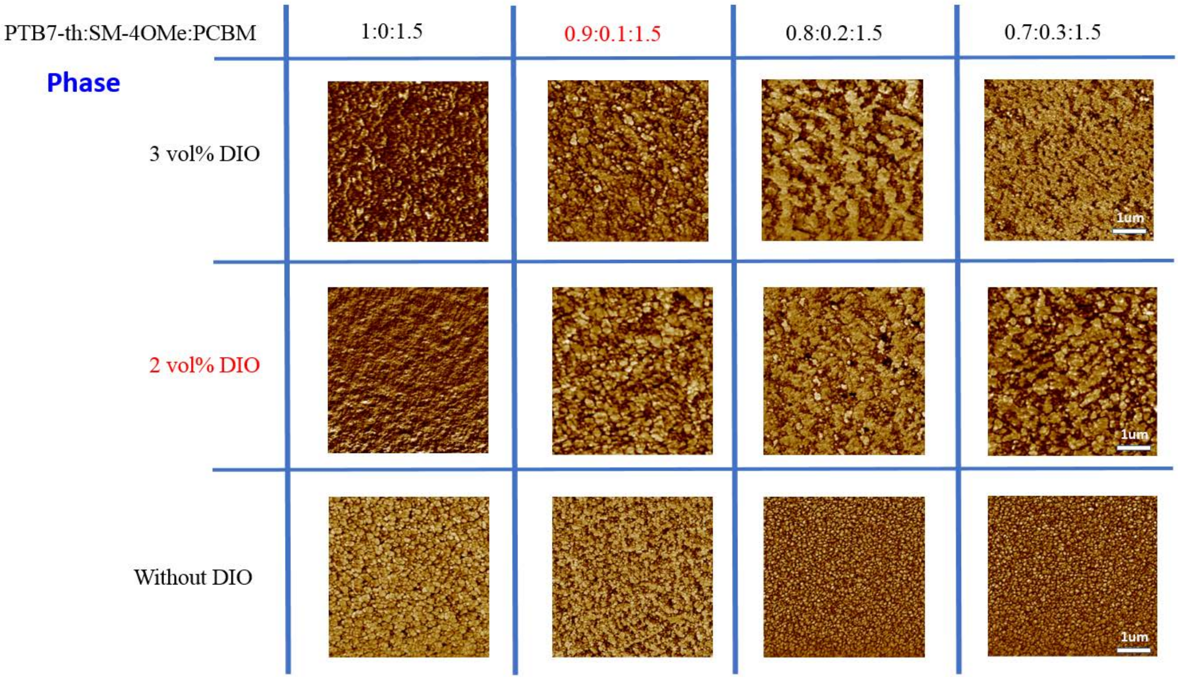


Figure 5: AFM height and phase images (5 × 5 μm) of the ternary blend films with different weight ratios of SM-4OMe

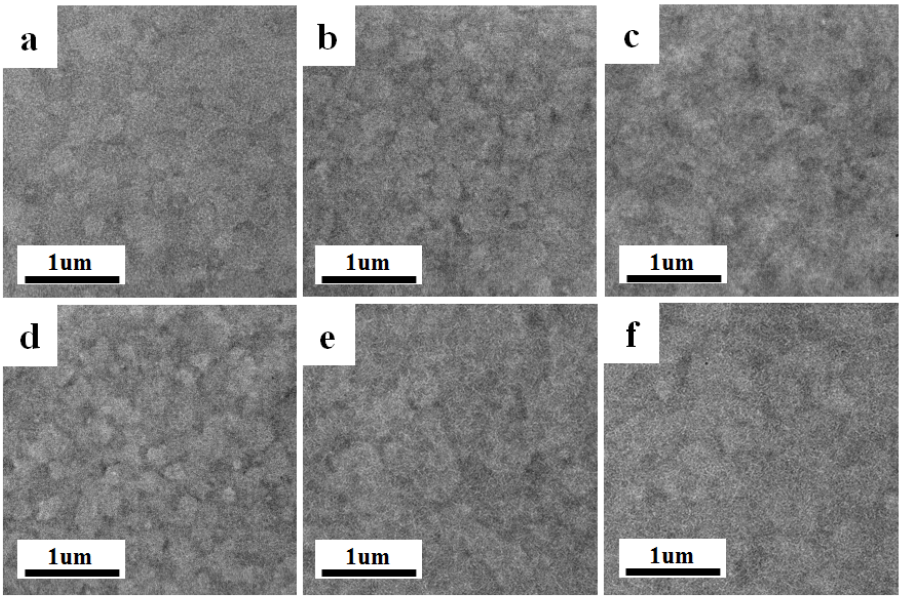


Figure 6: TEM images of films with a composition ratio of (a) 1:0:1.5 with 3 vol% DIO, (b) 0.9:0.1:1.5 with 3 vol% DIO, (c) 0.8:0.2:1.5 with 3 vol% DIO and (d) 0.9:0.1:1.5 with 2 vol% DIO, (e) 0.8:0.2:1.5 with 2 vol% DIO, (f) 0.7:0.3:1.5 with 2 vol% DIO.

Conclusion:

We found the power conversion efficiency of the device incorporates a ternary blends of PTB7-Th:SM-4OMe:$PC_{71}BM$ (0.9:0.1:1.5 by weight) as the active layer that was processed with 2 vol% DIO with CB increased to 10.4% from 8% for the device incorporating PTB7-th:$PC_{71}BM$(1/1.5 by weight) active layer that was processed with 2 vol% DIO in CB, an increase of 30%. This enhancement results from the energy transfer from a high bandgap small molecule SM-4OMe to a low bandgap polymer and optimum phase-separated morphology. This approach presents a simple but significant way for enhancing the absorption of the solar spectrum and thus the power conversion efficiency of polymer photovoltaics.

List of Publications and Significant Collaborations that resulted from your AOARD supported project:

d) manuscript is under preparation.

e) provide a list of any interactions with industry or with Air Force Research Laboratory scientists or significant collaborations that resulted from the work: We are working on a joint publication with Prof. Yang Yang, from UCLA.