Support Inforamation

An Alkylthieno-2-yl Flanked Dithieno[2,3-*d*:*2′*,*3′*-*d′*]benzo-[1,2-*b*:4,5-*b′*]dithiophene-based Low Band Gap Conjugated Polymer for High Performance Photovoltaic Solar Cells

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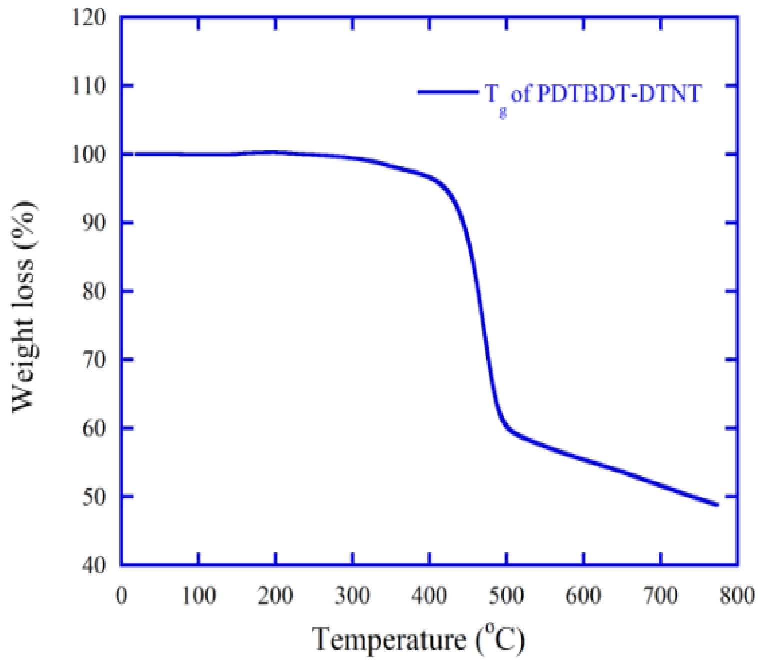
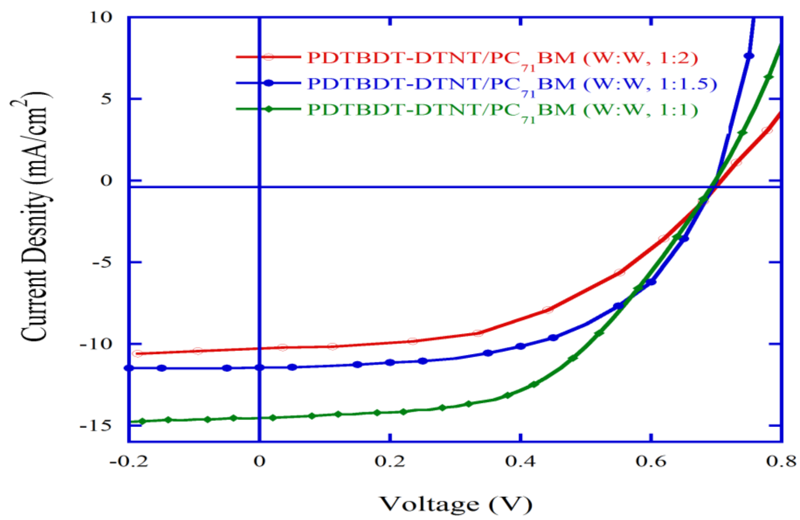
1. Thermal stability of the PDTBDT-DTNT



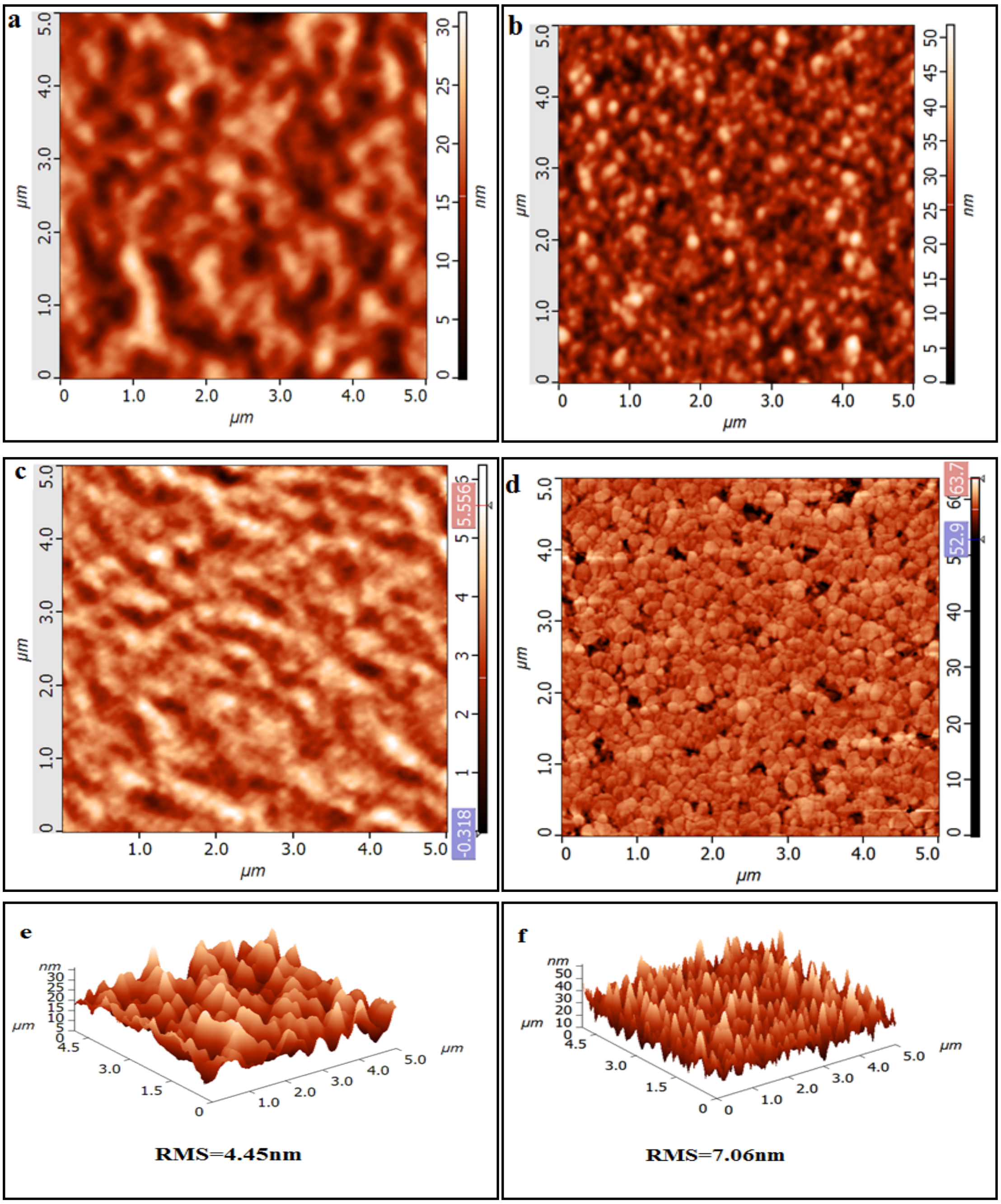
SFigure 1. T_G curve of **PDTBDT-DTNT**

2. Photovoltaic properties of PDTBDT-DTNT without solvent additives

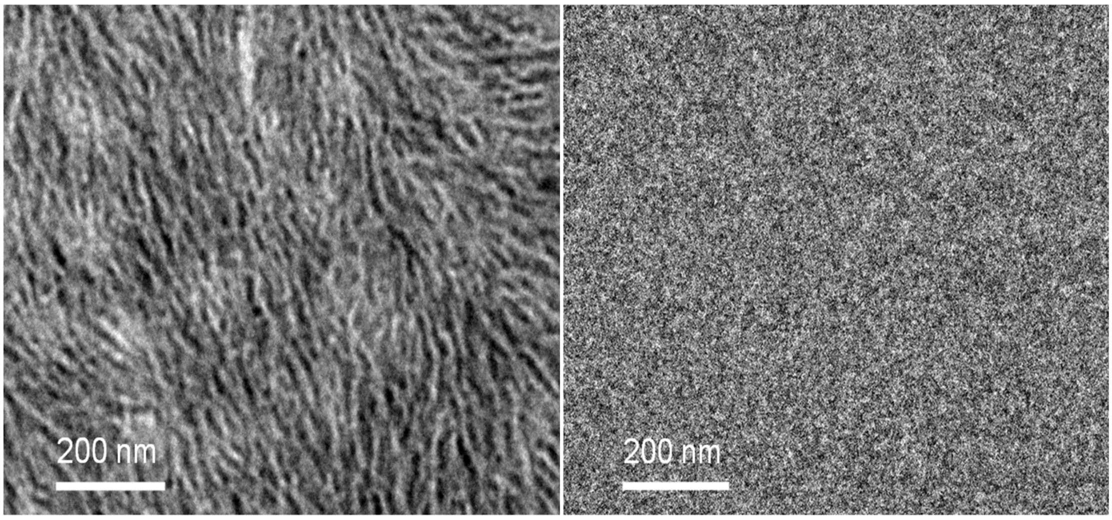


SFigure 2. J-V characteristics of the PVCs from **PDTBDT-DTNT/PC$_{71}$BM** without solvent additives

3. AFM and TEM images of the blend films of PDTBDT-DTNT/$PC_{71}BM$



SFigure 3. Tapping mode AFM topography images composite films of PDTBDT-DTNT/$PC_{71}BM$ with weight ratios of 1:1 without DIO (a, surface map; c, phase diagram; e, the surface of AFM 3D graph) and with 3% DIO (b, surface map; d, phase diagram; f, the surface of AFM 3D graph)



SFigure 4. TEM images composite films of PDTBDT-DTNT/$PC_{71}BM$ with weight ratios of 1:1 without DIO (left) and with 3% DIO (right)

4. Flux density inside the active layer and the calculated J_{sc} of the devices

The One Dimensional Transfer Matrix Formalism (TMF) is applied to decide the distribution of the optical electric field inside the solar cell. After solving the matrix equation, the monochromatic pointwise energy Q(x,λ) dissipated at a depth x per unit time and unit area in the material is calculated with the Poynting formula. Then we obtain Q(x,λ) for active layer as a function of depth and wavelength of equation (1) [1]:

$$Q(x,\lambda) = \frac{2\pi c\varepsilon_0 kn|E(x)|^2}{\lambda} \qquad (1)$$

(Where c is vacuum speed of light; ε_0 is permittivity of free space; λ is the light wavelength; n and k are the real and imaginary parts of the complex refraction index at the point x on active layer, and E(x) is the total optical electric field at the point of x). Only excitons generated within diffusion length of the D/A interface will contribute to the photocurrent. The effective absorption A(λ) for each wavelength is related to Q(x, λ) as equation (2) [2]:

$$A(\lambda) = \frac{1}{I(\lambda)} \int_{x \in active-layer} Q(x, \lambda) dx \qquad (2)$$

(Where $I(\lambda)$ is the light intensity transferred to the glass/ITO interface under AM 1.5 with irradiation of 100 mW/cm^2)

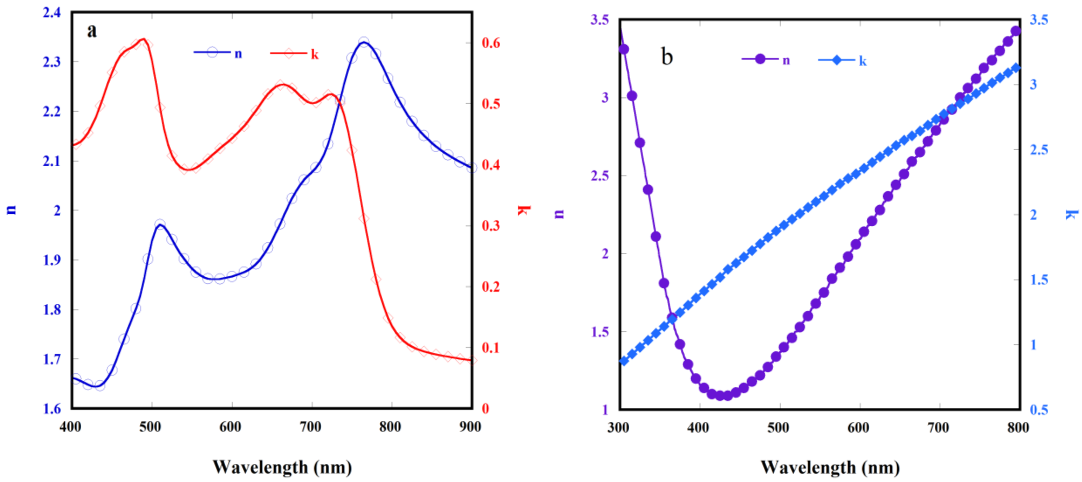
Following these, the Considering that, the photocurrent generation rates are shown as equation (3) [3]:

$$G(x) = \int_{\lambda_1}^{\lambda_2} \frac{\lambda}{hc} Q(x, \lambda) d\lambda \qquad (3)$$

and the maximum possible short current density (J_{sc} max) as a function of active layer thickness can be calculated as equation (4) [1] :

$$J_{SC} = \eta_{IQE} \int_{\lambda_1}^{\lambda_2} \frac{A(\lambda) I(\lambda)}{hc} \lambda q d\lambda \qquad (4)$$

In this study, the refractive indices (n) and extinction co-efficiencies (k) of ITO, PEDOT:PSS, MoO_3 and PFN layer were used the data reported in our recent work The refractive index (n) and extinction co-efficiency (k) of the Ca and the blend film from PDTBDT-DTNT and $PC_{71}BM$ (W:W, 1:1) and were measured on an ellipsometry (ELLiTOP) as shown in SFig 5a and Sfig 5b. The IQE of devices were applied to 85%. The refractive index (n) and extinction co-efficiency (k) were used as reported in reference. [4]



SFigure 5. the refractive indices (n) and extinction co-efficiencies (k) of blend film of

PDTBDT-DTNT/$PC_{71}BM$ (1:1) and Ca.

5. References

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