

Supplementary Information

Enhancement of power conversion efficiency in a polymer solar cell using a work-function-controlled $Ti_mSi_nO_x$ interlayer

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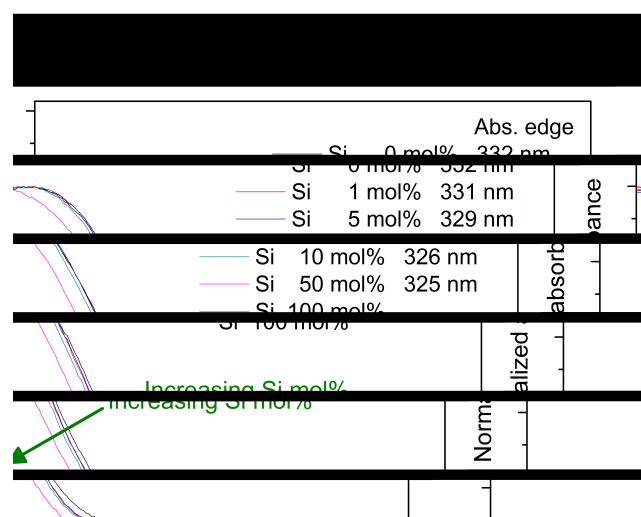


Fig. S1 UV-vis absorbance (normalized) of $Ti_mSi_nO_x$ as a function of Si mol%.

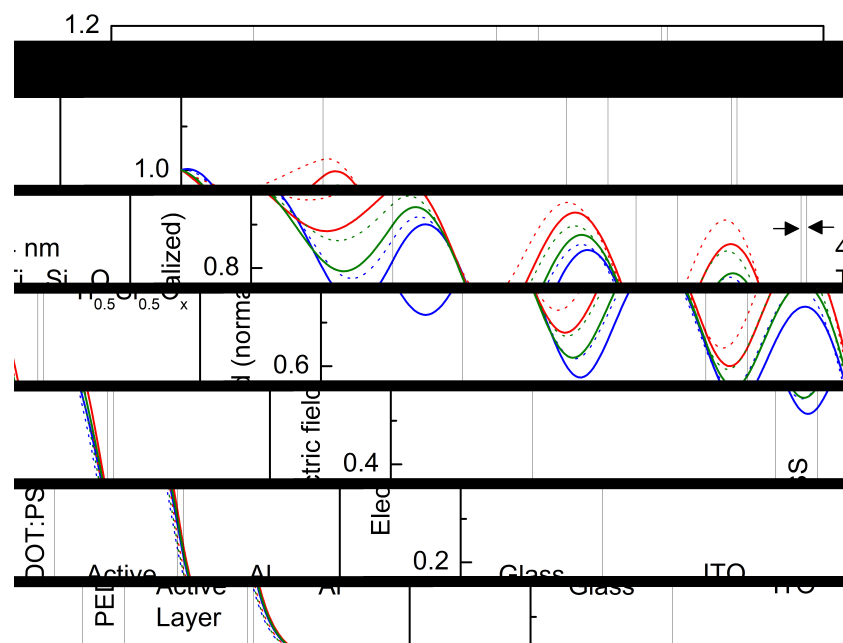


Fig. S2 Calculated electric-field intensities of 420-nm (blue), 430-nm (green) and 440-nm (red) lights as functions of position in the solar cells fitted with the Al-only (dotted line) and $\text{Ti}_{0.5}\text{Si}_{0.5}\text{O}_x/\text{Al}$ (solid line) cathodes.

The exception in comparison of IPCE between the devices fitted with the Al-only and the $\text{Ti}_{0.5}\text{Si}_{0.5}\text{O}_x/\text{Al}$ cathodes in the short wavelength region (Fig. 4 (b)) might be caused by the more remarkable difference in light absorption at shorter wavelength. The peaks of the electric fields at shorter wavelength are located in the middle of the active layer as shown in Fig. S2 while those at 650 nm are located near by the PEDOT:PSS/Al interface (Fig. 5). As the electric fields are well distributed in the middle of the active layer, the difference in light absorption in the shorter wavelength region is more significant. We think such higher absorption by the device fitted with the Al-only cathode induced the exceptionally higher IPCE in the region (400 – 480 nm). Accordingly, in the wavelength region, the total light absorption of the Al-only device is larger than that of the $\text{Ti}_{0.5}\text{Si}_{0.5}\text{O}_x/\text{Al}$ device but the difference seems to be too small to explain the difference fully.

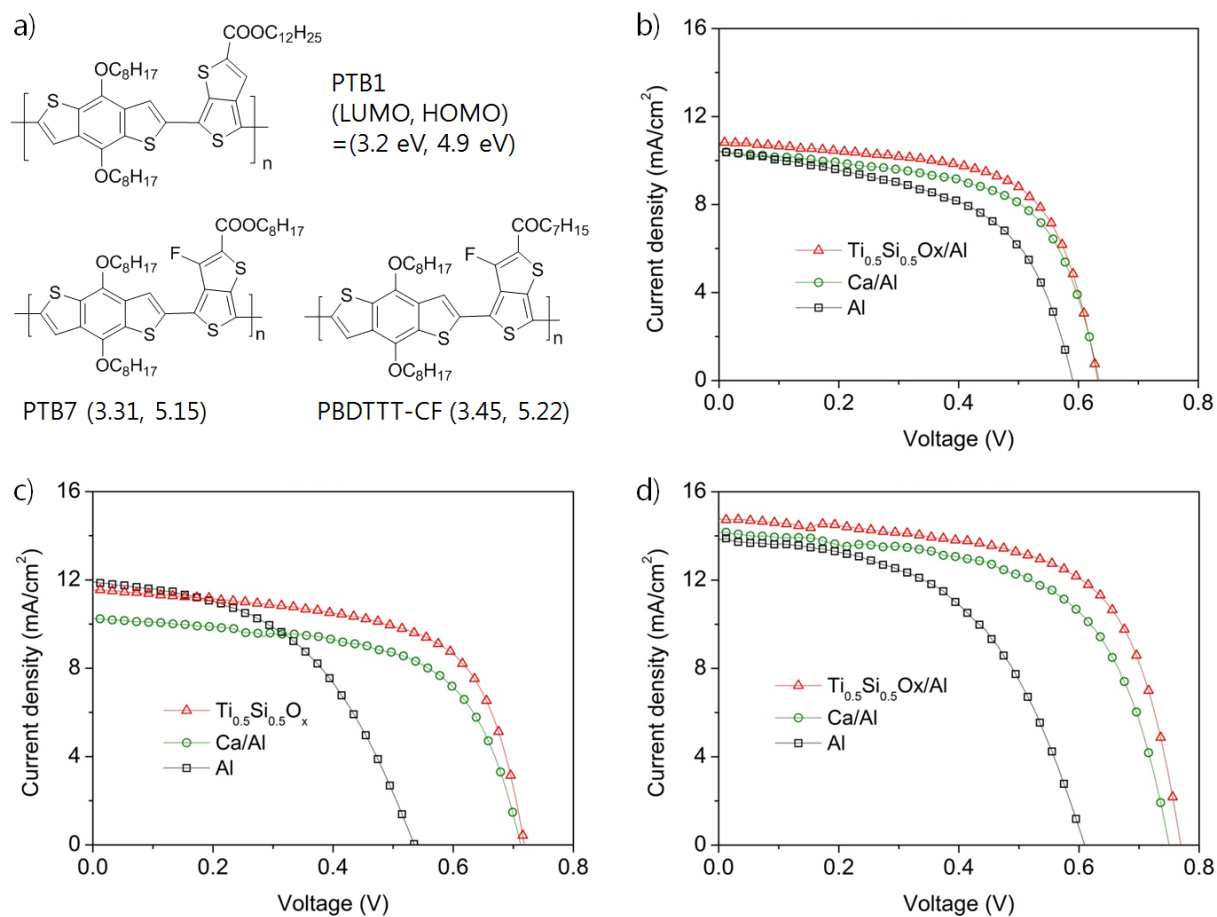


Fig. S3 a) The chemical structures of the tested polymers. $J-V$ characteristics of the PSCs based on the well-known donor polymers: b) PTB1, c) PTB7, and d) PBDTTT-CF combined with PC₇₁BM.

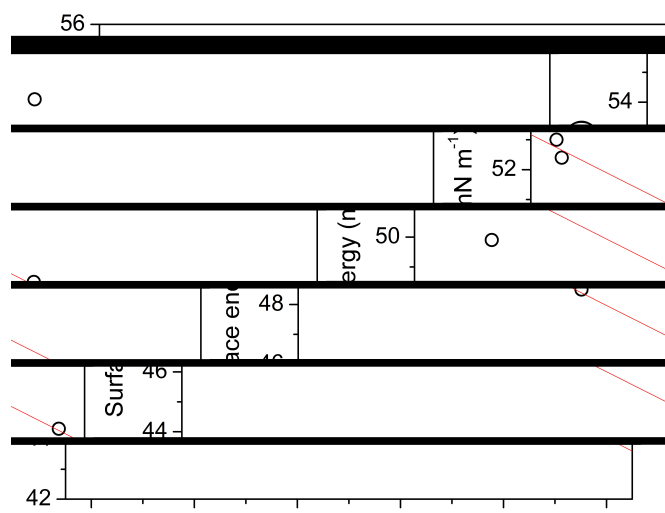


Fig. S4 Surface energy of $Ti_mSi_nO_x$ as a function of Si mol%.

The surface energies of the various interlayers were determined from contact angle measurements using distilled water and diiodomethane as probe liquids, and the Owens-Wendt-geometric mean equation (equation 1):^[1]

$$(1 + \cos)\gamma_{pl} = 2(\gamma_s^d \gamma_{pl}^d)^{0.5} + 2(\gamma_s^p \gamma_{pl}^p)^{0.5} \quad (1)$$

where γ_s and γ_{pl} are the surface energies of the substrate and the probe liquid, respectively.

The surface energy of substrate can be expressed as a sum of components based on dispersion (γ_s^d) and polar energies (γ_s^p): $\gamma_s = \gamma_s^d + \gamma_s^p$. The contact angles of water and diiodomethane droplets on the surfaces of the $Ti_mSi_nO_x$ films are summarized in Table S1.

Table S1. Measured contact angles of water and diiodomethane droplets on the surfaces of the $Ti_mSi_nO_x$ films.

Si mol%	Contact angle (deg.)	
	Water	Diiodomethane
0	52.9	29.5
1	53.7	30.0
5	49.7	31.8
10	56.6	34.7
50	60.4	36.3
100	64.6	41.6

Reference

- [1] D. K. Owens, R. C. Wendt, *J. Appl. Polym. Sci.* **1969**, *13*, 1741.