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

Supplementary information: **Optimal top electrodes for inverted polymer solar cells**

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Table S1. Photovoltaic parameters of PTB7: $PC_{71}BM$ inverted devices with different top electrodes.

Electrode	J_{SC} [mA/㎠]	V_{OC} [V]	*FF*	PCE [%]	R_s [Ω㎠]	R_{sh} [Ω㎠]
Al-1	14.19	0.75	0.66	7.00	6.1	498
Al-2	14.85	0.75	0.66	7.35	6.1	508
Al-3	14.74	0.75	0.65	7.16	6.0	495
Al-4	14.69	0.74	0.65	7.12	5.9	489
Al-5	14.71	0.74	0.65	7.09	5.9	489
Al Average	**14.64**	**0.75**	**0.65**	**7.14**	**6.00**	**496**
Ag-1	14.69	0.75	0.71	7.73	3.1	745
Ag-2	14.96	0.75	0.71	7.95	3.3	750
Ag-3	15.12	0.75	0.73	8.19	3.0	759
Ag-4	15.04	0.75	0.72	8.10	3.0	756
Ag-5	14.17	0.75	0.72	7.70	3.0	753
Ag Average	**14.78**	**0.75**	**0.72**	**8.00**	**3.08**	**753**
Au-1	13.14	0.75	0.70	6.84	4.5	606
Au-2	11.94	0.74	0.68	6.02	4.2	603
Au-3	13.46	0.75	0.69	6.93	5.8	612
Au-4	12.59	0.75	0.67	6.28	5.2	606
Au-5	13.26	0.74	0.69	6.84	4.9	607
Au Average	**12.88**	**0.75**	**0.69**	**6.58**	**4.92**	**607**

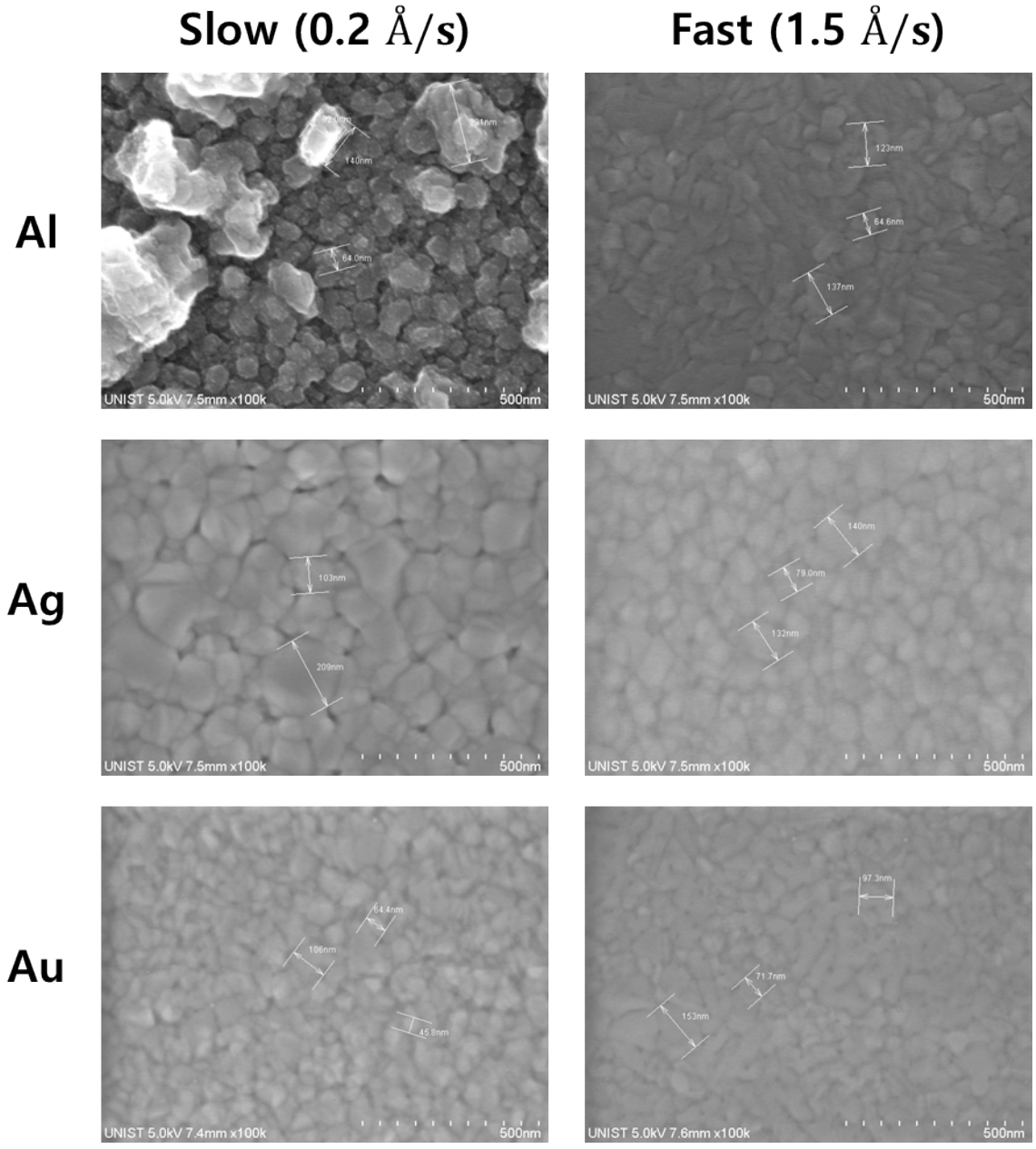

Figure S1. SEM images of different metal thin films (100 nm) prepared using slow and fast evaporation rates.

Table S2. Measured conductivity of metal thin films (100 nm) prepared using slow and fast evaporation rates.

Electrode	Conductivity [S/cm, $\Omega^{-1}cm^{-1}$]
ITO	5.2×10^3
Al (slow evaporation, 0.2 $\text{Å}/s$)	1.7×10^5
Al (fast evaporation, 1.5 $\text{Å}/s$)	3.5×10^5
Ag (slow evaporation, 0.2 $\text{Å}/s$)	3.7×10^5
Ag (fast evaporation, 1.5 $\text{Å}/s$)	3.9×10^5
Au (slow evaporation, 0.2 $\text{Å}/s$)	3.1×10^5
Au (fast evaporation, 1.5 $\text{Å}/s$)	3.0×10^5

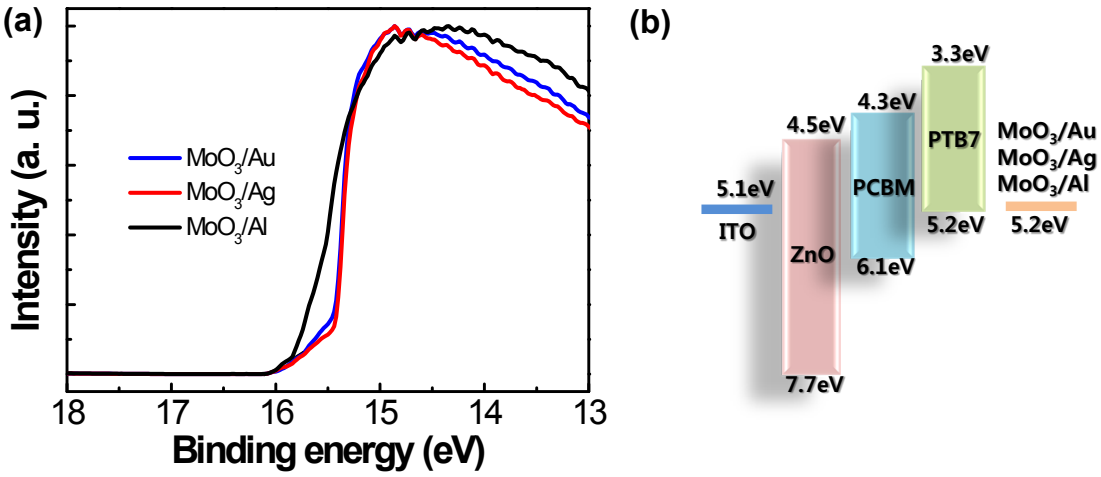

Figure S2. Energy band structures. a) UPS spectra for MoO_3/Au, MoO_3/Ag and MoO_3/Al. b) Energy band diagram for PTB7: $PC_{71}BM$ inverted devices.

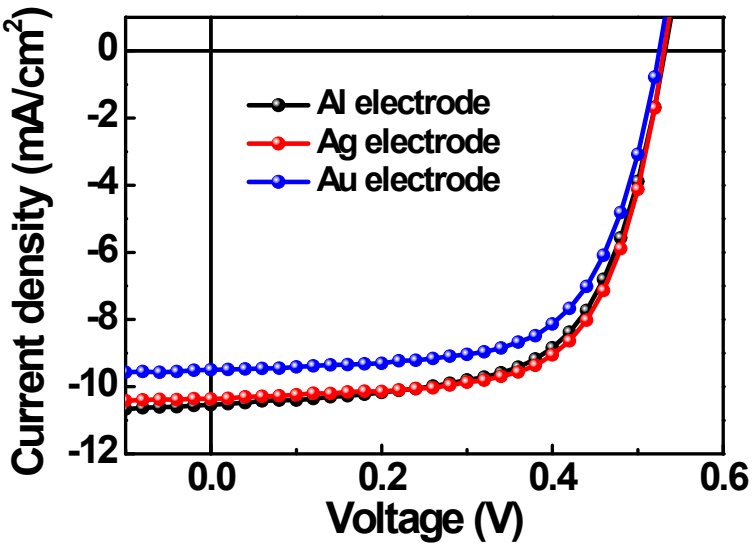

Figure S3. Comparison of *J-V* characteristics of P3HT: $PC_{61}BM$ inverted devices with different top electrodes

Table S3. Photovoltaic parameters of P3HT: $PC_{61}BM$ inverted devices with different top electrodes.

Device structure	J_{SC} [mA/㎠]	V_{OC} [V]	*FF* [%]	PCE [%]
ITO/ZnO/P3HT:$PC_{61}BM$/MoO_3(3.7 nm)/Al(100 nm)	10.5	0.53	0.63	3.54
ITO/ZnO/P3HT:$PC_{61}BM$/MoO_3(3.7 nm)/Ag(100 nm)	10.4	0.53	0.66	3.63
ITO/ZnO/P3HT:$PC_{61}BM$/MoO_3(3.7 nm)/Au(100 nm)	9.50	0.53	0.65	3.25

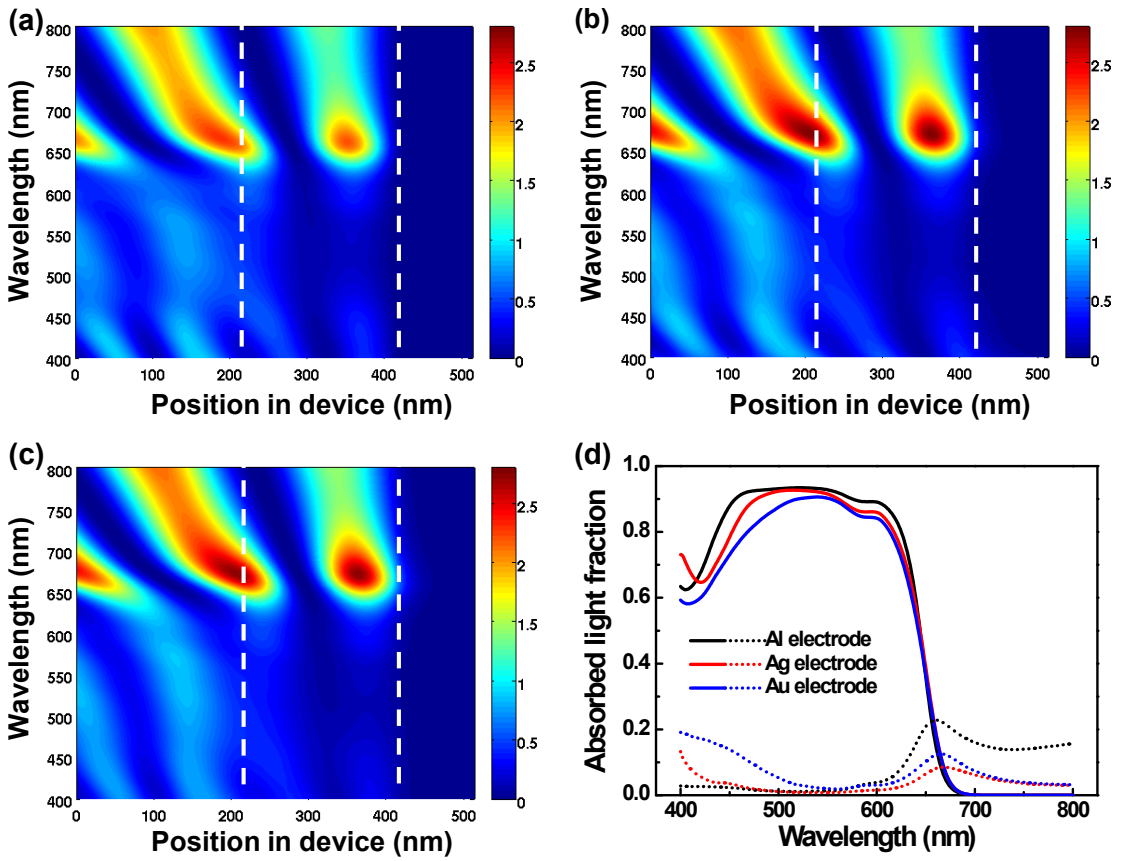

Figure S4. Simulated optical properties of P3HT:$PC_{61}BM$ inverted solar cells with different metal electrodes. (a)-(c) Normalized electric field intensity. (a), (b), and (c) are for devices having Al, Ag, and Au electrodes, respectively. White dashed lines indicate the position of the active layer. (d) Absorbed light fraction. Dashed lines indicate the absorption in the active layer. (Simulated J_{SC} : Al = 13.41, Ag = 13.05 and Au = 12.49)

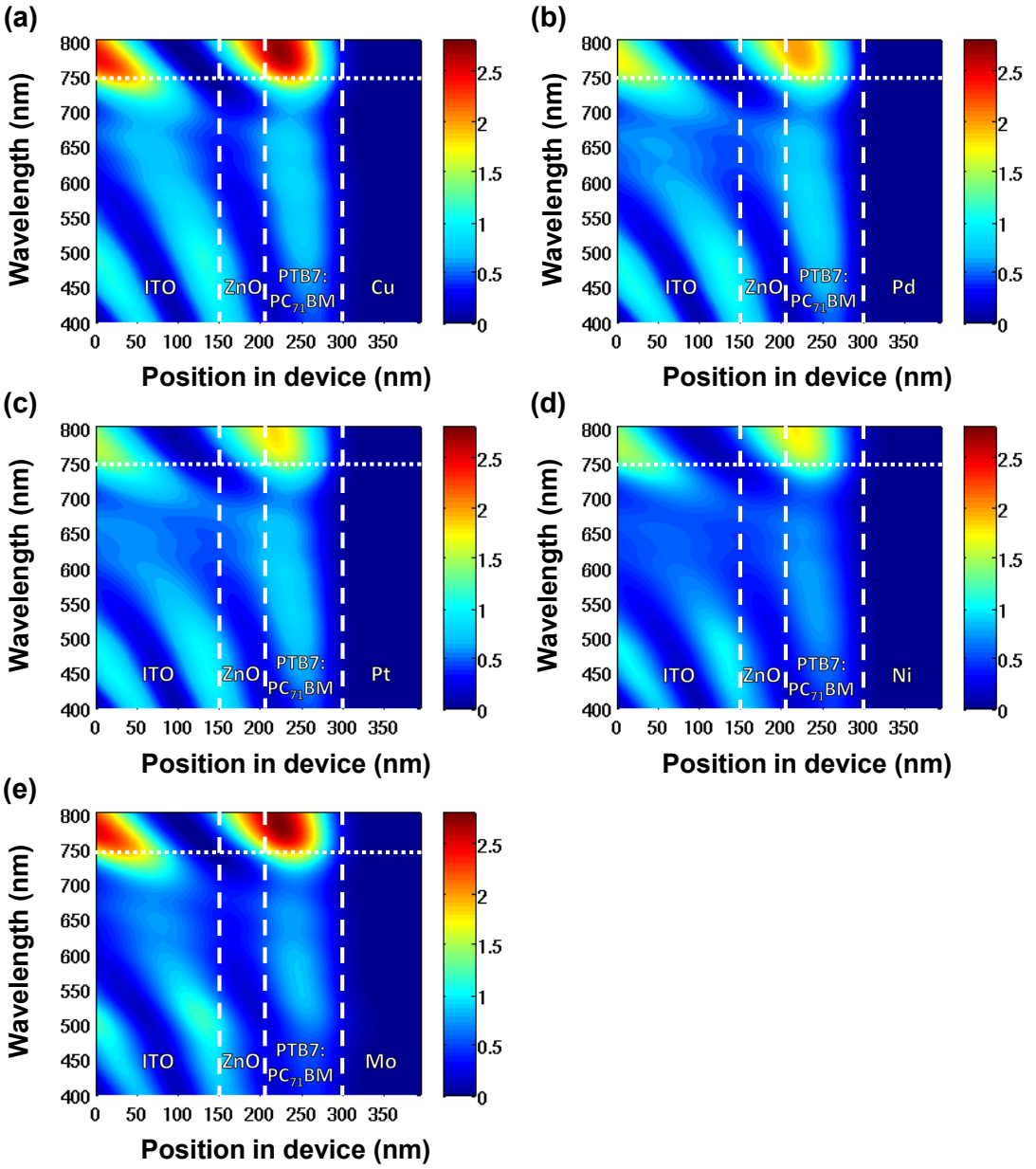

Figure S5. Spatial distribution of normalized electric field intensity in devices with different electrodes. (a), (b), (c), (d), and (e) correspond to devices with Cu, Pd, Pt, Ni, and Mo electrodes, respectively. White dashed lines indicate the boundaries of each layer and white dotted lines demark the absorption onset of PTB7:$PC_{71}BM$.

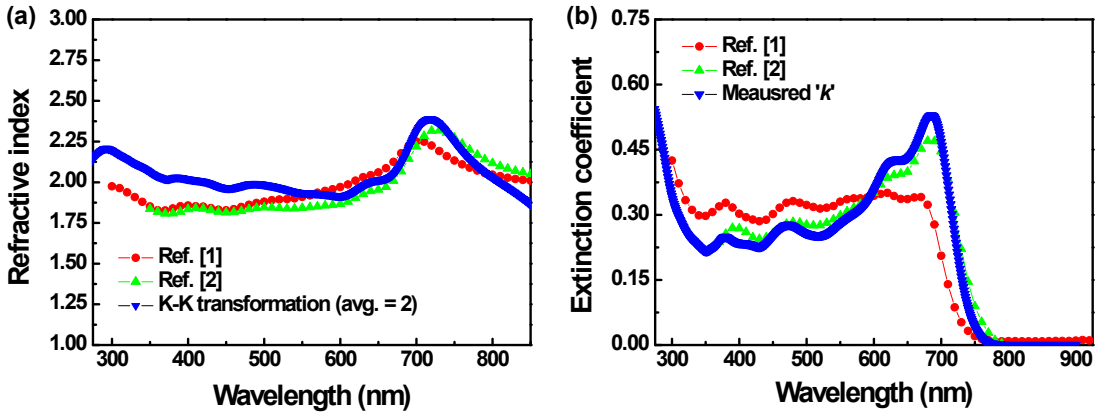

Figure S6. Complex refractive index of PTB7:$PC_{71}BM$ blends. (a) Refractive index (n). The calculated refractive index was compared with previously reported refractive index data which was obtained ellipsometrically.[S1,S2] All papers share same donor:acceptor ratio. (b) Extinction coefficient (k). Extinction coefficients were calculated from the measured absorption coefficient (α) of the active film.

References

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S2. G. J. Hedley, A. J. Ward, A. Alekseev, C. T. Howells, E. R. Martins, L. A. Serrano, G. Cooke, A. Ruseckas and I. D. W. Samuel, *Nat Commun*, 2013, **4**. 2867