Supplementary Information

Realizing 18.03% Efficiency and Good Junction Characteristics in Organic Solar Cells via Hydrogen-bonding Interaction between Glucose and ZnO Electron Transport Layer

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Experimental section

1 Materials

PTB7-Th and $PC_{71}BM$ were obtained from Organtec Ltd. and Lumtec of Taiwan, respectively. Anhydrous zinc acetate [$Zn(CH_3COO)_2$], 2-methoxyethanol ($CH_3OCH_2CH_2OH$) were purchased from Energy Chemical. Ethanolamine ($NH_2CH_2CH_2OH$) was ordered from Sigma-Aldrich Company. Gl was purchased from Macklin. All materials and solvents were used as received without further purification.

2 ZnO precursor and Glucose solution preparation

The ZnO precursor was prepared by dissolving 0.836 g of $Zn(CH_3COO)_2$ and 0.28 g of 2-methoxyethanol ($CH_3OCH_2CH_2OH$) in 10 mL of $NH_2CH_2CH_2OH$. The solution was stirred overnight for the hydrolysis reaction in the air.

The Gl solution concentration was 2 mg/mL with a mixed solvent of deionized water and ethanol (3:7 by volume).

3 Fabrication and characterization of OSCs

The ITO glass substrates (15 Ω square^{-1}) were cleaned in a sonication bath with detergent, deionized water, acetone, and isopropanol, then dried overnight in oven. Subsequently, ZnO precursor solution was spin-coated on top of the UV/ozone treated ITO substrate at 4000 rpm for 40 s, followed by 60 min annealing at 200 ℃. The Gl solution was spin coated onto the surface of ZnO at different rotation speeds. The samples were quickly transferred to a N_2-protected glovebox. Then, a blend of PM6:Y6 (1:1.2) in chloroform and 1-chloronaphthalene (99.5:0.5 by volume) with a donor concentration of 7 mg/ml was spin-coated on top of HTLs. A blend of PTB7-Th:$PC_{71}BM$ (1:1.5) was dissolved in the mixed solvents of CB and DIO (97:3 by volume) with a concentration of 25 mg/ml and was spin-coated on the ZnO or the ZnO/Gl(X) ETLs at 4000 rpm for 120 s. Finally, MoO_3 and Al electrodes were thermally deposited on the active layer continuously in a chamber with pressure < 4 × 10^{-4} Pa.

The current density–voltage (*J-V*) characteristics and external quantum efficiency (EQE) were measured by Newport solar simulator system. The *J-V* characteristics were carried under AM 1.5G, with a power intensity of 100 mW/cm^2. A calibrated monosilicon diode was fixed as the reference, exhibiting a response at 300−800 nm. A SPA-300HV atomic force microscopy (AFM) was utilized to investigate surface morphology. Zahner Electrochemical Workstation was used to measure the Electric impedance spectroscopy (EIS).

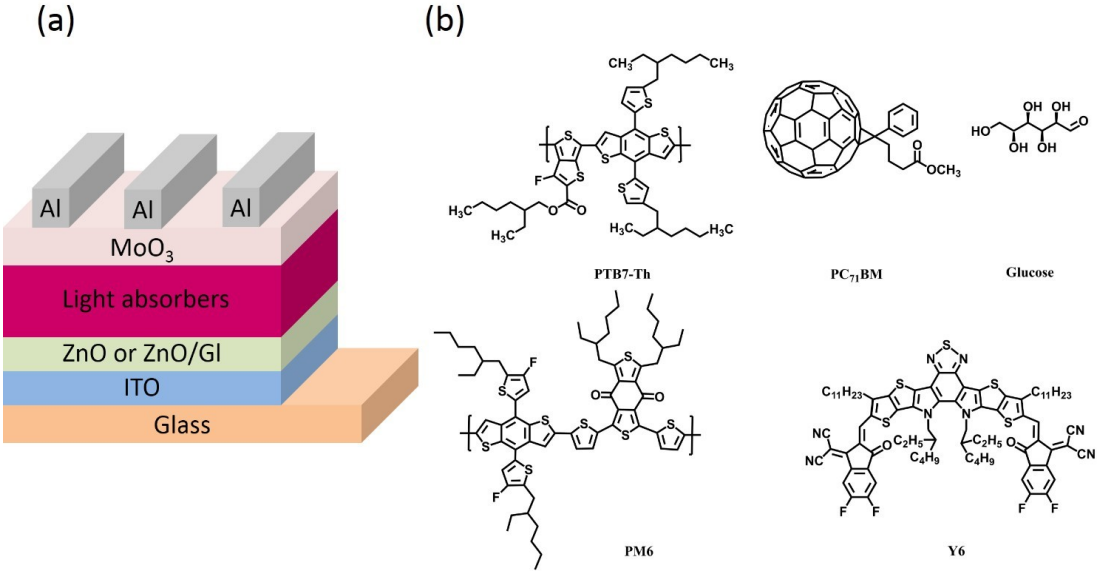

Fig. S1. (a) The architecture of OSCs. (b) Molecular structures of PTB7-Th, $PC_{71}BM$, Glucose, PM6, and Y6.

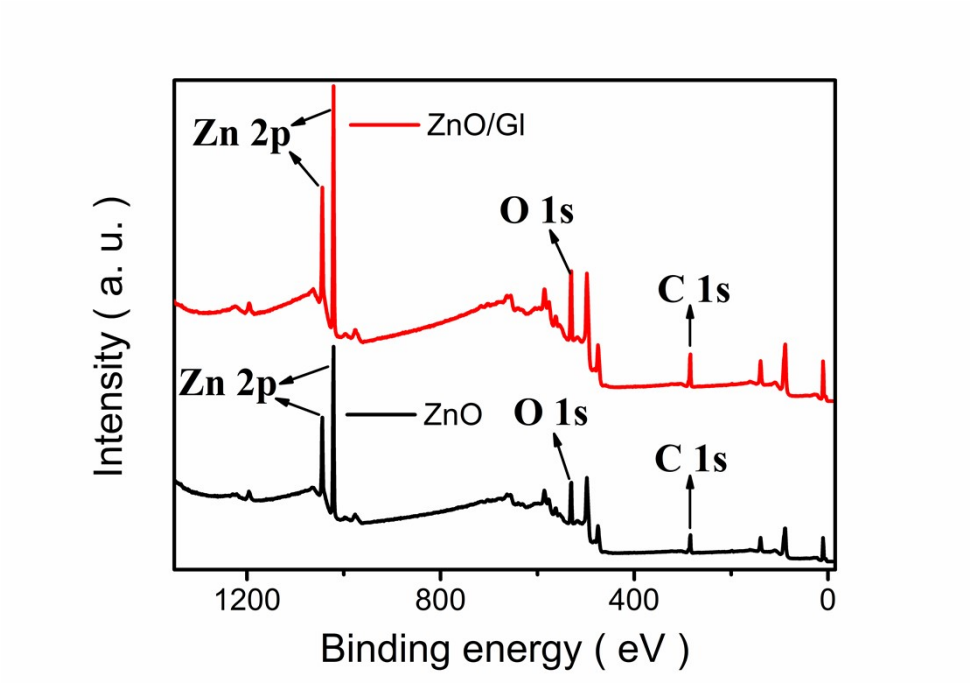

Fig. S2. XPS spectra of ZnO and ZnO/Gl samples.

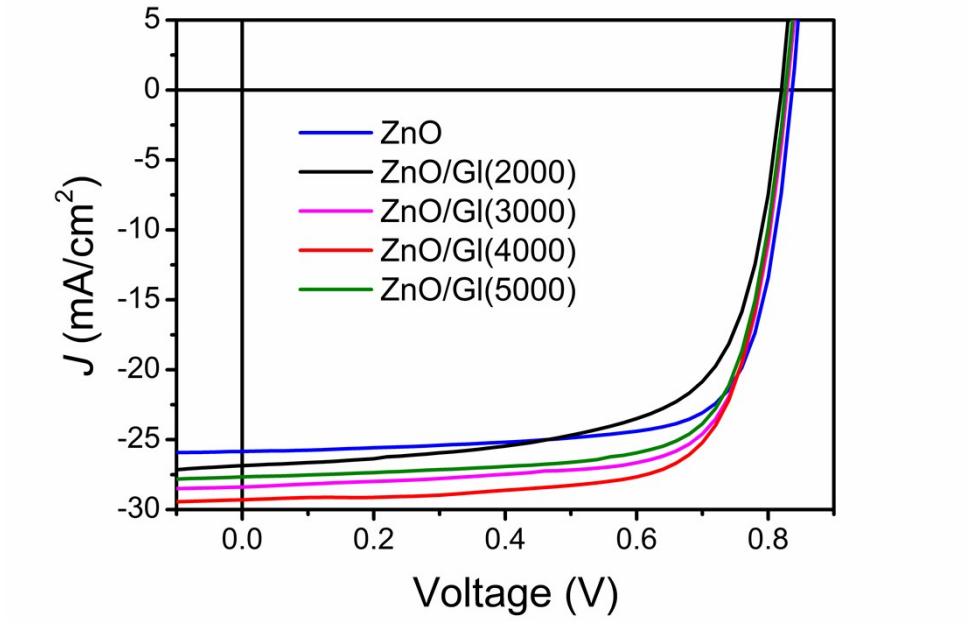

Fig. S3. *J–V* characteristics from cells with ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is the non-fullerene blend of PM6:Y6.

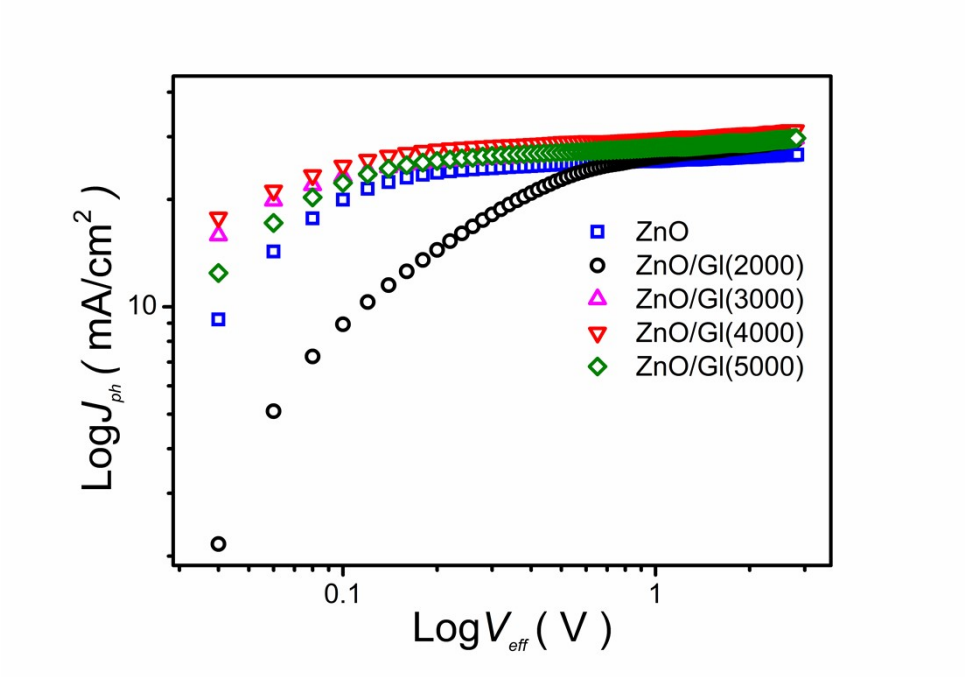

Fig. S4. Log J_{ph} versus Log V_{eff} plots of OSCs based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is the non-fullerene blend of PM6:Y6.

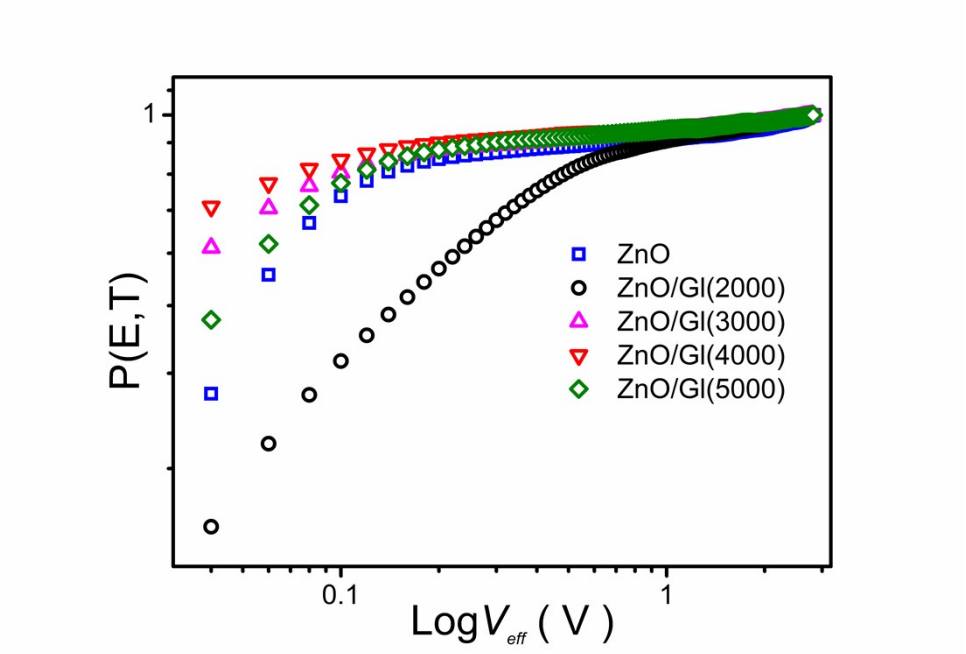

Fig. S5. $P(E, T)$ versus Log V_{eff} plots of OSCs based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is the non-fullerene blend of PM6:Y6.

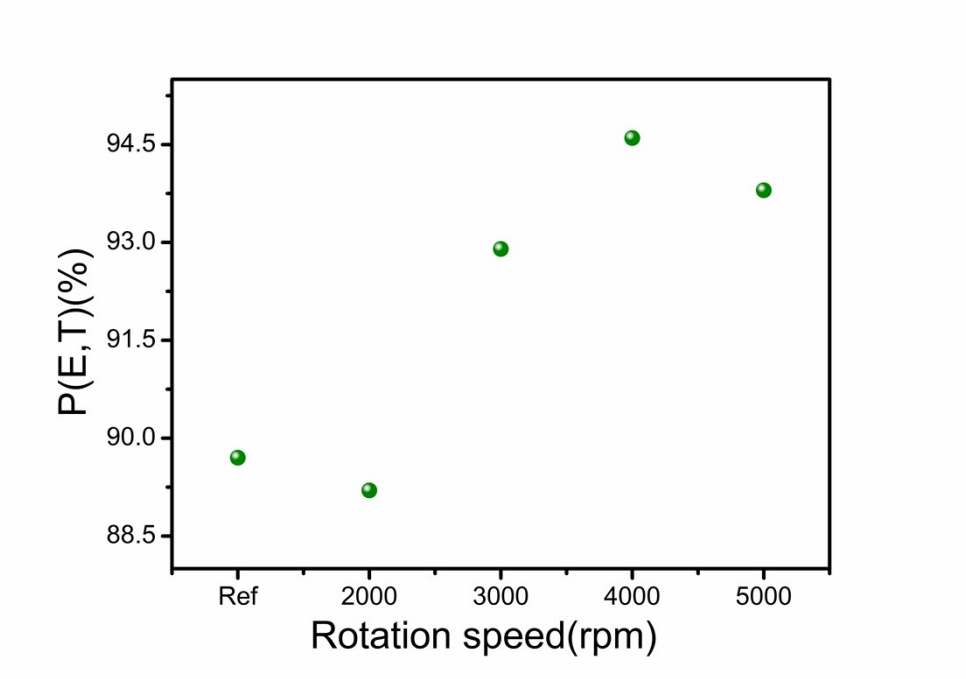

Fig. S6. $P(E, T)$ obtained from cells with ZnO and ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm under $V_0 = 0$ condition (V_0: built-in potential). The light absorber is the non-fullerene blend of PM6:Y6.

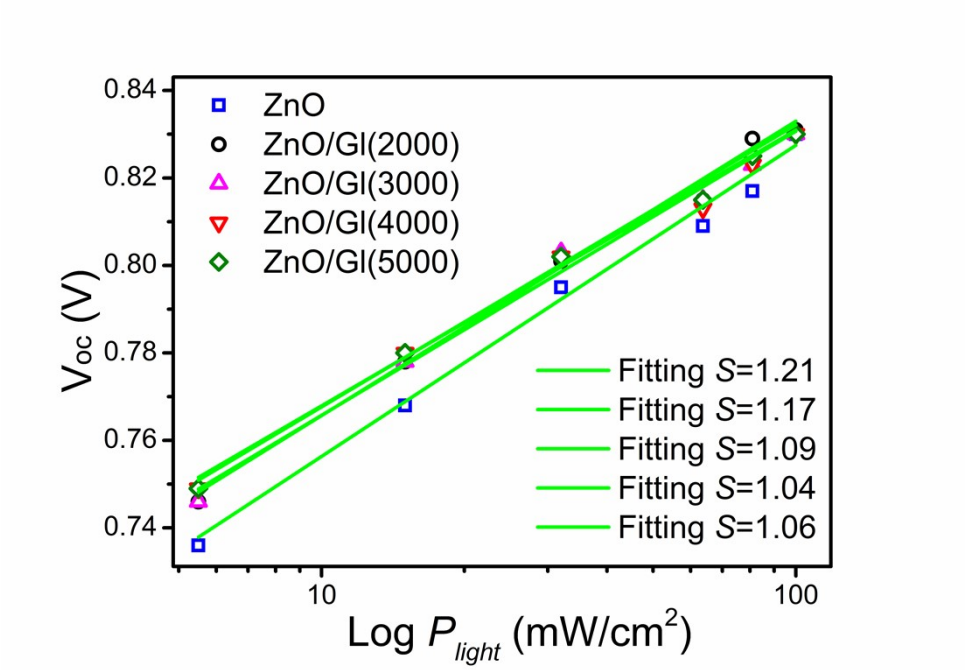

Fig. S7. Plots of V_{oc} versus log P_{light} of OSCs based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is the non-fullerene blend of PM6:Y6.

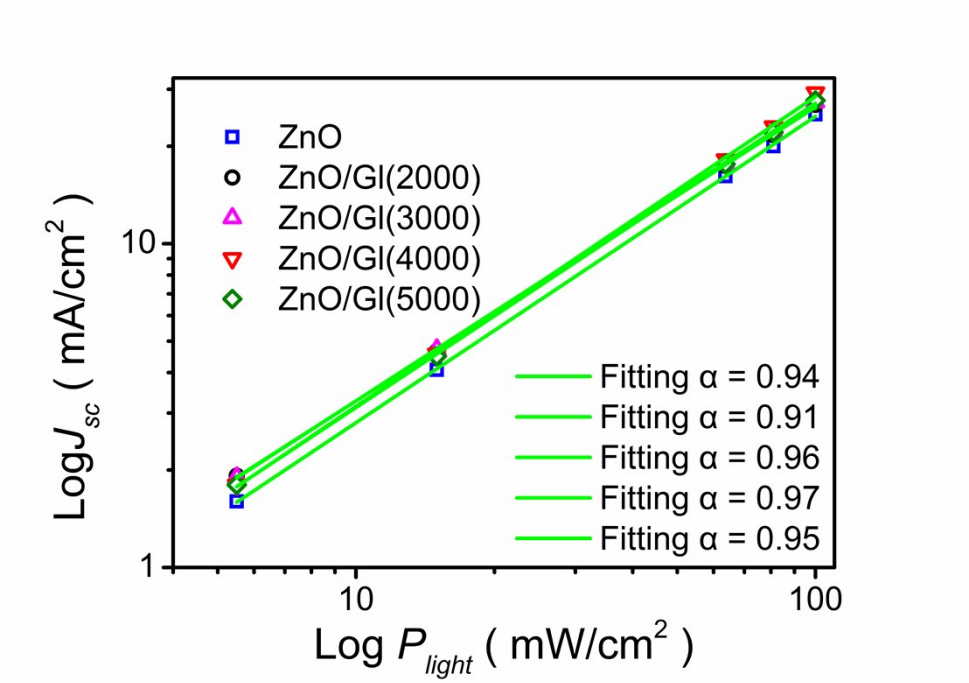

Fig. S8. Plots of log J_{sc} versus log P_{light} of OSCs based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is non-fullerene blend of PM6:Y6.

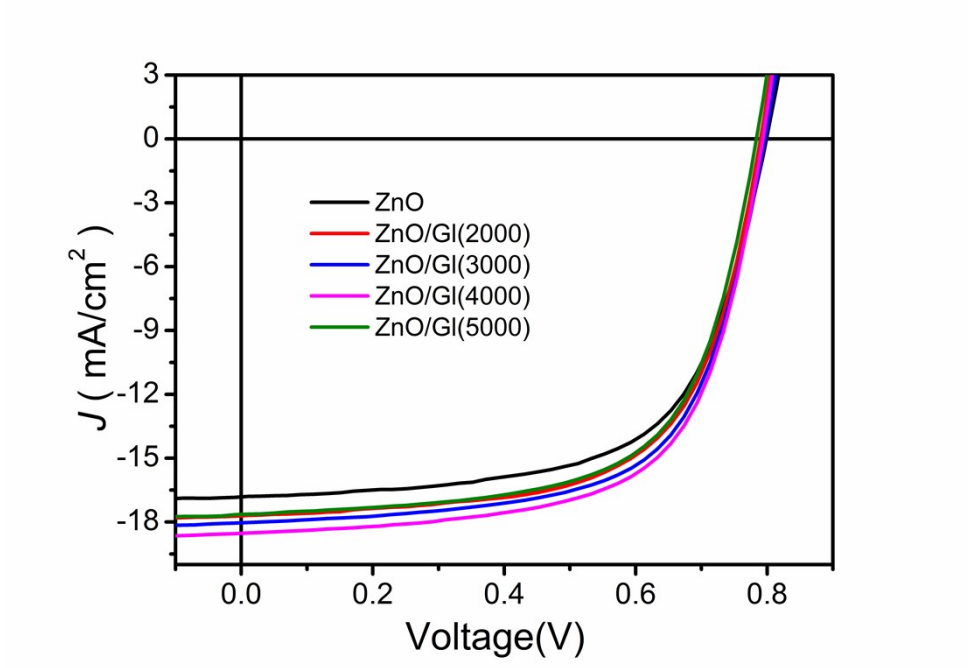

Fig. S9. *J–V* characteristics for cells based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

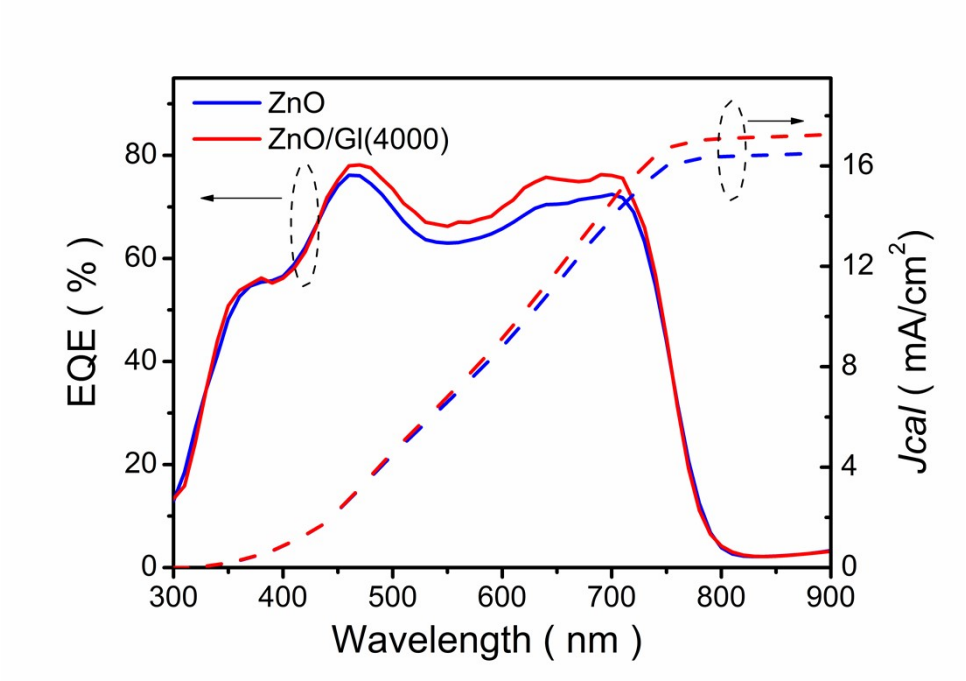

Fig. S10. External quantum efficiency (EQE) and integrated current density (J_{cal}) of cells using ZnO or ZnO/Gl(4000) as ETLs. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

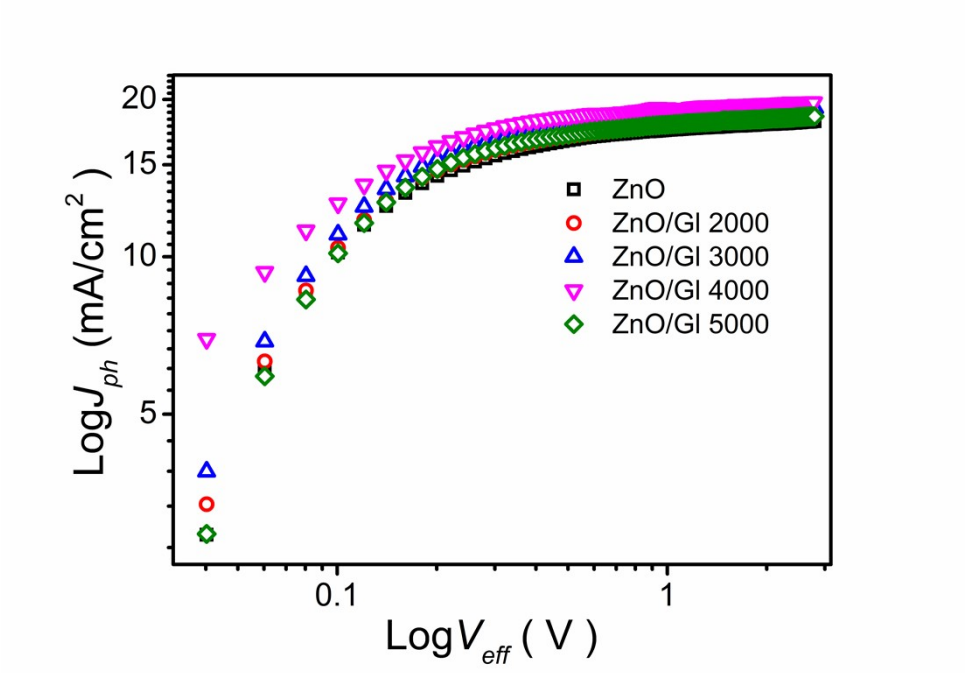

Fig. S11. Log J_{ph} versus Log V_{eff} plots of OSCs based on ZnO and ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

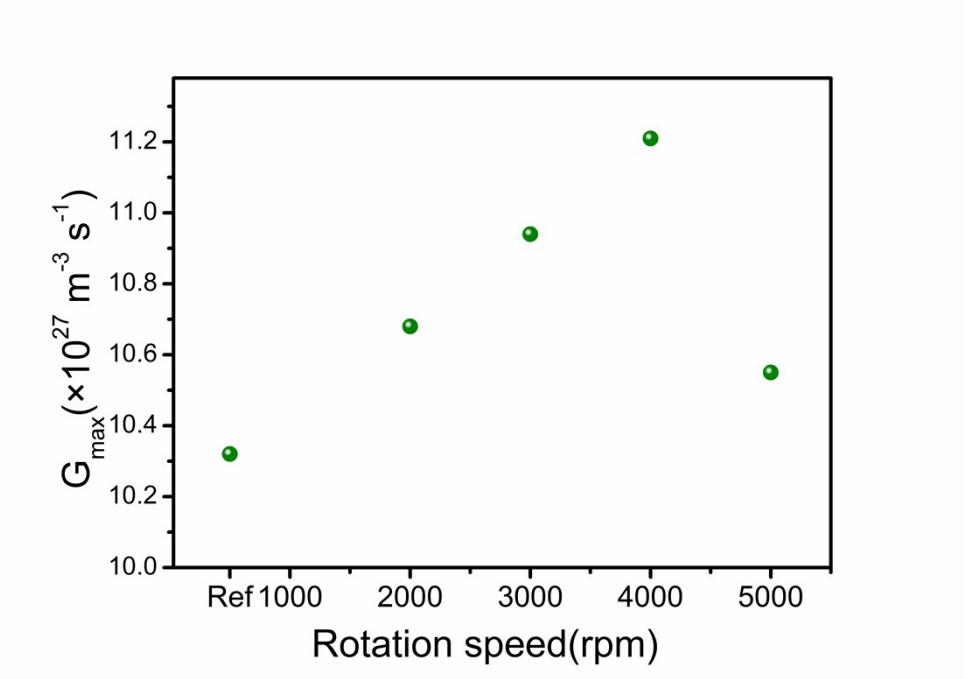

Fig. S12. *P*(*E*, *T*) obtained from cells based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm under V_0 = 0 condition (V_0: built-in potential). The light absorber is fullerene blend of PTB7-Th:$PC_{71}BM$.

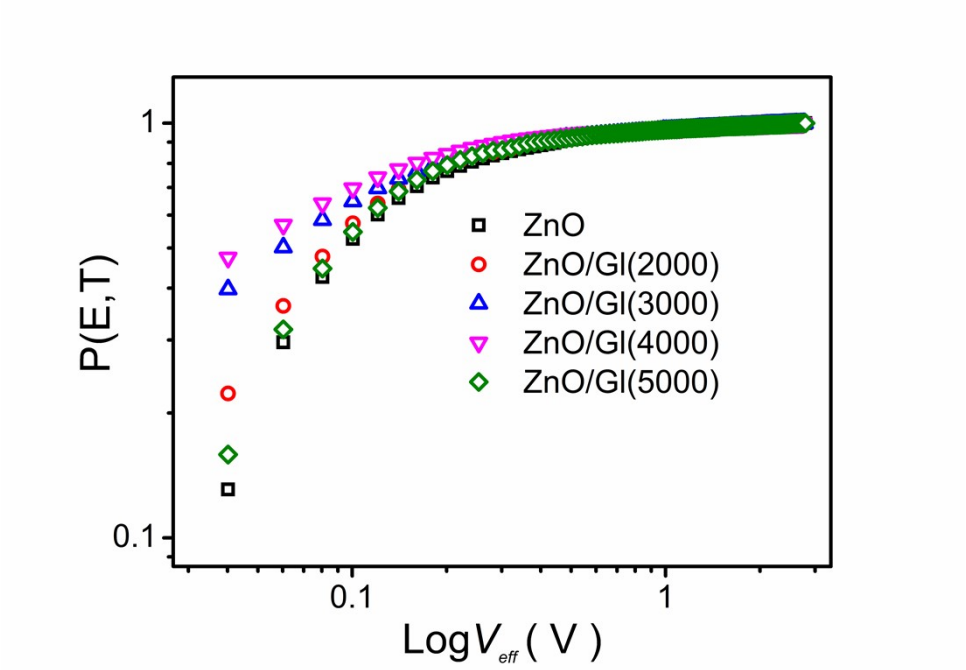

Fig. S13. *P*(*E*, *T*) versus Log V_{eff} plots of OSCs based on ZnO and ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

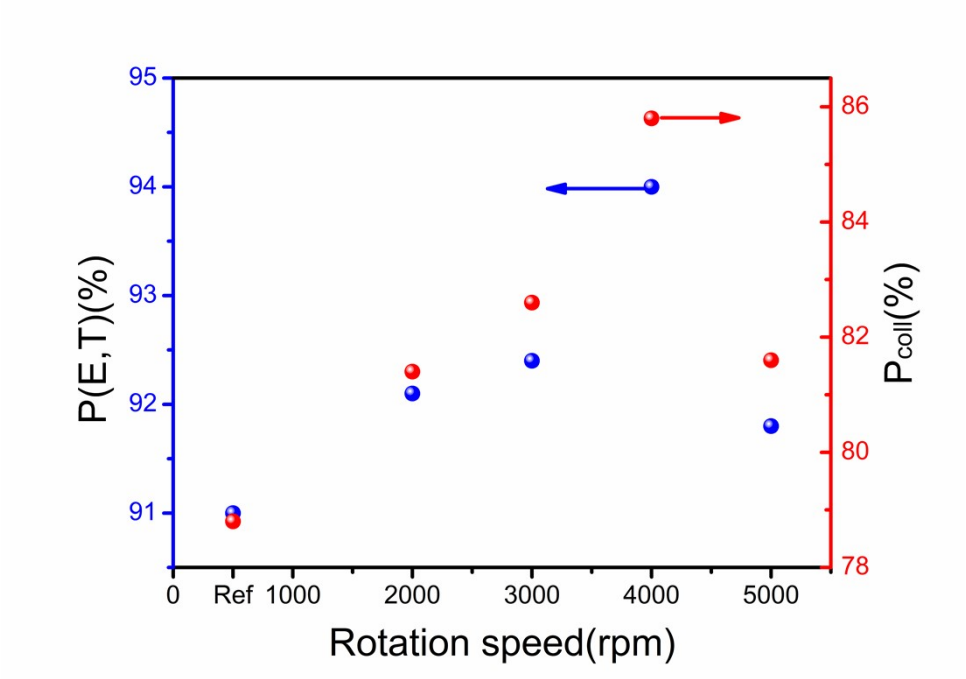

Fig. S14. $P(E, T)$ and P_{coll} obtained from cells based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

Table S1 Photovoltaic parameters of cells based on ZnO or ZnO/Gl(X) ETLs spin-coated with a rotation speed from 2000 to 5000 rpm. The light absorber is a blend of PTB7-Th:$PC_{71}BM$.

ETLs	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
ZnO	0.795	16.81	63.35	8.51
ZnO/Gl(2000)	0.790	17.67	62.05	8.66
ZnO/Gl(3000)	0.795	18.01	64.51	9.25
ZnO/Gl(4000)	0.794	18.50	64.64	9.49
ZnO/Gl(5000)	0.795	17.62	63.28	8.87