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Solvent-Mediated Surface Modification of Electron Transport Layer for Efficient PbS Quantum Dot Solar Cells

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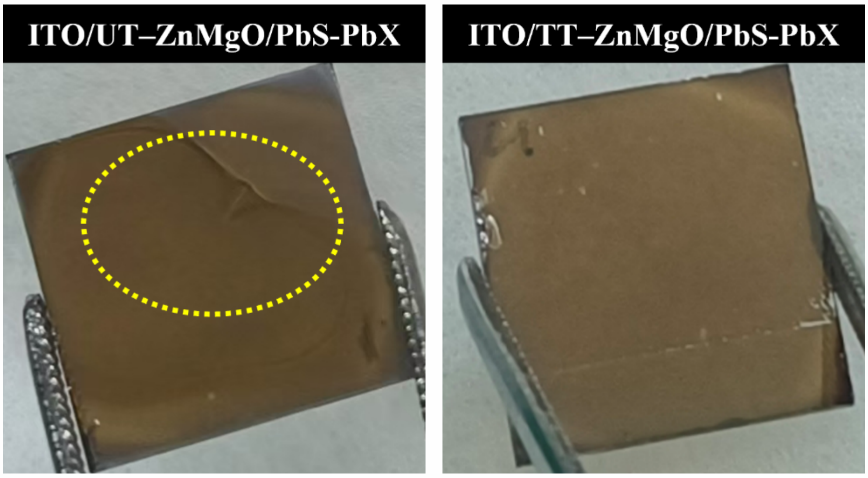


Figure S1. Pictures of PbS-PbX QDs deposited on UT-ZnMgO (left) and TT-ZnMgO (right) NP surfaces

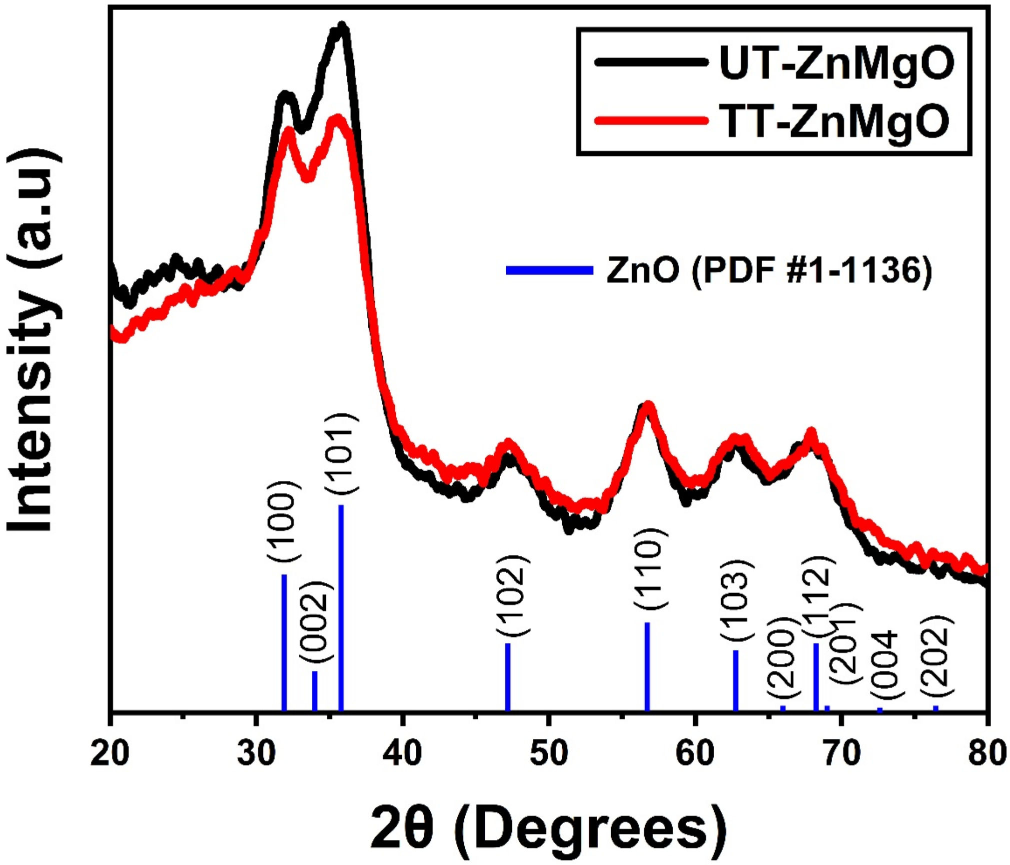
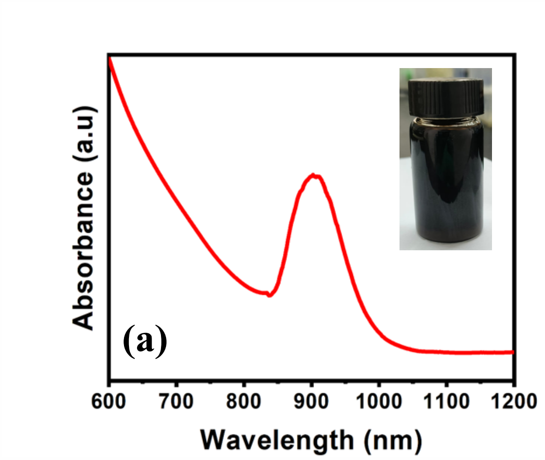


Figure S2. XRD patterns of UT-ZnMgO and TT-ZnMgo



Figures S3. UV-vis spectroscopy and crystalline structure of PbS-OA QDs (a) Absorption spectra of PbS CQDs (b) XRD pattern of PbS CQDs

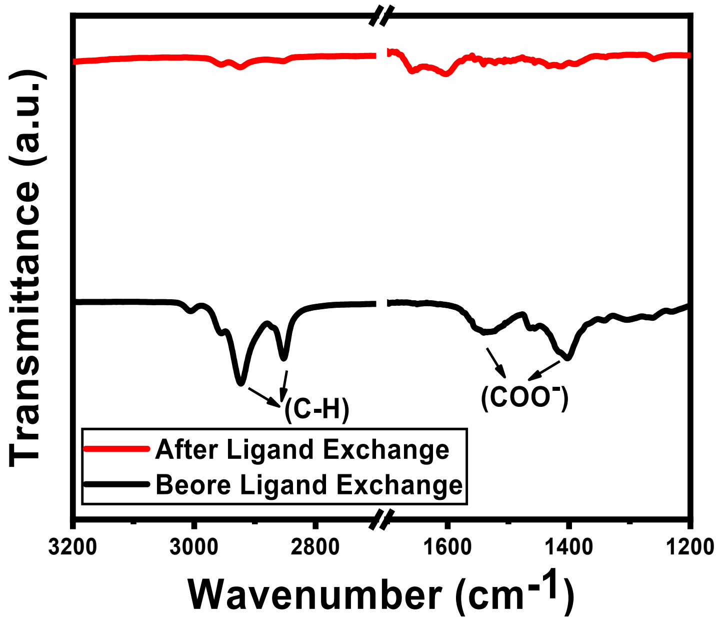


Figure S4. Fourier transformed infrared spectroscopy (FTIR) of PbS CQDs before (black line) and after ligand exchange (red line).

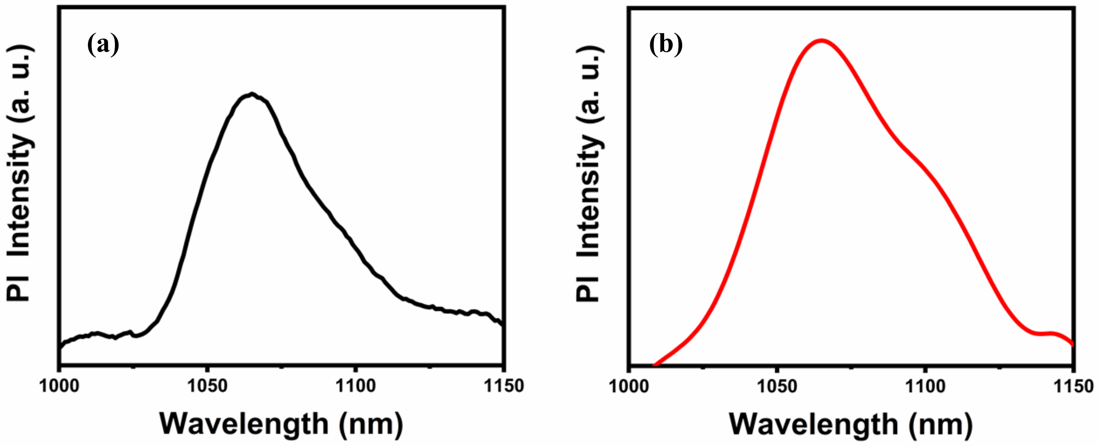


Figure S5. Near-IR Steady-state PL spectra of PbS-EDT of ITO/UT-ZnMgO/PbS-PbX/PbS-EDT (a) and ITO/TT-ZnMgO/PbS-PbX/PbS-EDT (b) full stacks.

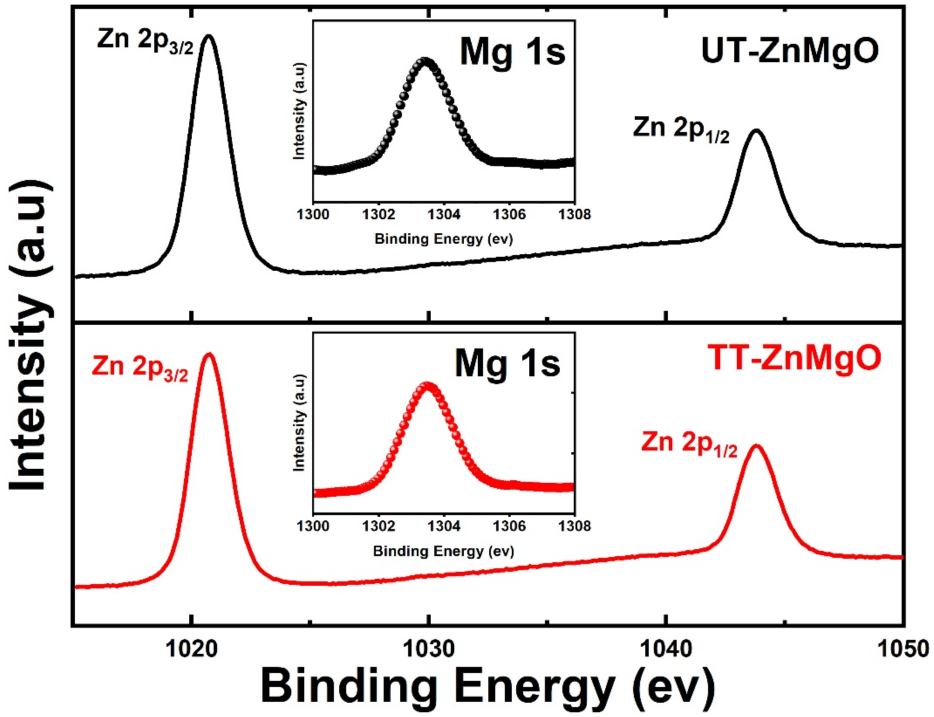


Figure S6.XPS Spectra of Zn 2p and Mg 1s (shown inset) core levels of UT-ZnMgO and TT-ZnMg

Table S1. Comparison of recent ZnMgO-based ETLs for PbS CQD solar cells and their reported PCEs.

Reference	ETL	Key Strategy	PCE
Xing et all [1]	Mg Doped ZnO	Mg Doping (defect reduction)	9.46
Ren et all [2]	Mg-ZnO + ZnO NC	Interface passivation	7.06
Gao et all [3]	MgCl2-treated ZnO	Surface defect passivation	8.2
Hu et all [4]	ZnMgO + graphene	Interface engineering	9.0
Zhang et all [5]	MgZnO nanocrystal	Enhanced Electron extraction	10.4
This work	ZnMgO + Toulene	Hydroxyl removal + wettability	6.73

Table S2**.** Contact angles of water on untreated (UT) and toluene-treated (TT) ZnMgO films, along with the corresponding approximate surface energies calculated using a water-only method**.**

Sample	**Contact Angle (°)**	**Approx. Surface Energy (mN/m)**
UT-ZnMgO	12.96	70.95
TT-ZnMgO	26.98	65.2

Table S3.Quantitative XPS O1s peak fitting areas with statistical error

Sample	**OI (%)**	**OII (%)**
UT-ZnMgO	17.28% +	82.72
TT-ZnMgO	29.09+	70.91

Table S4. Performance summary for the devices extracted from the J-V characteristics

Sample	***V*oc**	***J*sc**	**FF**	**PCE %**
UT-ZnMgO	0.22	9.43	0.27	0.56
TT-ZnMgO	0.54	27.85	0.45	6.73

Table S5. Extracted series resistance $R_s$and recombination resistance R_p values obtained from EIS fitting for untreated (UT-ZnMgO) and toluene-treated (TT-ZnMgO) PbS quantum dot solar cells. The higher $R_p$and lower R_sIn the TT-ZnMgO device, enhanced charge transport and reduced interfacial recombination are indicated, confirming the improved electronic quality of the treated ZnMgO layer.

Sample	**Rp.(Ω)**	**Rp·A (Ω·cm^2)**	**Rs.(Ω)**	**Rs·A (Ω·cm^2)**
UT-ZnMgO	72.59	5.81	12.37	0.99

TT-ZnMgO	296.13	23.69	9.06	0.73

References.

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