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Supporting Information

Ligand-dependent exciton dynamics and photovoltaic properties in PbS quantum dot heterojunction solar cells

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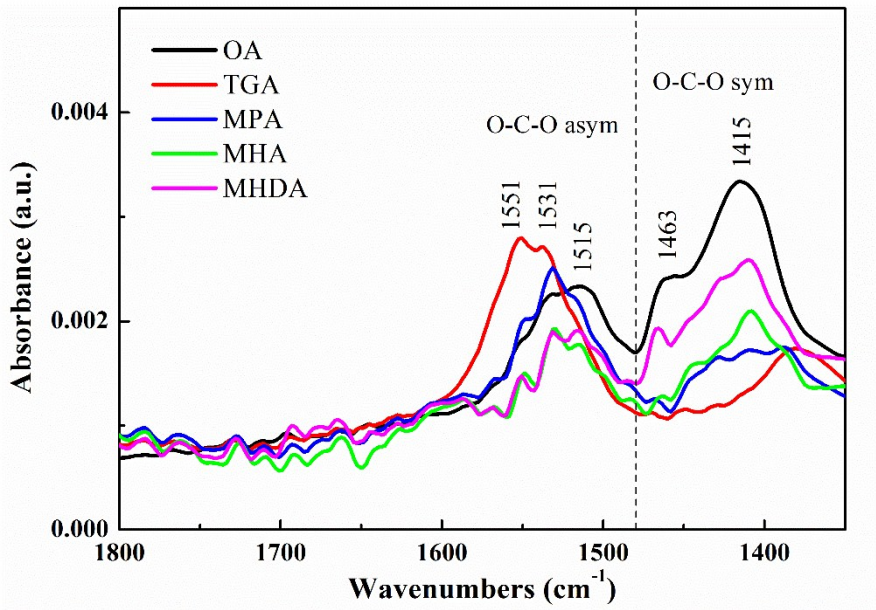

Fig. S1 Reflective FT-IT spectra (1800-1300 cm^{-1}) of PbS QD films capped with various surface ligands: OA, TGA, MPA, MHA and MHDA.

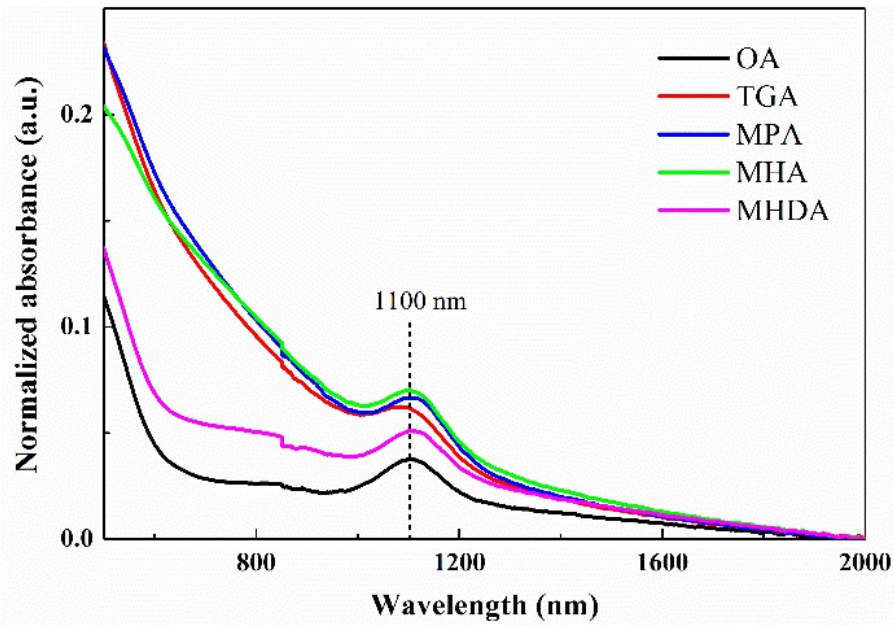

Fig. S2 (a) Room temperature UV-vis-NIR spectra of PbS QD films with various surface ligands. The films were fabricated by spin coating one cycle OA-capped PbS QDs on glasses, followed by solid-state ligand exchange in the case of TGA, MPA, MHA and MHDA-capped QDs.

Table S1. The photovoltaic parameters of PbS QDSCs with different surface ligands.

Ligands	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
TGA	10.8±0.56	0.45±0.004	0.38±0.008	1.81±0.04
MPA	15.3±0.21	0.46±0.001	0.38±0.001	2.64±0.05
MHA	6.76±0.16	0.53±0.002	0.33±0.002	1.20±0.02
MHDA	Electrically disconnected			

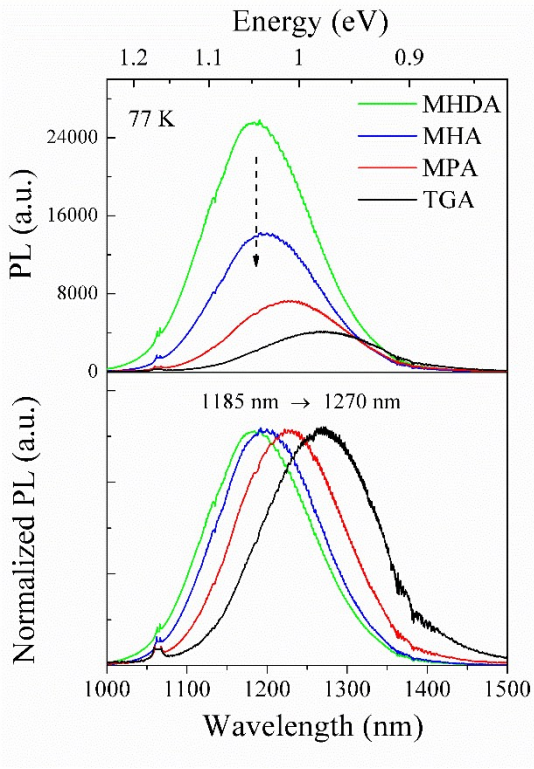

Fig. S3 PL emission and normalized spectra of PbS QD films with different length MAA ligands measured at 77 K.

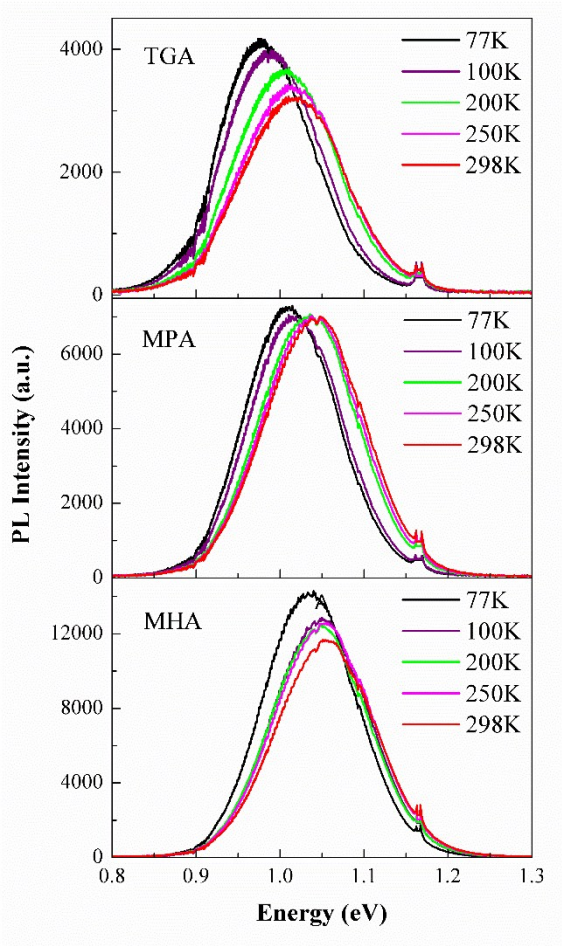

Fig. S4 PL spectra of PbS QD films with different ligands measured at various temperatures.

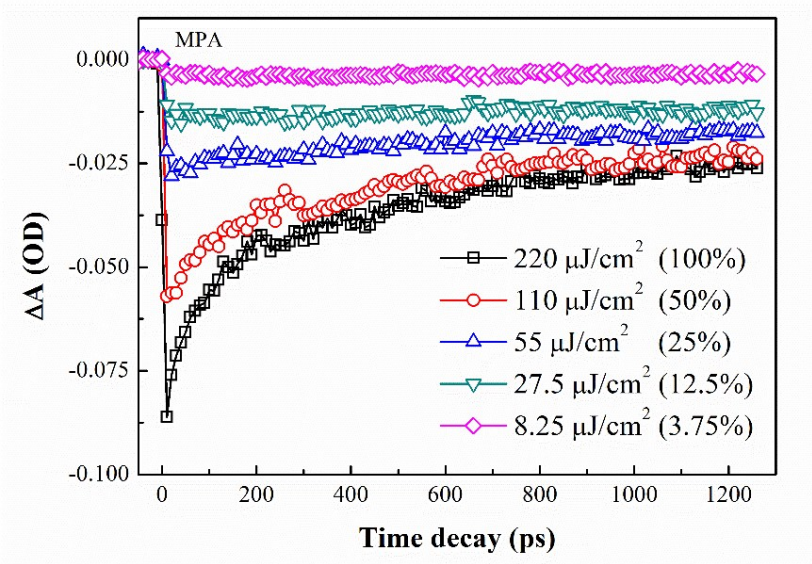

Fig. S5 The power dependent TA spectra of the PbS-MPA QD film.

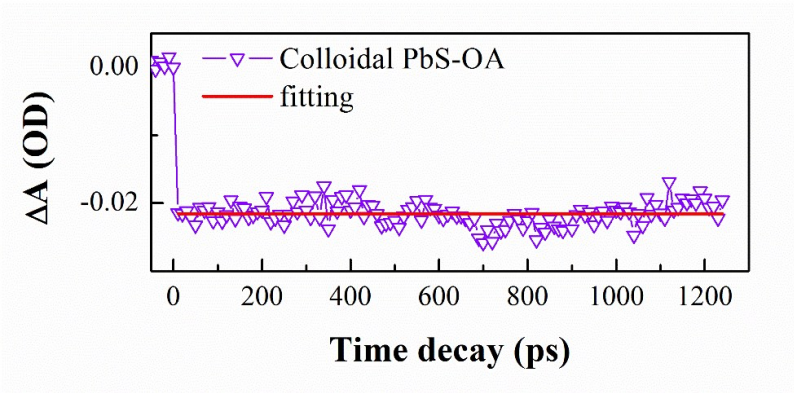

Fig. S6 TA spectrum of isolated PbS QDs dispersed in octane solution.

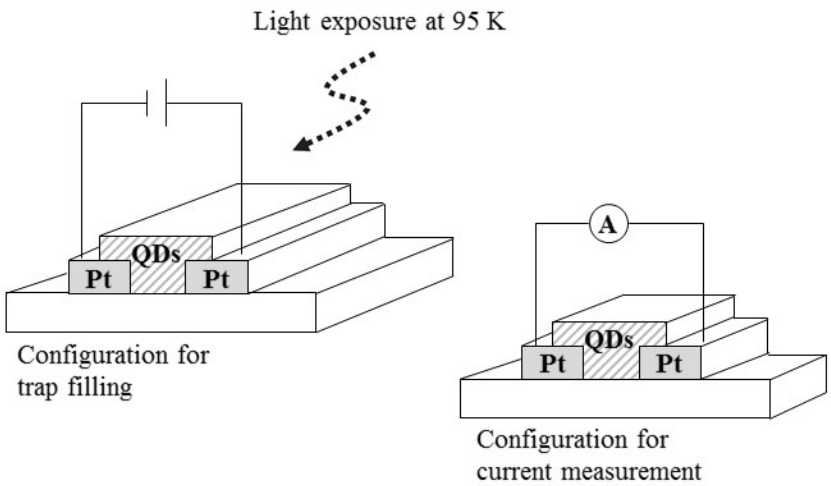

Fig. S7 Schematic illustration of the thermally stimulated current (TSC) measurement for QD films.

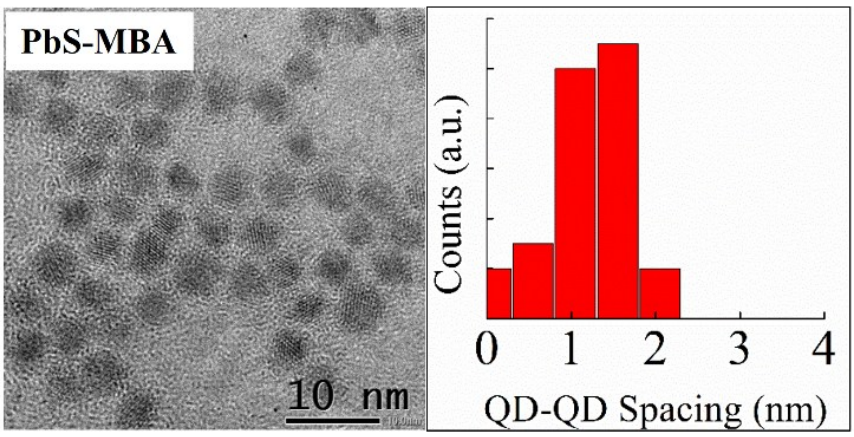

Fig. S8 (a,b) TEM images and the statistic QD-QD spacing of PbS QDs linked with MBA ligands.

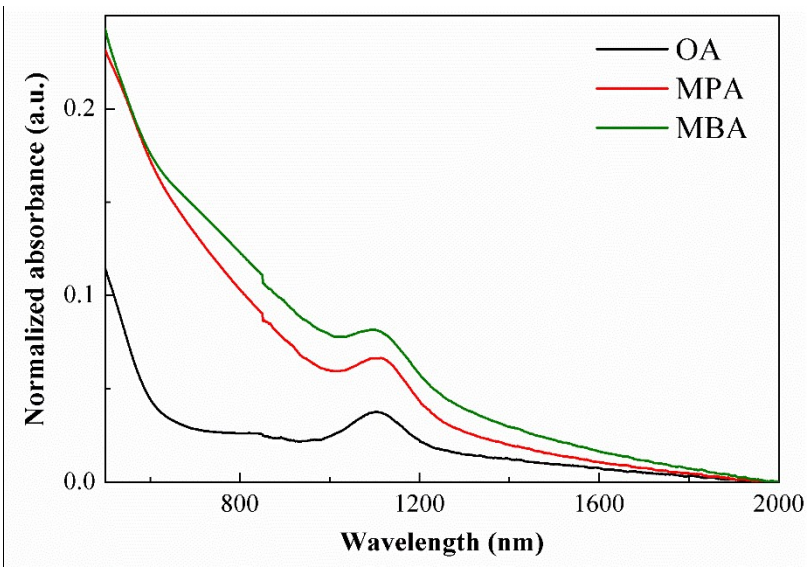

Fig. S9 Comparison of the UV-vis-NIR spectra of PbS QD films with OA, MPA and MBA ligands, respectively.

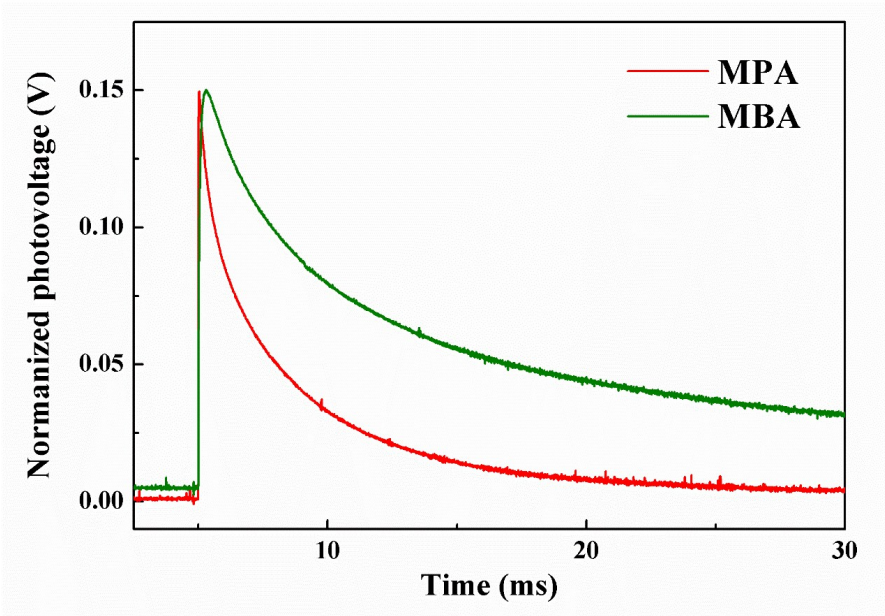

Fig. S10 The V_{oc} decay curves of PbS QDHSCs with MPA and MBA ligands, respectively.

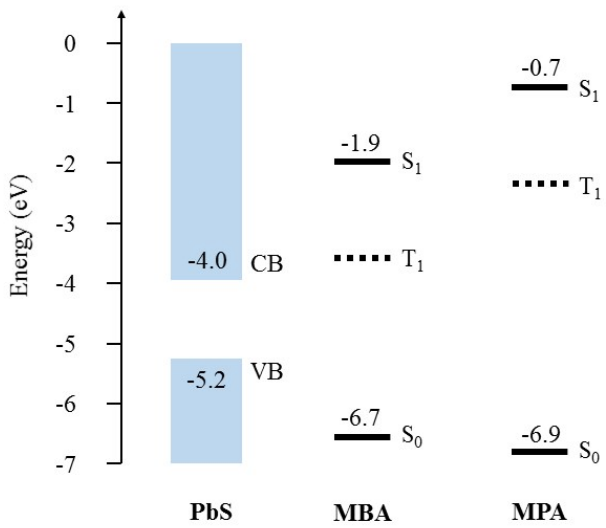

Fig. S11 Energy level diagram for PbS QD, MBA and MPA. The energy level of PbS QD was obtained from our previous work, while that of MBA and MPA was estimated from DFT calculation.