Electronic Supplementary Information

Ligands Affect the Lattice Structure and Photovoltaic Performance of Thin Films of PbSe Quantum Dots

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Figure S1. SEM images of PbSe QDs featuring various capping ligands. (A) OA-capped PbSe QD film; (B) OA-capped PbSe QD film subsequently treated with 1 mM EDT; (C) BA-exchanged PbSe QD film; (D) BA-exchanged PbSe QD film subsequently treated with 1 mM EDT. Scale bar: 100 nm.

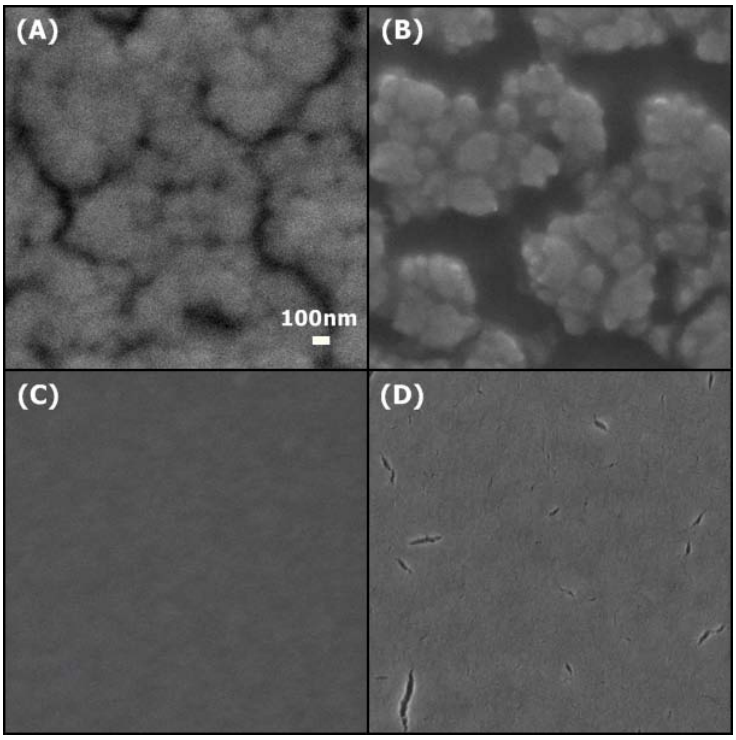


Figure S2. TEM image of monodisperse PbSe QDs with a first exciton absorption peak of 1455 nm. Average diameter of QDs: 4.6 nm.

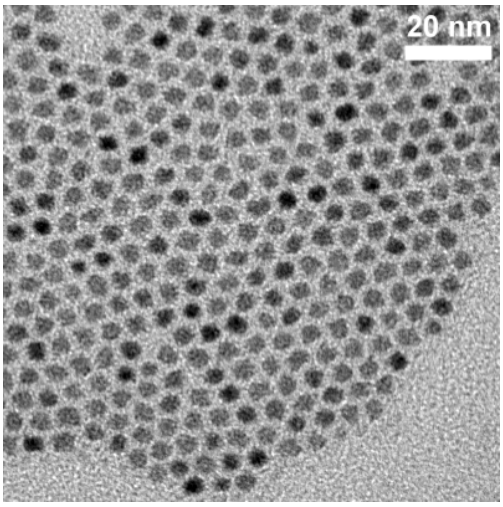


Figure S3. Synchrotron X-ray azimuthal scans of (i) OA-, (ii) BA-, and (iii) EDT-capped PbSe QD films, prepared through spin-coating onto Si substrates (log-normal scale).

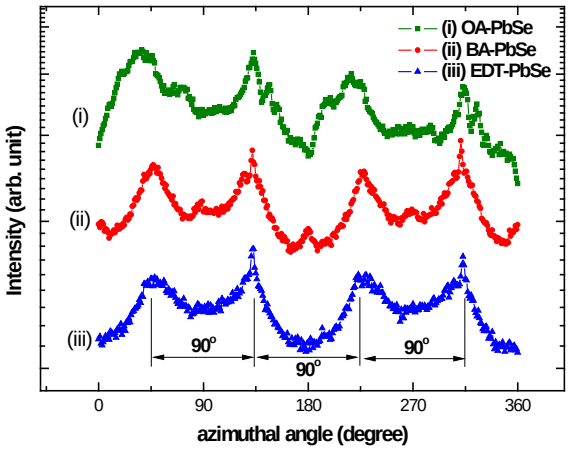
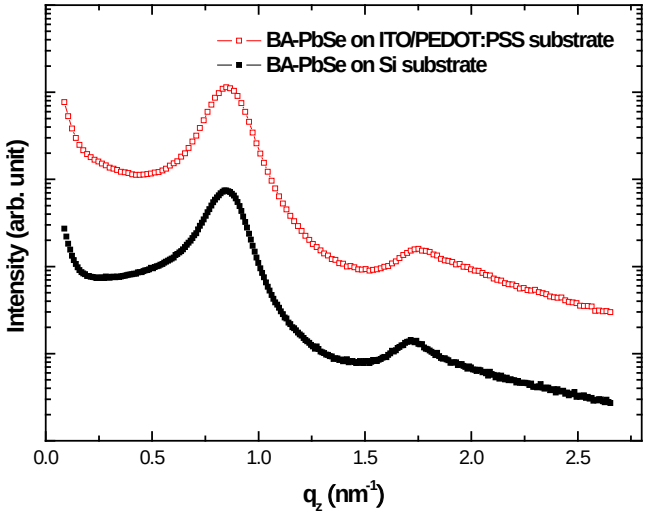


Figure S4. Synchrotron X-ray in-plane CTR and azimuthal scans of BA-capped PbSe QD films, prepared by spin-coating onto ITO/PEDOT:PSS and Si substrates.



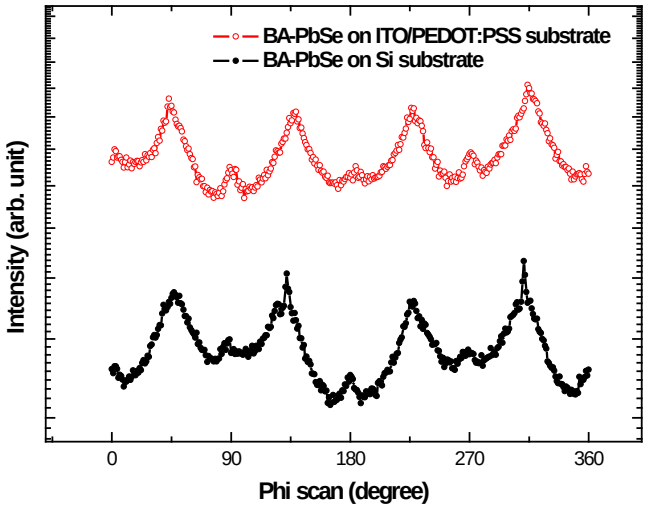


Table S1. Synchrotron XRR fitted parameters of the ligand-capped PbSe QD films.

PbSe-OA sample; grain size: 71.8 nm			
Layer	Thickness (nm)	Roughness (nm)	Density (g cm^{-3})
Si substrate	N.A.	$\sigma_{Si/SiO2}$ = 0.1	2.328
SiO_2	2.5	$\sigma_{SiO2/OA}$ = 0.3	2.27
PbSe-OA film	140	σ_s = 8	1.863
PbSe-BA sample; grain size: 31.8 nm			
Layer	Thickness (nm)	Roughness (nm)	Density (g cm^{-3})
Si substrate	N.A.	$\sigma_{Si/SiO2}$ = 0.1	2.328
SiO_2	2.5	$\sigma_{SiO2/OB}$ = 0.3	2.27
PbSe-BA film	62	σ_s = 3.8	3.561
PbSe-EDT sample; grain size: 31.6 nm			
Layer	Thickness (nm)	Roughness (nm)	Density (g cm^{-3})
Si substrate	N.A.	$\sigma_{Si/SiO2}$ = 0.1	2.328
SiO_2	3.3	$\sigma_{SiO2/EDT}$ = 0.45	2.27
PbSe-BA film	45	σ_s = 3.8	4.698

Figure S5. TEM images of the superlattices of the OA-capped PbSe QD film (a) before and (b) after exposure to air for 2 days; scale: 100 nm. The sample was prepared through spin-coating of a solution of PbSe QD (50 mg mL^{-1}) in octane in a N_2-filled glove box.