Supplementary Information

Direct Patterning of Colloidal Quantum Dots with Adaptable Dual-Ligand Surface

Donghyo Hahm,[1,†] Jaemin Lim,[1,†] Hyeokjun Kim,[2,†] Jin-Wook Shin,[3] Sungkwon Hwang,[4] Seunghyun Rhee,[1] June Hyuk Chang,[1] Jeehye Yang,[2] Beomgyu Choi,[1] Young-Shin Park,[5] Doh C. Lee,[5] Euyheon Hwang,[1] Seungjun Chung,[4] Chan-mo Kang,[3,*] Moon Sung Kang,[2*] and Wan Ki Bae[1,*]

[1]SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea

[2]Department of Chemical and Biomolecular Engineering, Sogang University, Seoul 04107, Republic of Korea

[3]Reality Display Research Section, Electronics and Telecommunications Research Institute (ETRI), Daejeon 34129, Republic of Korea

[4]Soft Hybrid Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Korea

[5]Department of Chemical and Biomolecular Engineering, KAIST Institute for the Nanocentury, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Korea

†These authors contributed equally to this work: Donghyo Hahm, Jaemin Lim, Hyeokjun Kim

Corresponding Authors

Correspondence to Wan Ki Bae (wkbae@skku.edu); Moon Sung Kang (kangms@sogang.ac.kr); Chan-mo Kang (nkcm@etri.re.kr)

Supplementary Note 1. Synthesis of quantum dots (QDs)

Chemicals. Indium acetate ($In(ac)_3$, 99.99%), zinc acetate ($Zn(ac)_2$, 99.99%), oleic acid (OA, 99%), 1-octadecene (ODE, 99%), tris(trimethylsilyl)phosphine ($(TMS)_3P$, 99.9%), *n*-trioctylphosphine (TOP, 99%), *n*-trioctylamine (TOA, 99%), selenium (Se, 99.9%), sulfur (S, 99.9%) are purchased from Uniam. Cadmium oxide (CdO, 99.5%, trace metals basis) and zinc chloride ($ZnCl_2$, anhydrous, ≥ 98 %) are purchased from Sigma-Aldrich. All chemicals are used as received.

Precursor preparation. All chemistry is carried out under Ar atmosphere with Schlenk line technique. 0.5 M indium oleate ($In(OA)_3$), 0.5 M zinc oleate ($Zn(OA)_2$), 0.5 M cadmium oleate ($Cd(OA)_2$), 2 M TOPSe, and 2M TOPS stock solutions are prepared prior to the QD synthesis. For a preparation of 0.5 M $In(OA)_3$ (or $Zn(OA)_2$) stock solution, 100 mmol of $In(Ac)_3$ (or $Zn(Ac)_2$) and a stoichiometric amount of OA are loaded into a flask and degassed under vacuum at 140 ℃ for 6 hours to obtain a clear solution. The reaction flask is back-filled with Ar, and the concentrations of the precursors are diluted to 0.5 M with 1-octadecene or tri-*n*-octylamine. The precursors are stored under Ar atmosphere at 80 ℃ for further use. For a preparation of 0.5 M $Cd(OA)_2$ precursor, a mixture of 10 mmol of CdO, 10 ml of OA, and 10 ml of ODE is degassed under vacuum at 110 ℃, and slowly heated up to 300 ℃ to obtain an optically transparent solution. The reaction flask is then cooled down to 110 ℃ and degassed under vacuum for an hour to remove the water. 2 M TOPSe and TOPS stock solutions are prepared by dissolving 100 mmol of Se and S in 50 ml of TOP at the elevated temperature (*ca.* 100 ℃) and stored under Ar atmosphere at room temperature.

Synthesis of InP cores. InP (r = 1.2 nm) QDs are synthesized following the previously reported method[1,2] with minor modifications. 2 mmol of $In(OA)_3$ precursor and 5 ml of ODE are loaded into a flask, degassed at 110 ℃ for 3 hour and backfilled with Ar. A mixture of 1 mmol of $P(TMS)_3$ diluted with 2 ml of TOP is rapidly injected into the reaction flask to form In-P complexes. The temperature is elevated up to 260 ℃ to instigate InP nucleation. The reaction temperature is maintained for 1 hour before cooled to room temperature. Synthesized InP QDs are washed repeatedly with acetone. Resulting InP (r = 1.2 nm) QDs show the atomic In/P ratio of 1.6. In order to synthesize larger InP (r = 1.9 nm) QDs, a mixture of 2 mmol of $In(OA)_3$ and 5 ml of ODE are placed into a reaction flask, degassed under vacuum at 110 ℃, and back-filled with Ar. 1 mmol of $P(TMS)_3$ diluted with 1 ml of TOP is injected into the reaction flask to form In-P complexes, and the reactant is heated up to 280 ℃ to generate InP nuclei. After 30 min of reaction, 5 mmol of indium and 2.5 mmol of phosphine precursor are added dropwise to promote InP growth. Synthesized InP QDs are purified twice *via* precipitation/redispersion method (acetone/toluene) and diluted with toluene for further use.

Synthesis of green- & red-emitting InP/$ZnSe_xS_{1-x}$ QDs. InP/$ZnSe_xS_{1-x}$ QDs are synthesized following the previously reported method[1,2] with minor modifications. For green-emitting InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs, a flask containing 5 mmol of $Zn(OA)_2$ and 10 ml of TOA is degassed at 110 ℃ for 1 hour, back-filled with Ar and heated up to 180 ℃. 100 mg of InP (r = 1.2 nm) QDs is injected to the reaction flask, and 2.9 mmol of 2M TOPSe precursor is added to promote ZnSe shell growth. The temperature is elevated to 320 ℃ and kept for 2

hours. 10 mmol of $Zn(OA)_2$ precursor, 2.1 mmol of TOPSe, and 4.2 mmol of TOPS are added stepwise for 3 hours to grow 2.3 nm thick $ZnSe_xS_{1-x}$ shell. For red-emitting InP (r = 1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QDs, a mixture of 100 mg of InP (r = 1.9 nm) cores, 10 ml of TOA, 0.5 mmol of $ZnCl_2$, and 5 mmol of $Zn(OA)_2$ are placed into a reaction flask and degassed under vacuum at 110 ℃ and back-filled with argon. For the growth of the ZnSe shell, 1.8 mmol of TOPSe is injected into the flask, and the temperature is quickly raised to 320 ℃ and maintained for an hour. The additional $ZnSe_xS_{1-x}$ shell is overcoated for 3 hours by adding 12 mmol of $Zn(OA)_2$, 6 mmol of TOPSe and 2 mmol of TOPS. The reaction mixture is cooled to room temperature, purified repeatedly *via* precipitation/redispersion method (acetone/toluene) and diluted with toluene for further use.

Synthesis of red-emitting and green-emitting $CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ QDs. Red-emitting $CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ QDs are synthesized referring to the method by Lim *et al*[3] with minor modifications. 0.2 mmol of $Cd(OA)_2$ and 10 ml of ODE are loaded into a flask, degassed under vacuum at 110 ℃ and back-filled with Ar. After heating up to 300 ℃, 0.1 mmol TOPSe is swiftly injected into the flask to form CdSe core (r = 1.5 nm). The additional injection of $Cd(OA)_2$ (0.3 mmol) and TOPSe (0.3 mmol) precursors at the elevated temperature yields larger CdSe cores (r = 2.5 nm) for red-emitting QDs. To overcoat $Cd_xZn_{1-x}Se$ layer onto the CdSe cores, 10 mmol of $Zn(OA)_2$ is injected at the elevated temperature, followed by stepwise injection of 2 mmol of $Cd(OA)_2$ and 8 mmol of TOPSe for 2 hours. For the growth of exterior $ZnSe_yS_{1-y}$ shell, 20 mmol of $Zn(OA)_2$ is added into the flask at the elevated temperature, followed by dropwise injection of 6.2 mmol of TOPSe and 9.1 mmol of TOPS for 3 hours. After cooled down to room temperature, the resulting QDs are purified repeatedly *via* precipitation/redispersion method (acetone/toluene) and diluted with toluene for further use. Green-emitting $CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ QDs are synthesized in the same manner with smaller CdSe core (r = 2.0 nm). $Cd_xZn_{1-x}Se$ shell is grown on CdSe cores by stepwise injection of 0.1 mmol of $Cd(OA)_2$ and 3.8 mmol of TOPSe following the injection of 5.5 mmol of $Zn(OA)_2$ precursors. After an hour of shell growth, the reaction flask is heated up to 320 ℃ to induce interdiffusion of cation and the reaction temperature is maintained until the emission wavelength moves to the green region. 20 mmol of $Zn(OA)_2$, 5 mmol of TOPSe, and 7 mmol of TOPS are added for $ZnSe_yS_{1-y}$ exterior shell growth. After cool down to room temperature, synthesized green-emitting $CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ QDs are purified repeatedly *via* precipitation/redispersion method (acetone/toluene) and diluted with toluene for further use.

Synthesis of blue-emitting $Cd_xZn_{1-x}S/ZnS$ QDs. Blue-emitting $Cd_xZn_{1-x}S/ZnS$ QDs are synthesized following the previously reported procedure[4] with minor modifications. As a typical synthesis, a mixture of 1 mmol CdO (1 mmol), $Zn(Ac)_2$ (10 mmol) and 7 ml of OA are loaded to a flask. The reaction flask is degassed under vacuum at 160 ℃ and filled with Ar. After 15 ml of ODE is added, the reaction temperature is heated to 300 ℃ to form cation solution. 1.6 mmol of elemental S dissolved in 2.4 ml of ODE is swiftly injected into the mixture and reacted for 3 min. 16 mmol of S powder dissolved in 32 ml of ODE is injected dropwise for 2 hours to grow exterior ZnS shell. Resulting QDs are purified repeatedly *via* precipitation/redispersion method (acetone/toluene) and diluted with toluene for further use.

Supplementary Note 2. Synthesis of photocrosslinkable ligands

Chemicals. 4,4'-difluorobenzophenone (> 99 %), 2-pyrrolidone (> 98 %), dimethyl sulfoxide (DMSO, > 99 %), 1,10-decanedithiol (> 98 %), potassium carbonate (K_2CO_3, > 99 %), N,N-dimethylformamide (DMF, > 99.5 %), 4-chlorobenzophenone (> 98 %), hydroquinone (> 99 %), 1,10-dibromodecane (> 95 %), tetrabutylammonium bromide (TBAB, > 98 %) are purchased from Tokyo Chemical Industry. Sodium hydrosulfide hydrate (NaSH, ≥ 60 %) is purchased from Sigma-Aldrich. All chemicals, unless otherwise stated, are used as received.

Synthesis of (4-((10-mercaptodecyl)thio)phenyl)(phenyl)methanone (S-BP). 4-chlorobenzophenone (5 g), 1,10-decanedithiol (5.7 g), K_2CO_3 (6.3 g), and 50 ml of anhydrous DMF are loaded into a flame dried RB flask under argon atmosphere. The mixture is heated to 60 ℃ for 8 hours before cooled to room temperature. The reactant is quenched with NH_4Cl and extracted with methylene chloride. After washing with brine, the organic layer is dried over $MgSO_4$ and concentrated under reduced pressure. The crude product is purified *via* recrystallization with MeOH. The solid residue is then dried under a vacuum to give the desired product as white solids.

^{1}H NMR (δ ppm; $CDCl_3$, 500 MHz): 7.78 (d, 2H), 7.73 (d, 2H), 7.58 (t, 1H), 7.48(d,2H), 7.32(t, 2H), 3.00 (t, 2H), 2.50 (q, 2H), 1.83~1.24 (m, 19H).

Synthesis of (4-((10-mercaptodecyl)oxy)phenyl)(phenyl)methanone (O-BP). A mixture of hydroquinone (15 g), 1,10-dibromodecane (34.1 g), K_2CO_3 (16 g), and 400 ml of anhydrous acetone are placed into a flame dried RB flask under argon atmosphere. The flask is heated to 60 ℃, and the temperature is maintained for 9 hours before the mixture is cooled to room temperature. After filtration of the mixture, the filtrate is washed with deionized water and the reactant is extracted with methylene chloride. The organic layer is dried over $MgSO_4$ and concentrated under reduced pressure. The residue is distilled to remove the unreacted reagent and purified by column chromatography (4:1 *n*-hexane:ethyl acetate) to yield a white solid (19.8 g). The intermediate product is collected without further characterization for subsequent reactions. The collected solid is placed into a RB flask containing NaSH (10.7 g), TBAB (4.61 g), and 160 ml of anhydrous DMF. The temperature is raised to 120 ℃ and maintained for 6 hours. The reaction is quenched with NH_4Cl, and the precipitate is purified by column chromatography (4:1 *n*-hexane:ethyl acetate) to give O-BP as an off-white solid.

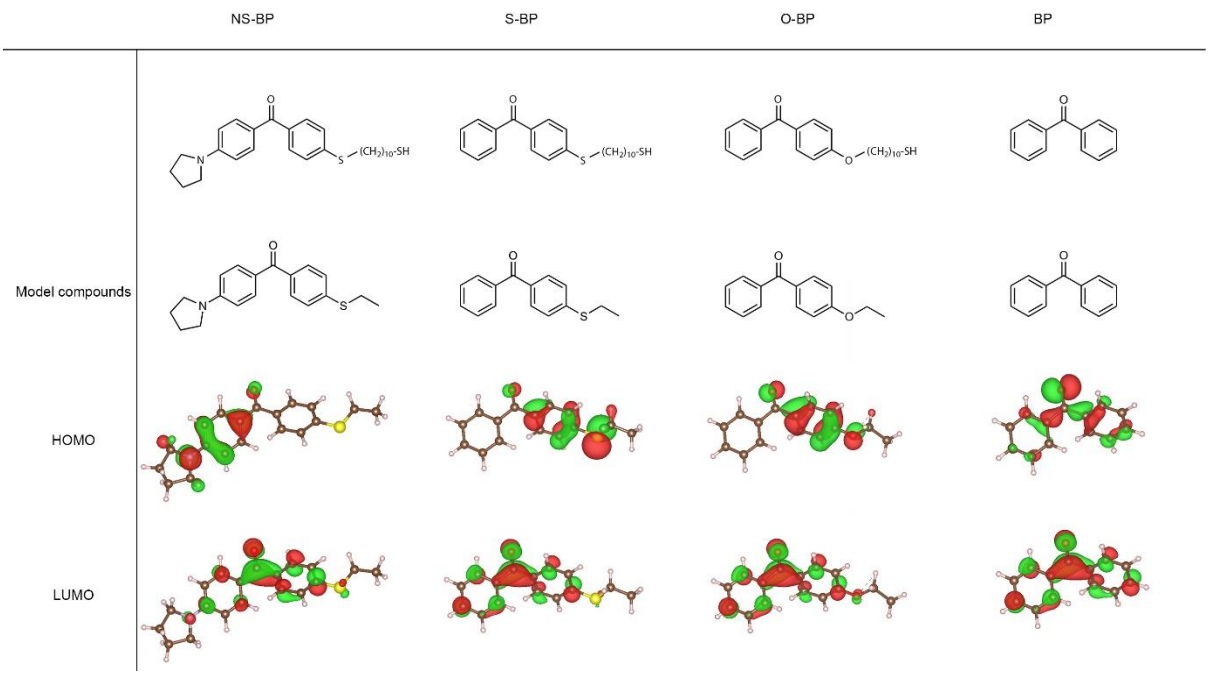
^{1}H NMR (δ ppm; $CDCl_3$, 500 MHz): 7.79 (d, 2H), 7.73 (d, 2H), 7.54 (t, 1H), 7.44 (t, 2H), 6.92 (d, 2H), 4.01 (t, 2H), 2.49 (q, 2H), 1.83~1.24 (m, 19H).

Supplementary Note 3. Density functional theory (DFT) calculation

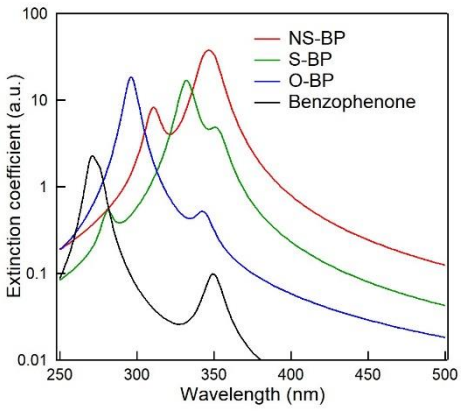
The calculations described in this paper are carried out using the plane-wave DFT software QUANTUM ESPRESSO[5] to obtain ground-state electronic properties using Optimized Norm-Conserving Vanderbilt Pseudopotential (ONCVPSP) for the most-widely used semilocal generalized gradient approximation (PBE-GGA)[6]. Kinetic energy cutoff for wavefunction and charge density are 70 Ry and 280 Ry, respectively. We set convergence threshold for self-consistency to 10^{-10} Ry. To get extinction coefficient we use the turboDavidson algorithm, which allows us to calculate absorption spectra of molecules using time-dependent density functional perturbation theory (TDDFPT). The interactions of electrons (Hartree and Exchange-Correlation effects) are taken into account fully *ab initio* and self-consistently.

Supplementary Note 4. Preparation of QD-PR patterns

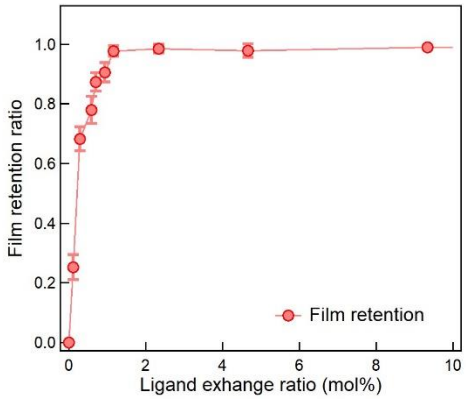
Native oleate ligands of InP (r =1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QDs are displaced by MMES prior to the preparation of a QD-PR solution. 30 mg of PXL-decorated QDs is added to 70 mg of commercial PR, supplied from DONGJIN SEMICHEM CO., LTD. The mixture is stirred at room temperature until it becomes clear. The resulting QD-PR is spun-cast onto a substrate at 1000 rpm for 30 s. Then, the film is soft baked on a hotplate at 90 °C for 100 s. After that, the film is selectively exposed to UV-A for 10 s by using a contact aligner (200 mJ/cm^2). The exposure gap between the film and photomask is 10 μm. Finally, the film was spray-developed by 0.1 % KOH solution for 60 s.



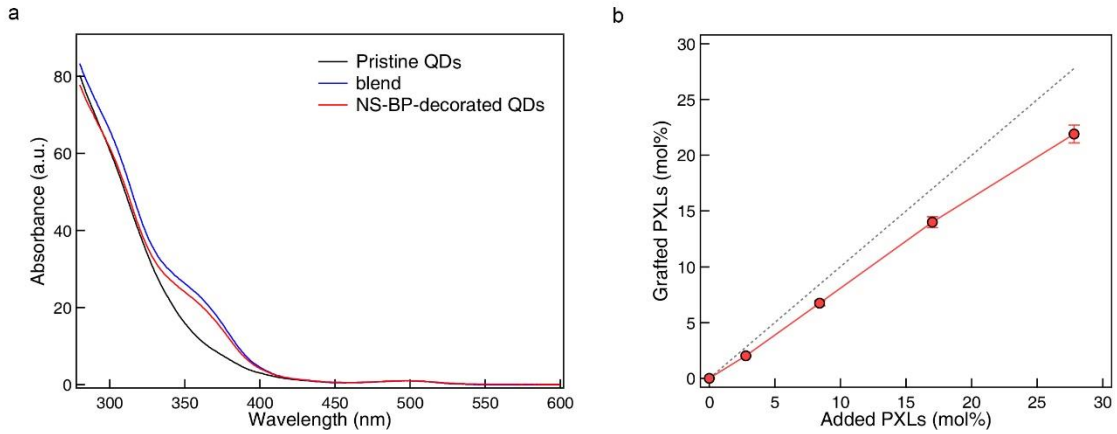
Supplementary Fig. 1 Chemical structures of NS-BP, S-BP, O-BP, benzophenone and model compounds, and calculated charge distribution within frontier molecular orbitals of these model compounds.



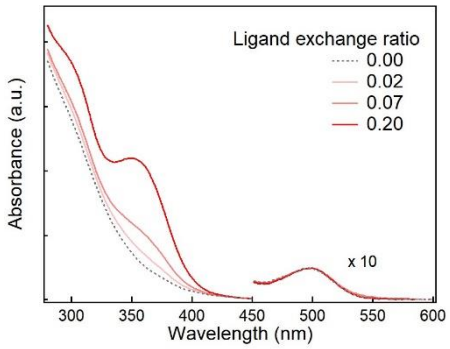
Supplementary Fig. 2 Calculated extinction coefficient of model compounds for NS-BP, S-BP, O-BP and benzophenone.



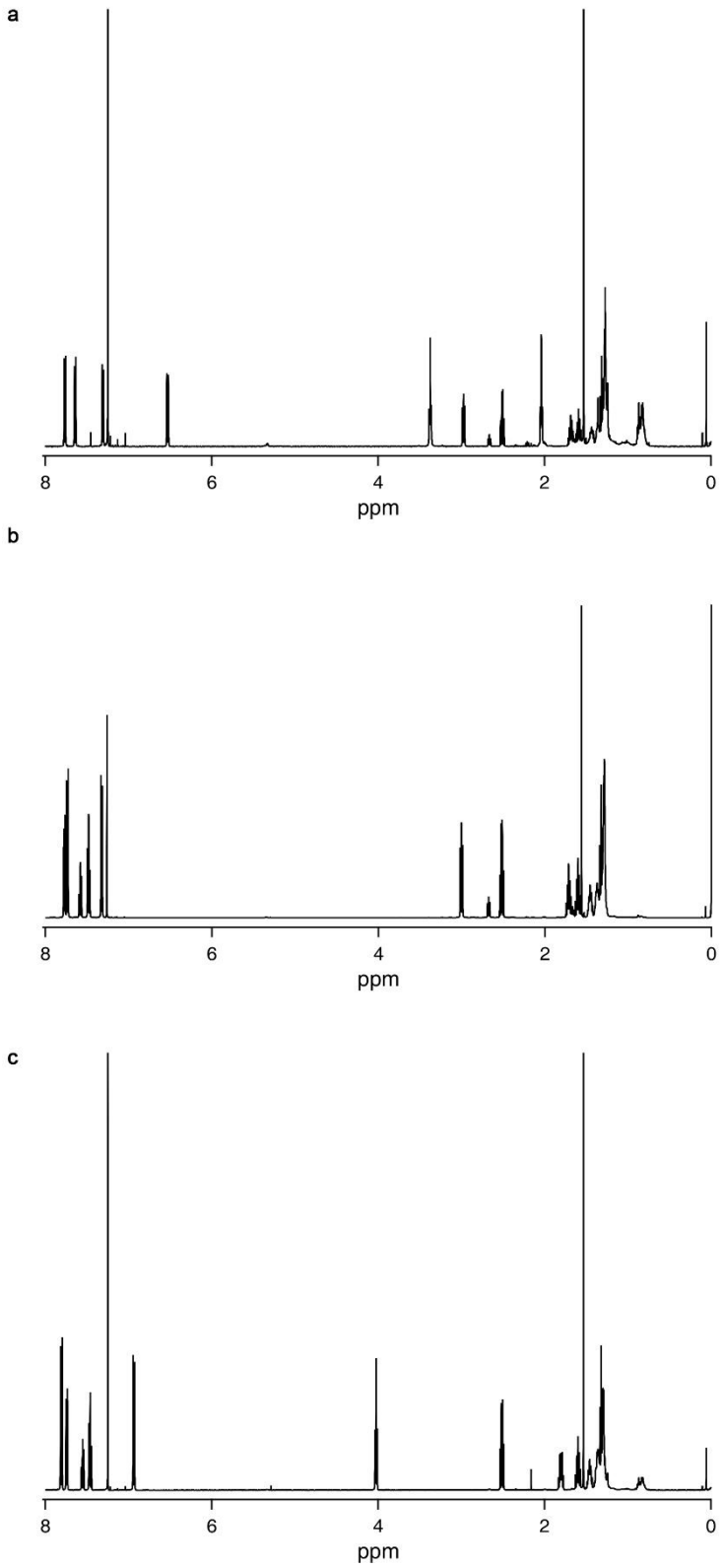
Supplementary Fig. 3 Maximum film retention ratios obtained with InP (r = 1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QD films with varying NS-BP contents.



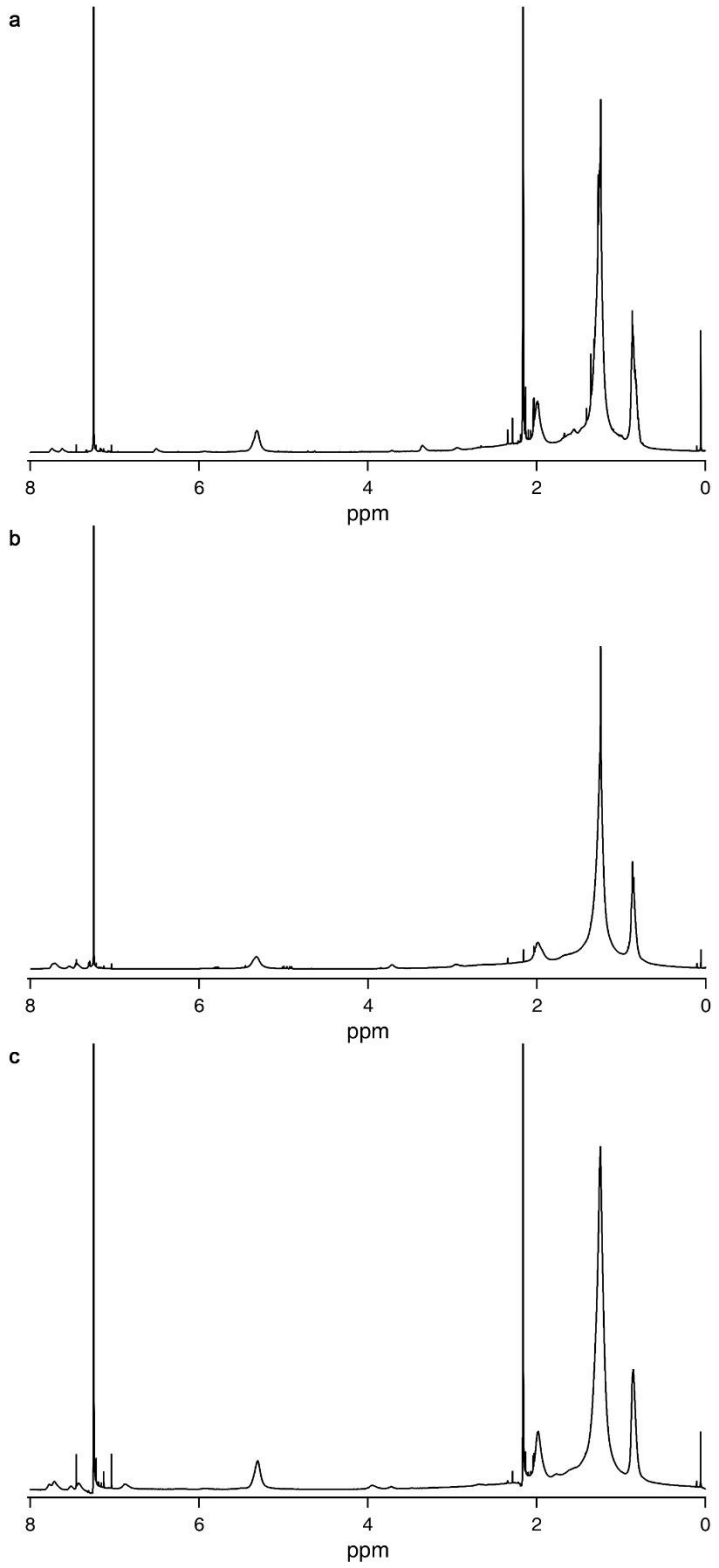
Supplementary Fig. 4 (a) Absorption spectra of InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs (black), a blend of InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs and NS-BP (blue), and NS-BP-grafted InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs after purification (red). (b) Amount of chemically grafted NS-BP onto the surface of InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs.



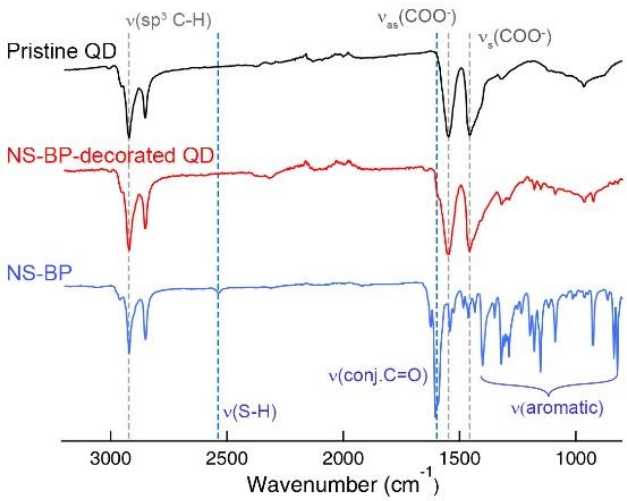
Supplementary Fig. 5 Absorption spectra of InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs grafted with varying NS-BP contents (0-20 mol%).



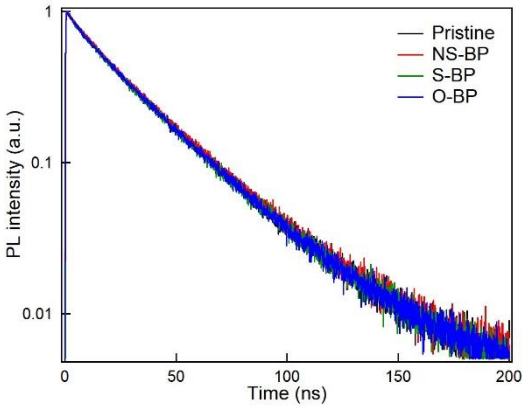
Supplementary Fig. 6 ^{1}H-NMR spectra of (a) NS-BP, (b) S-BP, and (c) O-BP.



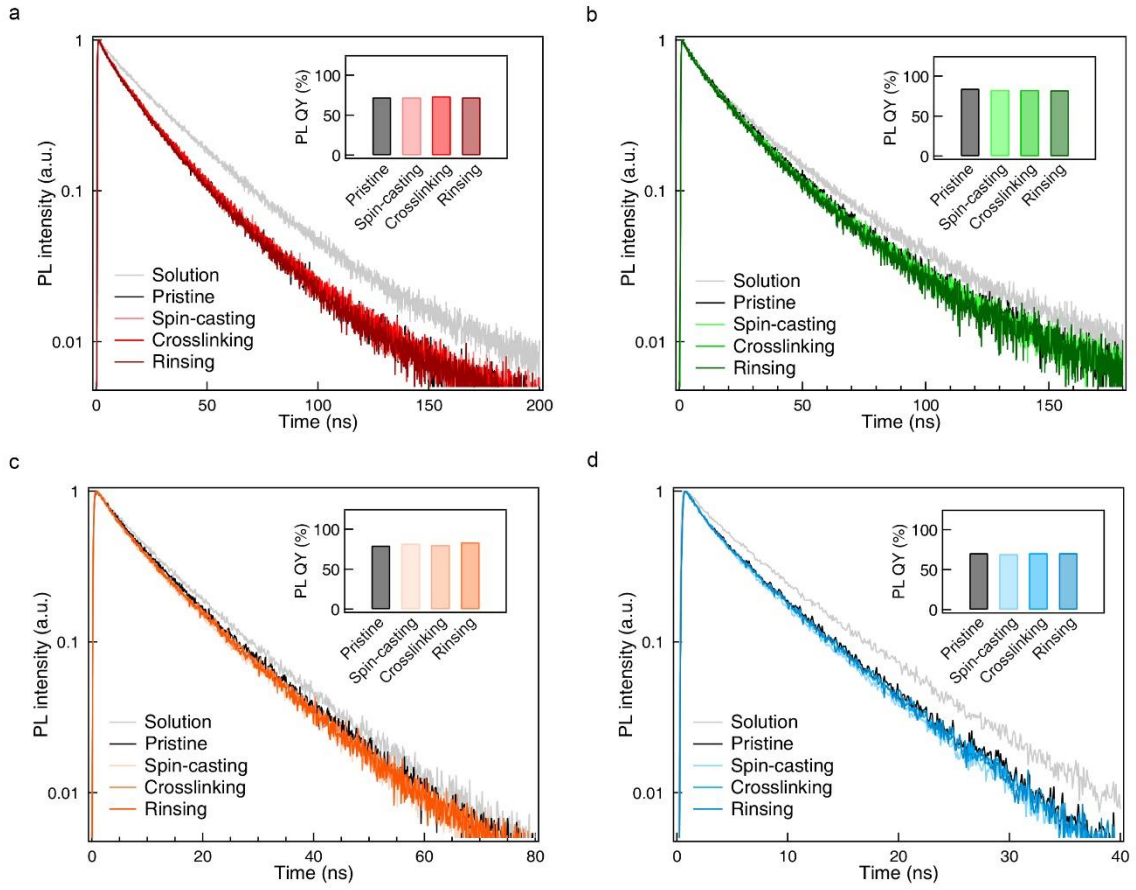
Supplementary Fig. 7 ^{1}H-NMR spectrum of PXL-grafted (7 mol%) InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs. (a) NS-BP, (b) S-BP, and (c) O-BP. The displacement ratios of PXLs are estimated based on the comparison between the integration of the characteristic peaks of PXLs and OA.



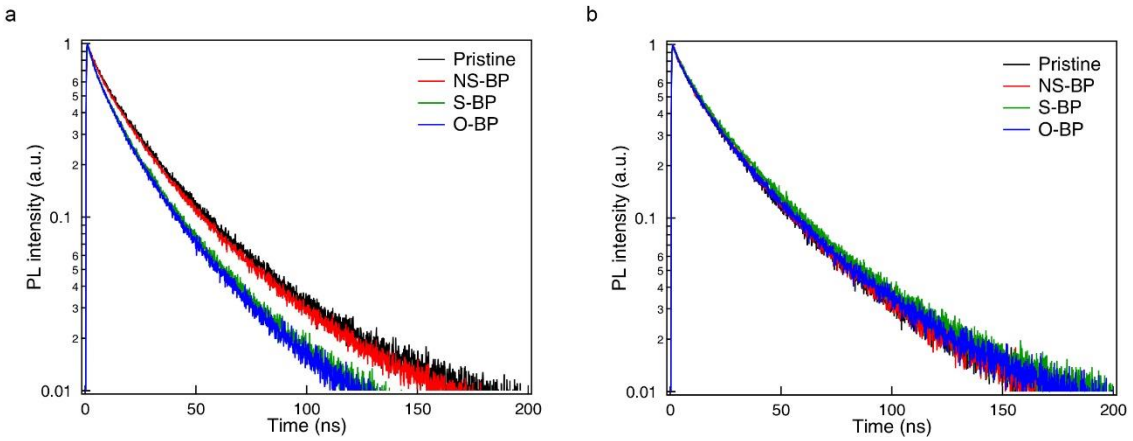
Supplementary Fig. 8 FT-IR spectra of pristine InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs (black), NS-BP-grafted InP/$ZnSe_xS_{1-x}$ QDs (red), and NS-BP (blue).



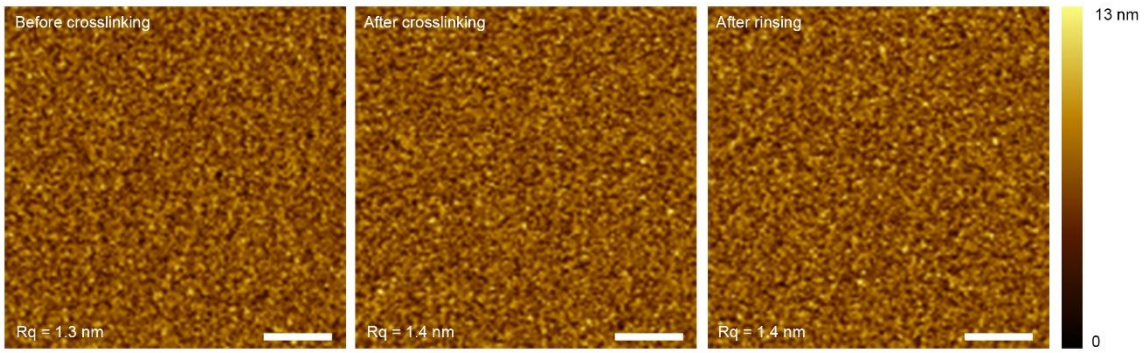
Supplementary Fig. 9 PL decay curves of pristine and PXL-grafted InP (r =1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QDs dispersed in toluene.



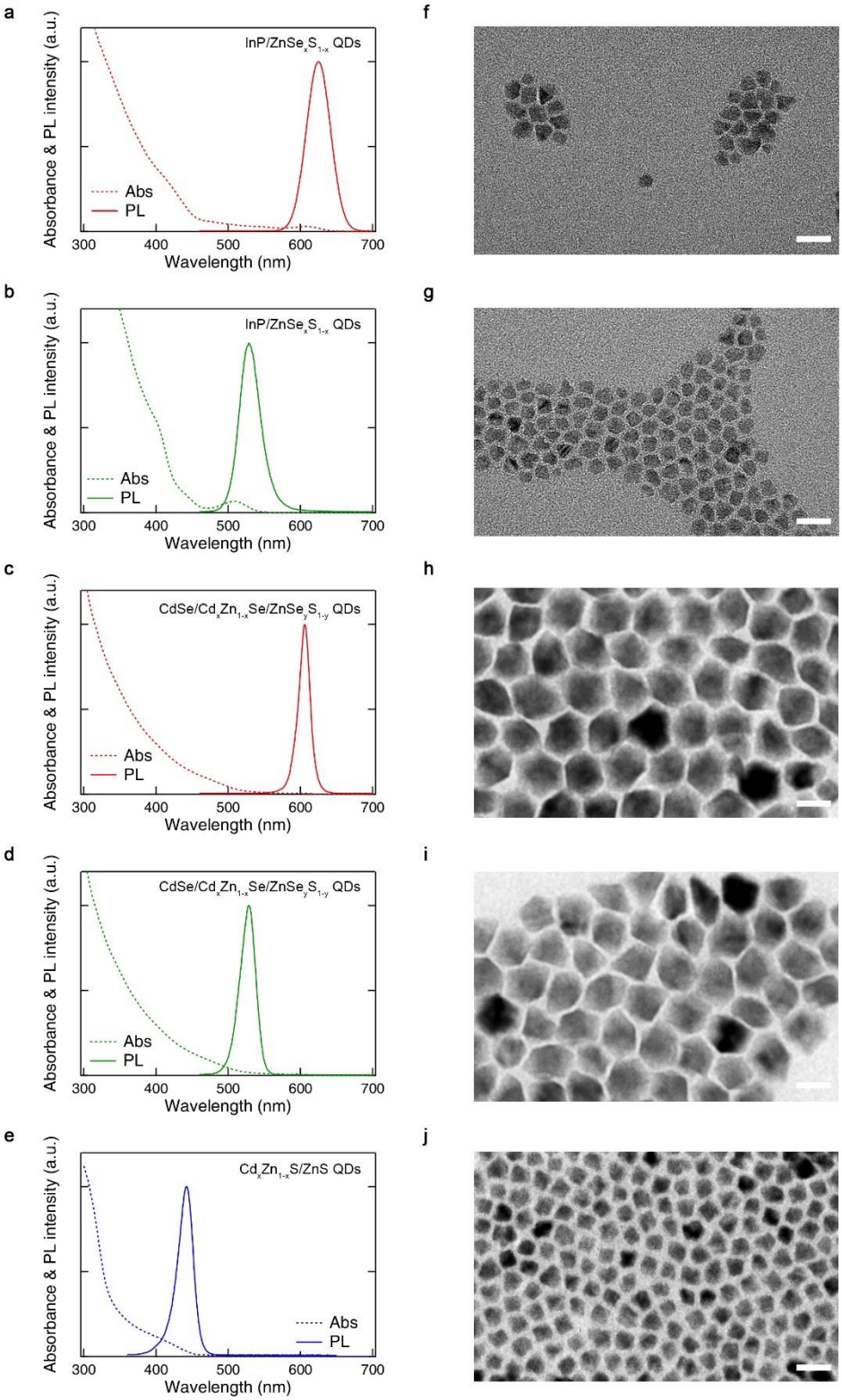
Supplementary Fig. 10 PL decay curves of NS-BP (7 mol%) grafted (a) red-emitting InP (r = 1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QDs, (b) green-emitting InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm), (c) red- and (d) green-emitting Cd-based QDs throughout the film spin-coating, crosslinking, and rinsing steps. PL decay curves of the pristine QD solution (grey) and film (black) is overlaid for comparison. Insets show film PL QYs of each film.



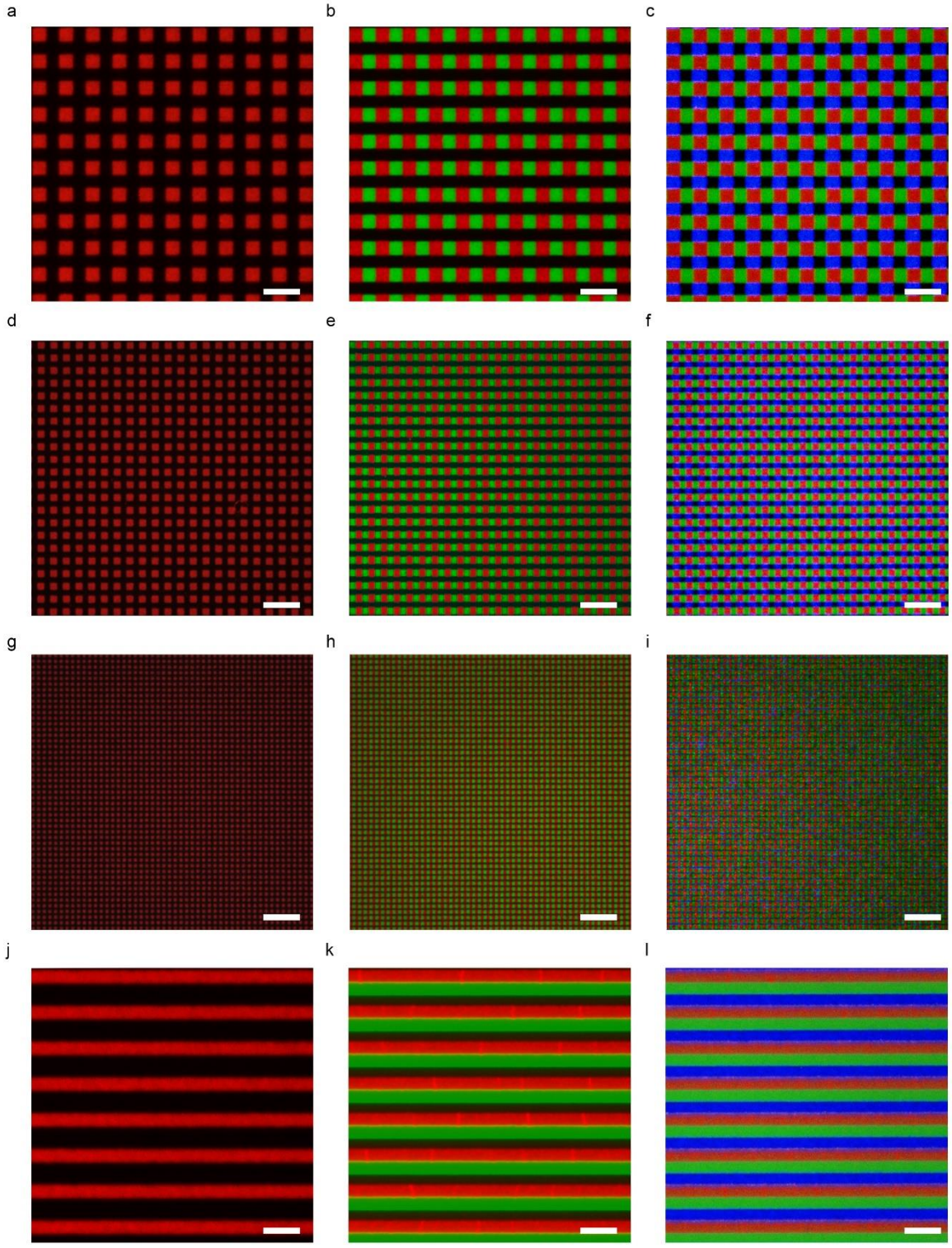
Supplementary Fig. 11 PL decay curves of photocrosslinked PXL-grafted InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QD films prepared at (a) an ambient condition and (b) an inert condition. PL decay of pristine QD films (black) are displayed for comparison.



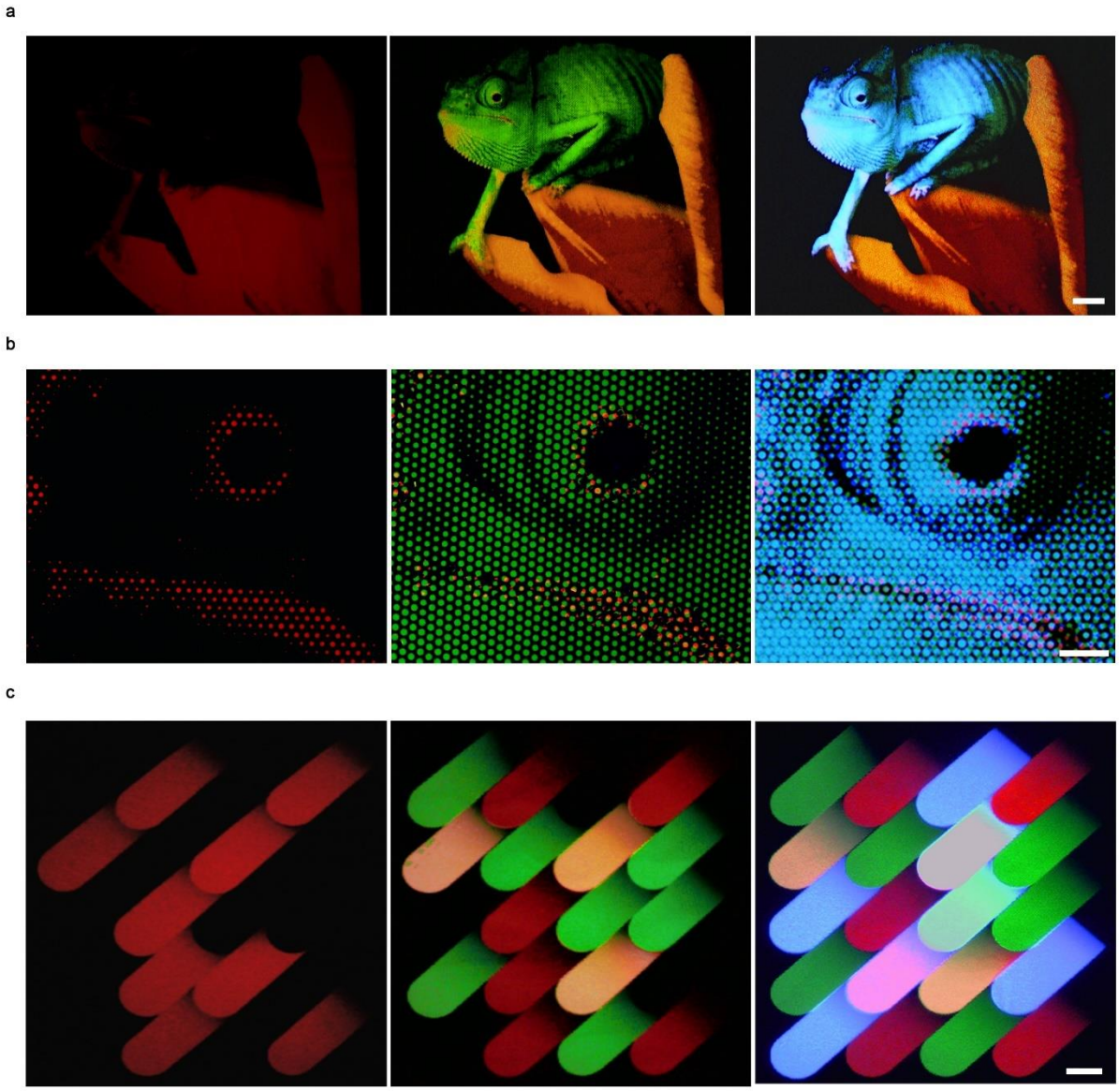
Supplementary Fig. 12 AFM images of crosslinked NS-BP-grafted InP (r =1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QD films before (left) and after (middle) UV-A irradiation and after being washed with toluene twice (right). Scale bar = 1μm.



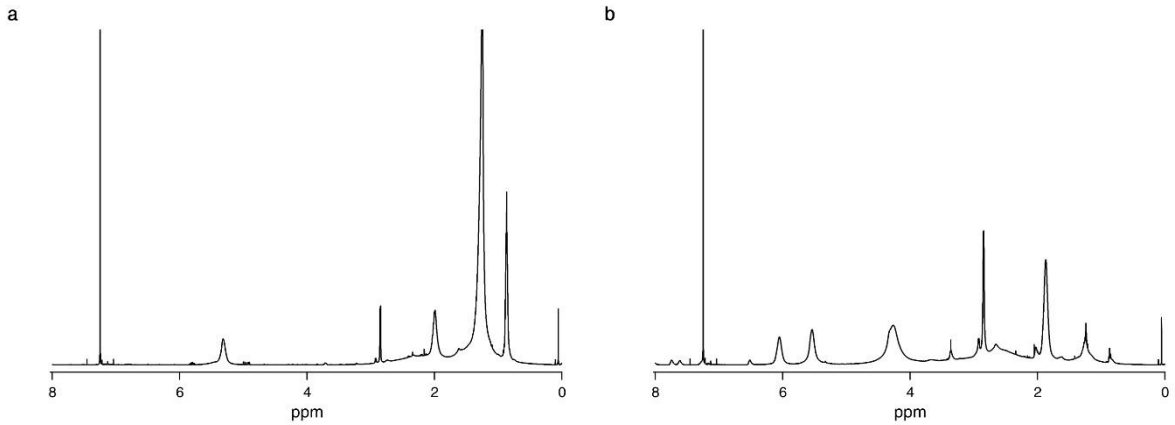
Supplementary Fig. 13 Absorption (dotted line) and emission (solid line) spectra (a-e), and TEM images (f-j) of (a,f) red- and (b, g) green-emitting InP/$ZnSe_xS_{1-x}$ QDs, (c, h) red- and (d, i) green-emitting CdSe/$Cd_xZn_{1-x}Se$/$ZnSe_yS_{1-y}$ QDs, and (e, j) blue-emitting $Cd_xZn_{1-x}S$/ZnS QDs. Scale bar = 50 nm.



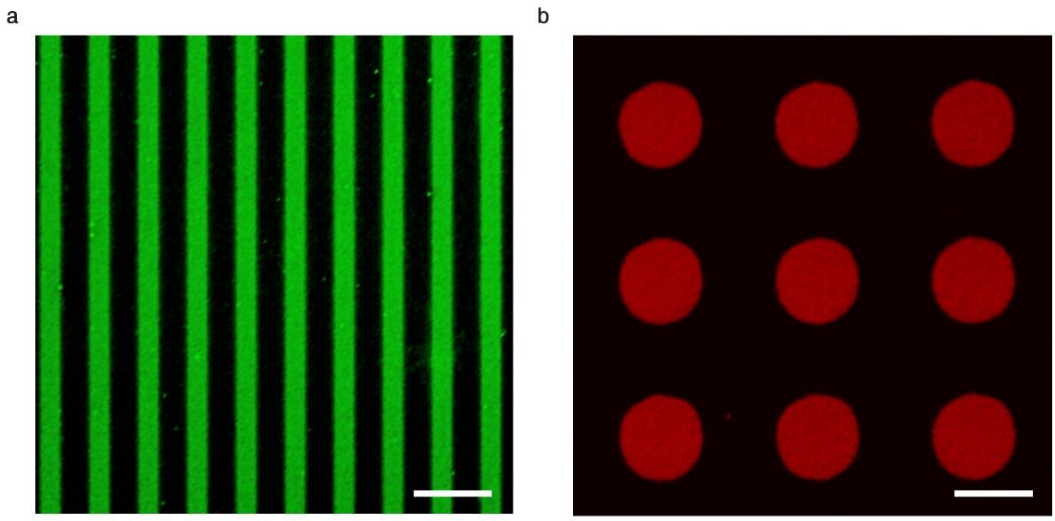
Supplementary Fig. 14 Fluorescence microscopic images of (a-i) square and (j-l) line patterns based on PXL decorated (a, d, g, j) R, (b, e, h, k) RG, and (c, f, i, l) RGB QDs. The widths of each pattern are (a-c) 3.8 μm, (d-f) 1.8 μm, (g-i) 0.8 μm and (j-l) 3.6 μm, respectively. Scale bars indicate 10 μm.



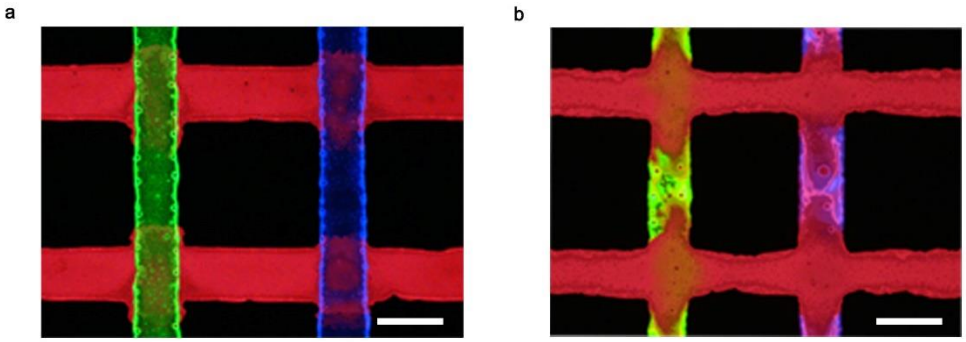
Supplementary Fig. 15 Fluorescence images made of R (left column), RG (middle column), and RGB (right column) QD patterns[7]. QDs are laterally positioned and vertically stacked to realize full color images. Scale bars indicate (a,c) 1 mm and (b) 200 μm, respectively.



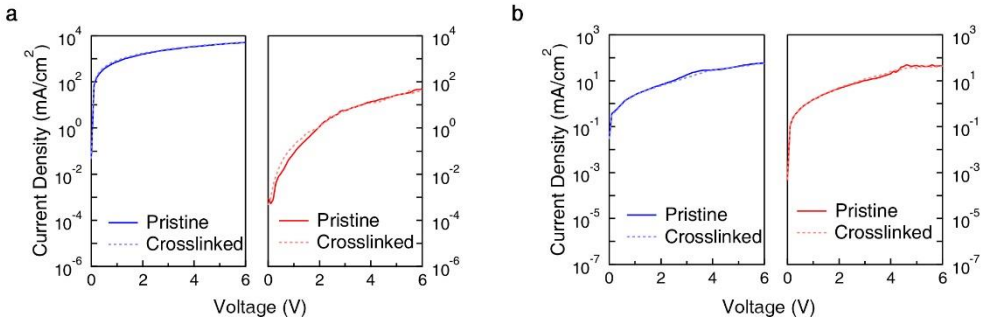
Supplementary Fig. 16 ^{1}H-NMR spectra (500 MHz, $CDCl_3$) of (a) InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs with OA dispersing ligands (b) and NS-BP-decorated (4 mol%) InP (r = 1.2 nm)/$ZnSe_xS_{1-x}$ (h = 2.3 nm) QDs with MMES dispersing ligands (96 mol%).



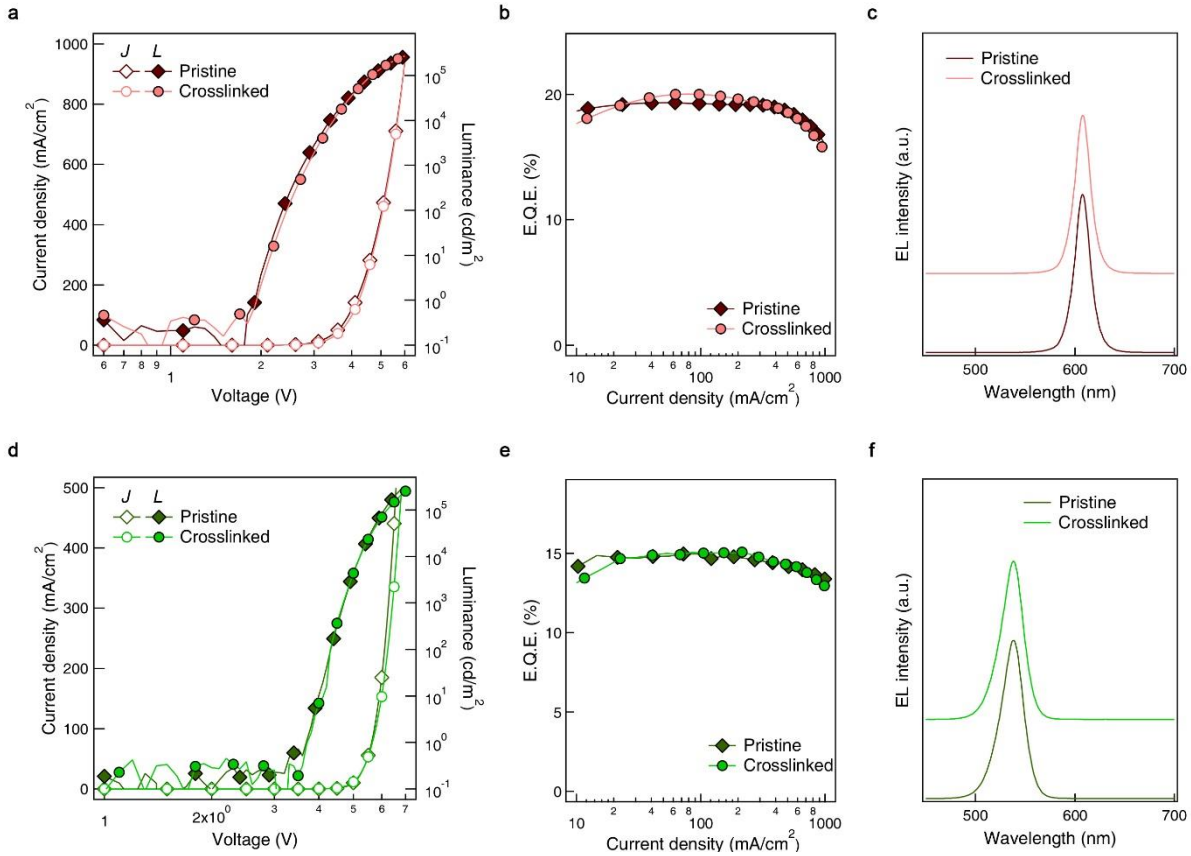
Supplementary Fig. 17 Fluorescence microscopic images of (a) line and (b) dot patterns based on PXL-decorated InP/$ZnSe_xS_{1-x}$ QDs. (a) MMES and (b) TFMBT are used for dispersing ligands to prepare QD casting solutions dispersed in PGMEA and TFT, respectively. Each film is exposed to UV-A with an exposure dose of (a) 42 mJ/cm^2 and (b) 210 mJ/cm^2 and rinsed with mother solvents. Scale bars = 100 μm.



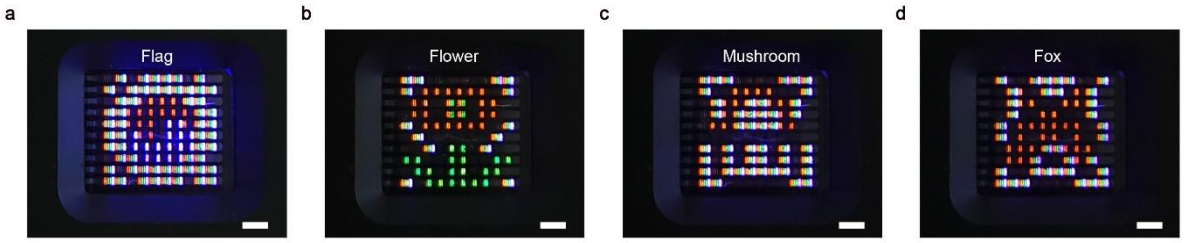
Supplementary Fig. 18 Magnified fluorescence images of inkjet-printed RGB cross-line patterns based on (a) PXL-decorated *versus* (b) pristine QDs (top, left). Scale bar = 200 μm.



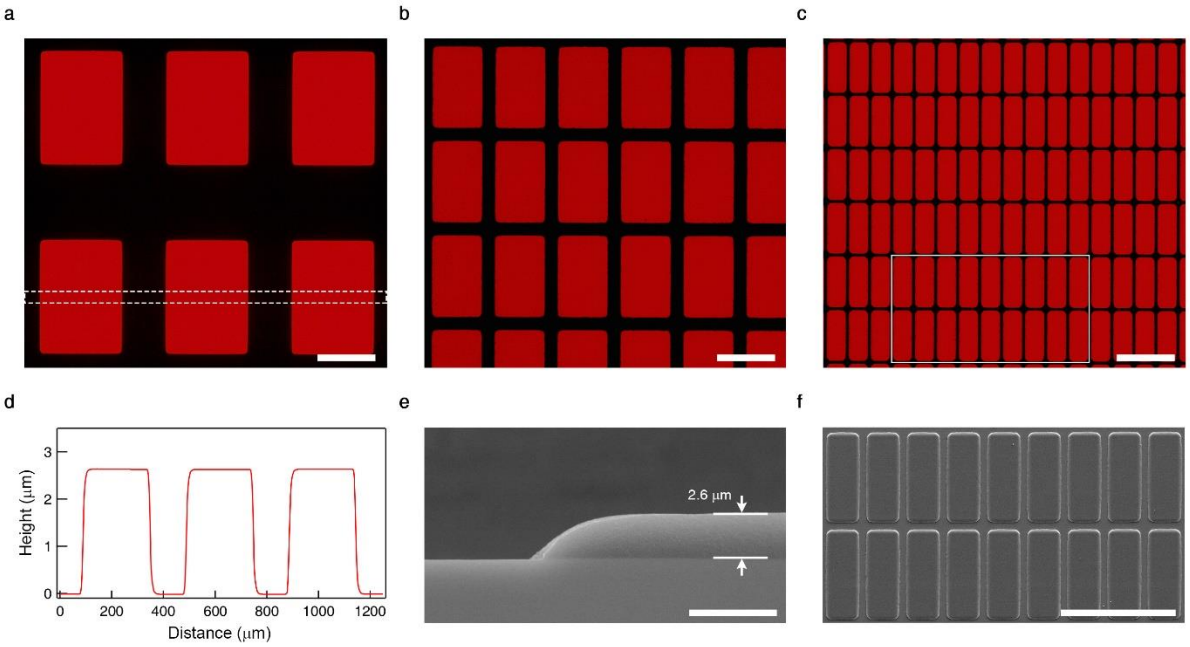
Supplementary Fig. 19 Current density−voltage characteristics of electron-only devices (left) and hole-only devices (right) implementing pristine *versus* photocrosslinked (a) InP (r = 1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) and (b) CdSe (r = 2.0 nm)/$Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ (h = 7.7 nm) QD films.



Supplementary Fig. 20 (a,d) Current density (J)–voltage (V)–luminance (L) (b,e) current density dependent external quantum efficiencies (EQEs), and (c,f) EL spectra of QD-LEDs employing pristine *versus* photocrosslinked (a-c) red- and (d-f) green-emitting CdSe/$Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$ QD films.



Supplementary Fig. 21 (a-d) Electroluminescent images of the RGB arrays with different patterns. Scale bars indicate 2 mm.



Supplementary Fig. 22 (a,b,c) Fluorescence microscopic images of patterned QD films based on PXL-grafted InP (r = 1.9 nm)/$ZnSe_xS_{1-x}$ (h = 3.2 nm) QDs and commercial photoresist. (b) Height profile of patterned QD film measured by a profilometer. Scanning electron microscopy (SEM) images of patterned QD films with (e) cross-sectional and (f) top view. Scale bars indicate (a,b,c,f) 200 μm and (e) 5 μm, respectively.

Supplementary Table 1. Structural and optical characteristics of RGB QDs used in the present study

Color	Compositions	Dimension (nm)		Peak PL (nm)	FWHM (nm)	PL QY (%)
		Core radius	Total shell thickness			
Red	$InP/ZnSe_xS_{1-x}$	1.9	3.2	625	36	93
	$CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$	2.5	8.0	606	18	95
Green	$InP/ZnSe_xS_{1-x}$	1.2	2.3	529	33	91
	$CdSe/Cd_xZn_{1-x}Se/ZnSe_yS_{1-y}$	2.0	7.7	529	26	92
Blue	$Cd_xZn_{1-x}S/ZnS$	2.7	3.6	443	25	84

Caption for Supplementary Video 1.

Electroluminescence of 10 × 10 RGB QD-LED arrays implementing photocrosslinked QD patterns. Real time movie of light emission from each primary color 10 × 10 QD-LED arrays and RGB QD-LED arrays.

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