

Supporting information for

Lead halide perovskites and other metal halide complexes as inorganic capping ligands for colloidal nanocrystals

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Materials and methods

I. Materials

Lead (II) acetate trihydrate ($\text{Pb}(\text{CH}_3\text{COO})_2 \times 3\text{H}_2\text{O}$, $\geq 99.99\%$, Aldrich), bis(trimethylsilyl)sulfide (TMS_2S , Aldrich), selenium dioxide (SeO_2 , 99.99%, Aldrich), cadmium oxide (CdO , 99.99%, Aldrich), 1-octadecene (ODE, 90%, Aldrich), oleic acid (OA, 90%, Aldrich), trioctylphosphine oxide (TOPO, 99%, Aldrich), trioctylphosphine (TOP, 97%, STREM), selenium powder (Se, 100 mesh, 99.99%, Aldrich), cadmium acetate hydrate ($\text{Cd}(\text{CH}_3\text{COO})_2 \times \text{H}_2\text{O}$, 99.99%, Aldrich), octadecylphosphonic acid (ODPA, 97%, PCI synthesis), myristic acid (MA, $\geq 99\%$, Aldrich), sulphur powder (S, 99.998%, Aldrich), 2,2'-dithiobis(benzothiazole) (MBTS, 99%, Aldrich), oleylamine (OAm, 70%, Aldrich), 1-hexanethiol (97%, ABCR), Indium (III) acetate ($\text{In}(\text{Ac})_3$, 99.99%, Aldrich), tris(trimethylsilyl)phosphine ($(\text{TMS})_3\text{P}$, 98%, Strem), Pd acetylacetonate ($\text{Pd}(\text{acac})_2$, 99%, Aldrich), 1,2-tetradecanediol (90%, Aldrich), dioctyl ether ($>97\%$, Aldrich), iron pentacarbonyl ($\text{Fe}(\text{CO})_5$, 99.999%, Aldrich), platinum acetylacetonate (98%, Strem), tetraline (1,2,3,4-tetrahydronaphthalene, 97%, Aldrich), tert-butylamine-borane complex (TBAB, Aldrich, 97%), gold(III) chloride trihydrate ($\text{HAuCl}_4 \times 3\text{H}_2\text{O}$, $\geq 99.9\%$, Aldrich), arsenic (III) sulfide (As_2S_3 , 99.999%, STREM), potassium sulphide (K_2S , 95%, STREM), methylamine solution in ethanol (33 wt%, Aldrich), hydroiodic acid (HI, 57 wt%, Aldrich), hydrobromic acid (HBr, 48 wt%, Aldrich), hydrochloric acid (HCl, 37 wt%, Aldrich), ammonium hydroxide (NH_4OH , 25%, Aldrich), lead iodide (PbI_2 , ABCR), lead bromide (PbBr_2 , ABCR), lead chloride (PbCl_2 , ABCR), potassium iodide (KI, Alfa Aesar), indium (III) chloride (InCl_3 , 99.99%, ABCR), indium (III) iodide (InI_3 , 99.999%, STREM), potassium chloride (KCl, Aldrich), iron (II) chloride (FeCl_2 , 99.5% anhydrous, ABCR), antimony (III) chloride (SbCl_3 , 99.999%, ABCR), zinc chloride-diethyl ether complex (ZnCl_2 , 2.2M solution in dichloromethane, Fluka), sodium sulphide nonahydrate ($\text{Na}_2\text{S} \times 9\text{H}_2\text{O}$, $\geq 98\%$, Aldrich), sodium stannate ($\text{Na}_2\text{Sn}(\text{OH})_6$, 95%, Aldrich), infrared dye IR-26 (Exciton Inc.), Rhodamine 6G (Aldrich), ethanol (Fluka), hexane (Aldrich), acetone (Aldrich), N-methylformamide (MFA, 99%, ABCR), propylene carbonate (PC, anhydrous, Acros), 1-octylamine (99%, Aldrich), hexamethylphosphoramide (HMPA, anhydrous, TCI), N,N-dimethylformamide (DMF, 99.8%, Aldrich), acetonitrile (ACN, 99.8% anhydrous, Aldrich), dimethylsulfoxide (DMSO, Aldrich), tetrachloroethylene (TCE, 99%, Aldrich), 1,2-dichloroethane (DCE, Fluka), toluene ($\geq 99.9\%$, Aldrich), methanol ($\geq 99.9\%$, Aldrich), 2-propanol (Scharlau), dimethylsulfoxide deuterated (DMSO-d₆, 99.9atom%, Cambridge Incomp Lab) were used as received. Squalane (99%, Aldrich) and ODE) were dried under vacuum, then stored and handled inside a glovebox.

II. Syntheses of colloidal nanocrystals capped with organic ligands

All syntheses were performed airless using Schlenk-line technique. As-synthesized nanocrystals (NCs) were capped with long-chain organic ligands providing colloidal stability in nonpolar organic solvent (hexane, toluene, chloroform).

3-8nm PbS NCs were synthesized according to the method of Hines et al.¹ with slight modifications. For obtaining 4.5 nm PbS NCs, $\text{Pb}(\text{CH}_3\text{COO})_2 \cdot 3\text{H}_2\text{O}$ (1.5g, 4mmol), ODE (35 mL) and oleic acid (15 mL, 42.4 mmol) were mixed in a three-neck flask. The mixture was degassed under vacuum at 120°C for 2 hours and heated to 150°C under nitrogen flow. The heating mantle was removed and solution of TMS_2S (0.42 mL, 2 mmol) in 10 mL ODE (dried) was injected into vigorously stirring lead oleate solution at 143°C. After 3 min, the reaction mixture was cooled down to room temperature. NCs were washed three times with toluene/ethanol solvent/nonsolvent pair, redissolved in hexane and filtered through 0.2 μm PTFE filter. Smaller and larger NCs can be obtained by varying the amount of oleic acid in the initial reaction mixture.

5.6nm zinc-blende CdSe (ZB-CdSe) NCs were synthesized according to the method of Cao et al.² with slight modifications. SeO_2 (55.5mg, 0.5 mmol), cadmium oleate in ODE (1.75 mL of 0.3M solution) and ODE (30 mL) were mixed and quickly heated up to 240°C. After 1-hour growth at 240°C, solution was cooled down to room temperature, NCs were washed three times with hexane/acetone, dissolved in hexane and filtered through 0.2 μm filter.

3.1-4.7nm wurtzite CdSe (WZ-CdSe) NCs were synthesized according to the procedure reported by Bawendi group.³ CdO (30 mg, 0.234 mmol), ODPa ((140 mg, 0.418 mmol), and TOPO (1.5g) were mixed, heated to 150 °C, degassed under vacuum for 1 hour and then heated to 320 °C under nitrogen flow. 0.5 mL TOP was added after a colourless clear solution was formed. Then reaction mixture was heated to 380 °C and TOPSe/TOP (30 mg Se in 0.25 mL TOP) solution was swiftly injected into the flask. After 10-min growth, the reaction was terminated by fast cooling. The resulting CdSe NCs were washed 3 times by acetone/hexane, redispersed in hexane and filtered through 0.2 μm filter. Size and concentration of NCs were estimated from the optical absorption spectra, using method reported in Ref.⁴

4.7nm CdS NCs were synthesized according to Cao et al.⁵ with 10-fold up-scaling. Briefly, cadmium acetate hydrate (267 mg, 1 mmol), myristic acid (457 mg, 2 mmol), ODE (63mL), sulphur (16 mg, 0.5 mmol), and MBTS initiator (10.4 mg, 31.3 μmol) were mixed and dried at 120 °C under vacuum for 2 hours, and then heated to 240 °C under nitrogen flow, maintained for 90 min at 240 °C and cooled down to room temperature. CdS NCs were extracted into hexane by multiple mixing of hexane with the crude solution. All hexane fractions were mixed together, concentrated and washed three times with hexane/ethanol. Purified CdS NCs were redispersed in hexane and filtered through 0.2 μm filter.

CdSe/CdS core/shell NCs were synthesized according to method of Chen et al.,³ using WZ-CdSe NCs as seeds. 100 nmol of WZ-CdSe in hexane was mixed with 3 mL ODE and 3 mL OAm and degassed under vacuum at room temperature for 90 min and at 110 °C for 15 min, and then heated to 310 °C under nitrogen flow and maintained for 2 hours. During the heating, when the temperature reached 240 °C, the solutions of cadmium oleate in ODE and hexanethiol in ODE began to be injected dropwise with syringe pump at the rate of 3 mL/hr. Total of 0.422 mmol $\text{Cd}(\text{Oleate})_2$ in 6 mL ODE and 74 μL hexanethiol in 6 mL ODE were added during 2 hours. Afterwards, 1 mL oleic acid was injected and the solution was further annealed at 310 °C for 1 hour. The resulting CdSe/CdS core/shell NCs were washed 3 times with acetone/hexane, redissolved in hexane and filtered through 0.2 μm filter.

InP NCs capped with MA were synthesized using a modified method of Peng et al.⁶ $\text{In}(\text{Ac})_3$ (0.4 mmol), MA (1.54 mmol) and squalane (4 g) were loaded into a three-neck flask and dried for 75 minutes under vacuum at 125°C. The mixture was heated to 188°C under N_2 flow. $(\text{TMS})_3\text{P}$ (0.2 mM) and dried 1-octylamine (2.4 mmol) in squalane (1.5 mL) were mixed in a glovebox, loaded into syringe and swiftly injected into the hot reaction mixture. The reaction temperature was decreased down to 178°C immediately after the injection and was kept at this value for 215 minutes for the growth of InP NCs. The

NPs were washed with toluene and a mixture of methanol–isopropanol (1:1) several times and stored in toluene (3 mL). Before ligand exchange, NCs were transferred to hexane by evaporating toluene and redissolving in hexane.

5nm OAm-capped Au NCs were prepared according to the method of S. Sun et al.⁷ with minor modifications. Tetraline (10 ml), OAm (10 mL) and $\text{HAuCl}_4 \times 3\text{H}_2\text{O}$ (0.1 g) were mixed at room temperature and stirred for 20 min under nitrogen purge. A solution containing 0.5 mmol TBAB complex (0.0435g), 1 ml oleylamine and 1 ml tetraline was injected into the precursor solution. The reaction mixture turned yellow to dark purple in 2-5 s. Stirring was continued for 30 minutes before the washing procedure. 40 ml acetone and 8 mL methanol were added to precipitate the NCs, followed by centrifugation. The precipitate of Au NCs was redispersed in 8 mL toluene. A minimally sufficient amount of methanol was added to precipitate Au NCs second time. After centrifuging, Au NCs were redispersed in toluene or in hexane (for ligand-exchange).

4.0nm Pd NCs were synthesized based on the protocols reported by Hyeon et al.⁸ with minor modifications. The flask containing OAm (10 mL) and TOPO (0.25 g) was heated to 50 °C under vacuum for 30 min. 2 mL of the OAm-TOPO mixture was withdrawn and mixed with a solution of 0.1g $\text{Pd}(\text{acac})_2$ in 0.3 mL TOP (prepared in a glovebox) and the resulting mixture was injected into the reaction flask. The flask was heated to 100 °C under vacuum. The solution was heated under nitrogen to 250 °C at the rate of ~3 °C/min, kept at 250 °C for 30 min and cooled to room temperature. To purify Pd NCs, toluene (2 mL) and ethanol (30 mL) were added, followed by centrifugation. Collected precipitate of NCs was redispersed in toluene (3 mL).

3.8 nm FePt NCs were synthesized by slightly modified method of Sun et al.⁹ Platinum acetylacetonate (197 mg, 0.5 mmol), 1,2-tetradecanediol (345 mg, 1.5 mmol) and dioctyl ether (20 mL) were mixed and heated to 100°C under airless conditions. At this temperature, a solution of oleic acid (0.16 mL, 0.5 mmol), OAm (0.17mL, 0.5mmol) and $\text{Fe}(\text{CO})_5$ (0.13 mL, 1 mmol) was injected, and the mixture was further heated to reflux (295°C). The refluxing was continued for 30 min. Then the reaction mixture was cooled to room temperature. The black product was precipitated by adding toluene (10 ml) and ethanol (60 ml) and separated by centrifugation. The black precipitate was redissolved in toluene (~10 ml) in the presence of oleic acid (10 μL) and oleylamine (10 μL), and then centrifuged to remove any insoluble NCs or byproducts. The NCs were additionally precipitated by adding 30-40 ml ethanol followed by centrifugation. The NCs were redispersed in toluene.

III. Synthesis of halometallate and chalcogenidometallate ligands

K_3AsS_4 was prepared by mixing As_2S_3 (98 mg, 0.4 mmol), S (25.6mg, 0.8mmol) and K_2S (132 mg, 1.2 mmol) in water (2mL) at room temperature. After 24-hour stirring, the mixture was filtered through 0.45 μm PTFE filter and K_3AsS_4 was precipitated by acetone (20mL). Precipitate was dried by multiple washing with acetone. Final product was stored in a glovebox.

$\text{K}_4\text{Sn}_2\text{S}_6$ was synthesized analogously to Ref.¹⁰ by exchanging Na_2S with K_2S .

$\text{CH}_3\text{NH}_3\text{I}$, $\text{CH}_3\text{NH}_3\text{Br}$ were synthesized as described in Ref.¹¹ 24 mL of a 33 wt% methylamine solution in absolute ethanol was added to 10 mL hydroiodic (hydrobromic) acid and 100 mL ethanol and stirred under N_2 atmosphere at room temperature for 4 hours. Water and ethanol were then removed by rotary evaporator. The product composition and purity were confirmed by XRD.

IV. Ligand exchange with metal halide and metal chalcogenide complexes, and neutral metal halide salts

Typically, 50 μmol of desired ligand was dissolved in 1 mL MFA (N-methylformamide). Solutions of metal halide complexes were prepared by simple mixing of metal halide with equimolar amount of the corresponding methylammonium, ammonium or potassium halide. Ligand solution in MFA was mixed with 1 mL hexane solution of NCs capped with organic ligands (2-5 mg). The biphasic system was stirred vigorously for 3-12 hours (72 hours for Au-InCl₃ combination), until the complete migration of NCs from nonpolar to polar organic phase. The nonpolar phase was removed and the polar phase was rinsed 3-4 times with pure hexane. To remove the excess of metal halide ligands, NCs were precipitated from MFA by adding a nonsolvent, centrifuged and redispersed in MFA or PC. Further details are below.

For **PbS-MAPbI₃**, **PbS-MAPbBr₃**, **PbS-KPbI₃** NC-ligand pairs, acetone was used as a nonsolvent and MFA or PC were used as solvents. After redispersion, only concentrated (>25 mg/1 mL) solutions in MFA were stable, whereas dilution immediately resulted in NC precipitation. Purified solutions in PC were stable in a wide range of concentrations (0-50 mg/mL).

For **PbS-PbI₂**, **PbS-PbBr₂** and **PbS-InI₃** NC-ligand pairs, either acetone or DMF were used as a nonsolvent and PC was used as a solvent. After precipitation with DMF NCs were well soluble in PC. After precipitation with acetone NCs were not soluble in pure PC. Addition of 1% of HMPA or DMF allowed stabilization of colloids. Solutions in PC were stable in a wide range of concentrations (0-50 mg/mL).

For **CdSe-InCl₃**, **CdSe-InI₃**, **CdSe-KInCl₄**, **CdSe-FeCl₂**, **CdS-InCl₃**, **CdS-FeCl₂** and **FePt-InCl₃** NC-ligand pairs, acetone or HMPA were used as nonsolvents and PC was used as a solvent. Solutions in PC were stable in a wide range of concentrations (0-50 mg/mL).

For **CdS-SbCl₃**, **CdSe-SbCl₃** and **PbS-SbCl₃** NC-ligand pairs, HMPA was used as nonsolvent and PC was used as a solvent. Only diluted solutions were stable.

For **CdSe/CdS-CH₃NH₃CdBr₃**, **CdSe/CdS-KInI₄**, **CdSe/InI₃**, **Au/InCl₃** and **Pd/InCl₃** NC-ligand pairs, HMPA was used as a nonsolvent and PC was used as solvent. Solutions in PC were stable in a wide range of concentrations (0-50 mg/mL).

For **CdSe/CdS-CdBr₂**, **CdSe-CH₃NH₃CdBr₃**, **CdS-CH₃NH₃CdBr₃** and **CdSe-NH₄CdCl₃** NC-ligand pairs HMPA:toluene (1:2) mixture was used as nonsolvent and PC was used as solvent.

For **CdSe/CdS-(NH₄)₂ZnCl₄**, **CdSe-(NH₄)₂ZnCl₄**, **CdS-(NH₄)₂ZnCl₄**, **CdSe-ZnCl₂** NC-ligand pairs acetone was used as nonsolvent and PC with 1% of HMPA was used as solvent.

For **CdSe/CdS-InCl₃** NC-ligand pair HMPA:acetone (1:3) mixture was used as nonsolvent and PC with 1% of HMPA was used as solvent.

For **CdS-CH₃NH₃InI₄** NC-ligand pair toluene was used as nonsolvent and PC with 1% of HMPA was used as solvent.

For **InP-InCl₃** NC-ligand pair acetone was used as nonsolvent. After precipitation with acetone NCs were not soluble in pure PC. Addition of 1% of HMPA allowed stabilization of the colloid.

The ligand exchange with **K₃AsS₄** and **K₄Sn₂S₆** was conducted analogously to Ref.¹² For PbS NCs, 5 mg (17 μmol) of K₃AsS₄ was dissolved in 1 mL of MFA and mixed with 5 mg PbS NCs dissolved in 1 mL of hexane. Two-phase system was stirred vigorously for 30 min. The polar phase was then washed 3 times with 1 mL of hexane and filtered through 0.45 μm PTFE filter. NCs were then precipitated by 1 mL ACN and minimum amount of toluene (depends on NC size). Resulting NCs were redissolved in PC or MFA and filtered once again through 0.45 μm PTFE filter. For CdSe/CdS NCs ligand exchanges with K₃AsS₄ or K₄Sn₂S₆ were conducted identically but with higher amount of inorganic ligand (10mg).

V. Characterization

Fourier transform infrared (FTIR) spectroscopy. Attenuated total reflectance (ATR) FTIR spectra were recorded using Thermo Scientific Nicolet iS5 FTIR spectrometer.

UV/vis/IR absorption spectra were collected using a Jasco V670 spectrometer.

Transmission electron microscopy (TEM). TEM images were recorded using JEOL JEM-2200FS microscope operated at 200kV.

X-ray diffraction (XRD) Powder XRD patterns were collected with STOE STADI P powder diffractometer, operating in transmission mode. Germanium monochromator, Cu $K_{\alpha 1}$ irradiation and silicon strip detector Dectris Mythen were used.

Dynamic light scattering (DLS) DLS was used to the distribution of hydrodynamic diameters in colloidal solutions (Figure S3). DLS patterns were collected using Zetasizer Nano-ZS (Malvern Instruments, Inc.).

Electrophoretic mobility. Electrophoretic mobility was measured using Zetasizer Nano-ZS (Malvern Instruments, Inc.). Colloidal solutions were measured using a dip-cell setup with Pd electrodes. Typical measurements of electrophoretic mobility included several scans of 100 runs each in the high-resolution mode. Dilution was optimized for each sample to achieve >100 kcps count rate and the best signal-to-noise ratio. The voltage applied to colloidal solutions was typically between 5 V and 10 V for polar solvents (MFA, PC) and 40V for nonpolar (toluene). Table S3 summarises ζ -potentials for some solutions of NCs capped with inorganic ligands. For all NC/ligand pairs ζ -potential was negative. Typical absolute value was in range 30-40 mV for lead-halide-based ligands and 25-35 mV for all other ligands.

ICP elemental analysis (Table S4) was performed by Bachema analytical laboratories (<http://www.bachema.ch/>) using inductively coupled plasma mass spectrometry (ICP-MS) and inductively coupled plasma optical emission spectrometry (ICP-OES, for Fe only). In this study, we used ICP for the accurate quantification of metals, chalcogens (S, Se) and iodine. The atomic ratio between the metal from NC core (NC metal) to the one from the ligand (ligand metal) for carefully washed samples (2 precipitations and redispersions in PC) provide a strong evidence for the chemisorption of metal halides onto the NC surface.

Elemental analysis by energy-dispersive X-ray spectroscopy (EDX, Table S4) was performed with two scanning electron microscopes (Zeiss Gemini 1530 and Hitachi, S-4800).

Steady state PL spectroscopy and PL QY measurement. For PbS NCs, Fluorolog iHR 320 Horiba Jobin Yvon spectrofluorimeter equipped with an InGaAs detector was used to acquire steady state PL spectra. The excitation wavelength was 960 nm, provided by a 450W Xenon lamp dispersed with a monochromator. Measured intensities were corrected to take into account the spectral response of the InGaAs detector. NCs capped with oleic acid were dissolved in TCE. NCs capped with metal-halide complexes were dissolved in PC. NCs capped with K_3AsS_4 were dissolved in dimethylsulfoxide-d6 (DMSO-d6). PL QYs were estimated as reported previously,¹² using IR-26 dye molecule as a standard.

For CdSe/CdS NCs, Fluoromax-4 Horiba spectrofluorimeter equipped with a visible PMT detector was used to acquire the steady state PL spectra of solutions of CdSe/CdS core/shell NCs and for quantum yield estimations. The excitation wavelength was 530 nm with bandwidth of 1 nm. PL QYs were estimated as reported previously,¹³ using of Rhodamine-6G as a standard.

Time-resolved PL spectroscopy. Time-resolved photoluminescence (PL) was measured on a NanoLog FL3 Horiba spectrofluorimeter, using a monochromator-based time-correlated single-photon counting (TCSPC) method and an infrared photomultiplier tube (PMT). The PL was excited by a laser diode at 785 nm (DeltaDiode-785L) with a pulse width of ~80 ps operating at 100 KHz, using a defocused laser beam (spot diameter ~ 2 mm) to allow spatial averaging over the probed samples. The system exhibits a time resolution of ~50 ps after reconvolution with the instrument response function. The PL decays were obtained while monitoring the NC emission peaks with a spectral bandwidth of 20 nm and were corrected to take into account the spectral response of the detector.

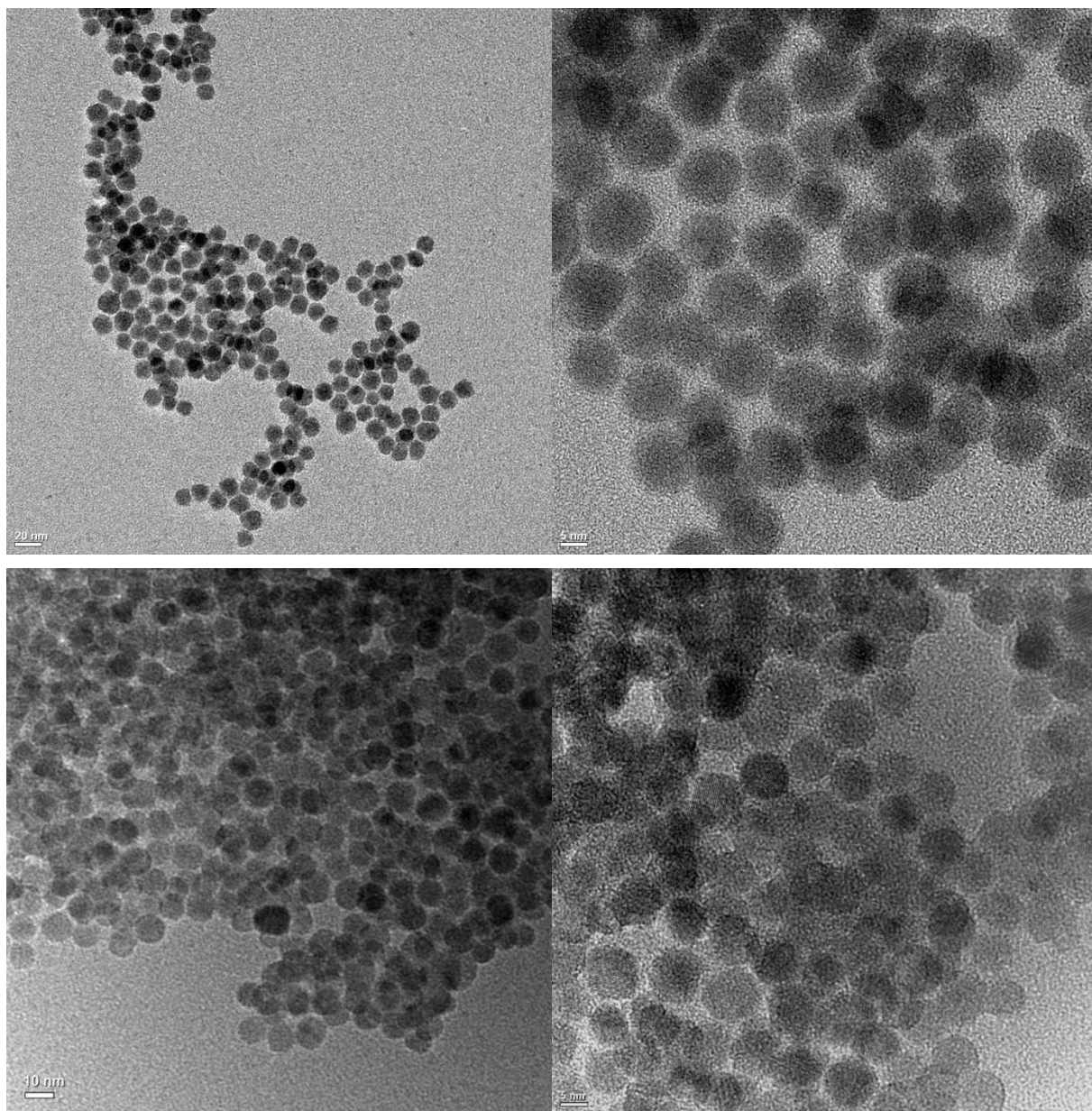


Figure S1. TEM images of CdSe/CdS core/shell NCs capped with MACdBr₃ (top panel) and with (NH₄)₂ZnCl₄ (bottom panel) and deposited from PC solution.

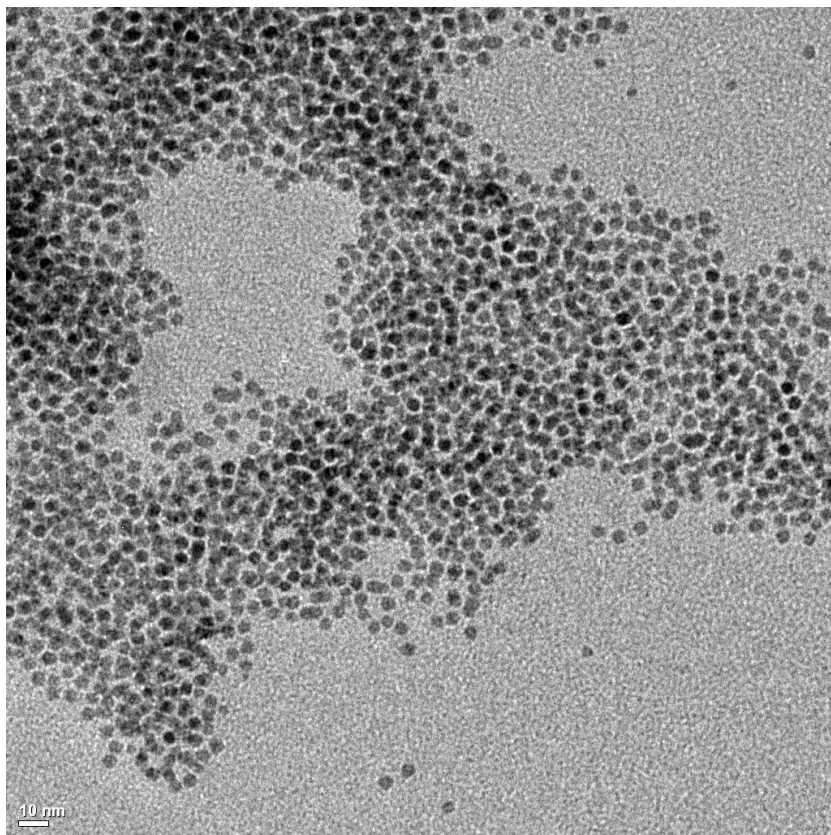


Figure S2. TEM image of Pd NCs capped with InCl_3 and deposited from PC solution.

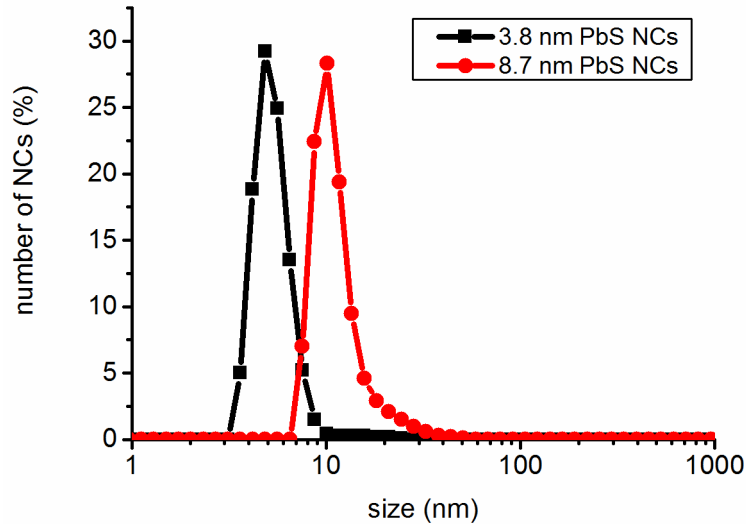


Figure S3. Size-histograms obtained by DLS measurements for solutions of PbS-MAPbI₃ NCs in PC.

Table S1. NC-Ligand combinations which form colloiddally stable solutions after redispersion in PC or MFA. No PL signal could be detected after ligand exchange for all CdS, CdSe and InP samples. In contrast, PbS and CdSe/CdS NCs retained strong PL, as discussed in the main text.

NCs	Ligands
PbS	MAPbI ₃ , MAPbBr ₃ , KPbI ₃ , PbI ₂ , PbBr ₂ , InI ₃ , SbCl ₃
CdSe	InCl ₃ , InI ₃ , KInCl ₄ , FeCl ₂ , MACdBr ₃ , CdBr ₂ , (NH ₄) ₂ ZnCl ₄ , ZnCl ₂ , NH ₄ CdCl ₃ , SbCl ₃
CdS	InCl ₃ , FeCl ₂ , MACdBr ₃ , (NH ₄) ₂ ZnCl ₄ , MAInI ₄ , SbCl ₃
CdSe/CdS	MACdBr ₃ , CdBr ₂ , (NH ₄) ₂ ZnCl ₄ , KInI ₄ , InCl ₃
InP	InCl ₃ , MAInI ₄
Au	InCl ₃
Pd	InCl ₃
FePt	InCl ₃ , MAPbBr ₃ , PbBr ₂

Table S2. Elemental atomic ratios in CdS (4.7nm), PbS (4.5nm) and CdSe (3.1nm) NCs capped with oleate and with metal halide ligands, estimated by ICP (ICP-OES for Fe, ICP-MS for all other elements) and by EDX analysis. **NM** - not measured, **EDX1** – by Zeiss Gemini 1530; **EDX2** - by Hitachi S-4800.

NC/ligand pair	elements	ICP atomic ratio EDX1 atomic ratio EDX2 atomic ratio
CdS/OA	Cd : S	1 : 0.758 1 : 0.747 1 : 0.805
CdS/KInI ₄	Cd : S : In : I	1 : 1.368 : 0.321 : 0.304 1 : 1.303 : 0.253 : 0.225 1 : 1.404 : 0.411 : 0.238
CdS/FeCl ₂	Cd : S : Fe	1 : 0.966 : 0.092 1 : 0.9 : 0.026 NM : NM : NM
CdSe/OA	Cd : Se	1 : 0.609 1 : 0.61 NM : NM
CdSe/InI ₃	Cd : Se : In : I	1 : 1.276 : 0.242 : NM 1 : 1.01 : 0.230 : 0.195 1 : 1.247 : 0.246 : 0.206
PbS/OA	Pb : S	1 : 0.871 1 : 0.864 1 : 0.916
PbS/KPbI ₃	Pb : S : I	1 : 0.840 : 0.453 1 : 0.811 : 0.347 1 : 0.711 : 0.411
PbS/MAPbI ₃	Pb : S : I	1 : 0.845 : 0.411 1 : 0.851 : 0.400 1 : 0.939 : 0.466
PbS/PbI ₂	Pb : S : I	NM : NM : NM 1 : 0.733 : 0.34 1 : 0.772 : 0.425
PbS/InI ₃	Pb : S : In : I	NM : NM : NM 1 : 0.984 : 0.065 : 0.305 1 : 1.077 : 0.070 : 0.358
InI ₃	In : I	NM : NM NM : NM 1 : 2.9
KInI ₄	In : I	NM : NM NM : NM 1 : 3.58

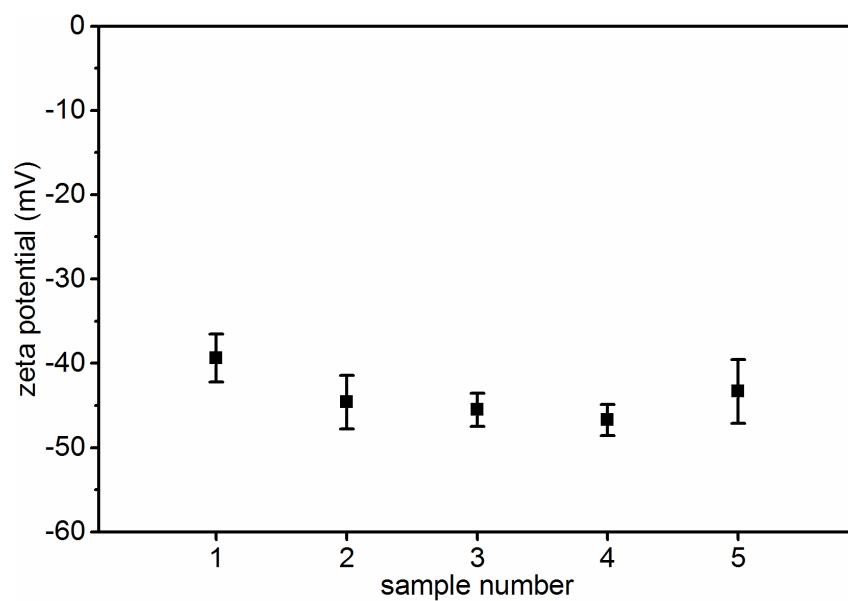


Figure S4. Reproducibility of the measured ζ -potential for 5 different samples of 8.7nm PbS NCs capped with MAPbI₃. Error bars show standard deviation among 6 measurements for the same sample.

Table S3. ζ -potentials for solutions of NCs capped with inorganic ligands in PC.

NC	Ligand	ζ -potential, mV
PbS	MAPbI ₃	-48.8
	MAPbBr ₃	-39.2
	KPbI ₃	-25.5
	PbI ₂	-44.9
	PbBr ₂	-47.6
CdSe	InCl ₃	-27.1
CdS	SbCl ₃	-32.3
InP	InCl ₃	-23.3
CdSe/CdS	MACdBr ₃	-31.9
Au	InCl ₃	-23.3
Pd	InCl ₃	-32.8
FePt	InCl ₃	-27.1

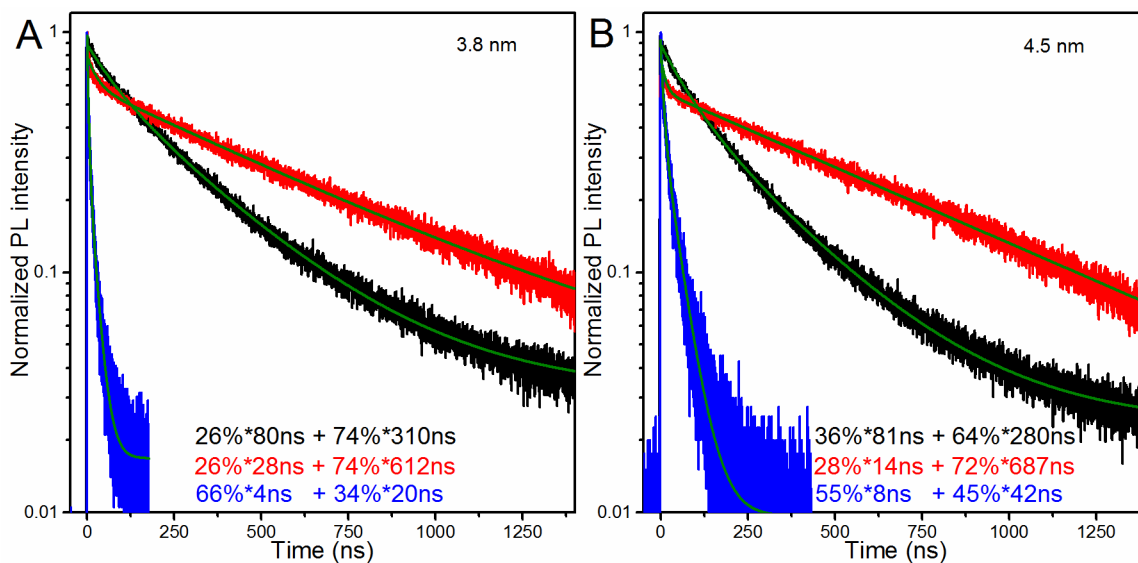


Figure S5. Normalized time-resolved PL decays obtained from solutions of 3.8 nm (A) and 4.5 nm (B) PbS NCs capped with oleic acid (black), MAPbI₃ (red) and K₃AsS₄ (blue). Green lines indicate biexponential fits. Model used: $I(t) = A_1 * e^{-\frac{t}{t_1}} + A_2 * e^{-\frac{t}{t_2}} + I_0$, where $t_{1,2}$ are the two decay constants, $A_{1,2}$ - their relative amplitudes and I_0 constant background (dark counts, scattering etc.)

Table S4. Fitting parameters for the PL decay curves shown in Figure S5.

Sample		A ₁	t ₁ (ns)	A ₂	t ₂ (ns)	I ₀
3.8 nm PbS NCs	Oleic acid-capped	0.225	80	0.631	310	0.032
	MAPbI ₃ -capped	0.194	28	0.575	612	0.027
	K ₃ AsS ₄ -capped	0.628	4	0.327	20	0.017
4.5 nm PbS NCs	Oleic acid-capped	0.308	81	0.556	280	0.023
	MAPbI ₃ -capped	0.219	14	0.566	687	0.000
	K ₃ AsS ₄ -capped	0.504	8	0.414	42	0.010

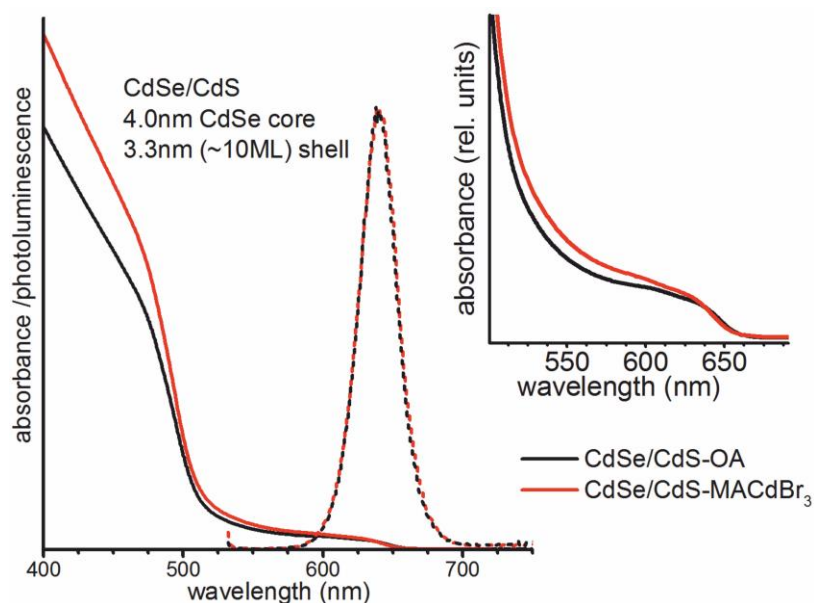


Figure S6. Absorption and emission spectra of the largest studied CdSe/CdS NCs capped with oleate ligands in toluene (PL QY=75%) and with MACdBr₃ in PC (PL QY=65%).

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