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Size controlled synthesis of monodisperse PbTe quantum dots: using oleylamine as capping ligand

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Table S1 PbTe QDs Yield Calculation*

Sample #	Input Mass of $PbCl_2$ (g)	Output Mass of PbTe QDs (g)	Theoretical Yield of PbTe (g)	Yield (%) based on the theoretical yield of PbTe
QD-1	0.093	-	0.110	-
QD-2	0.094	0.018	0.110	16
QD-3	0.093	0.057	0.110	52
QD-4	0.095	0.040	0.110	36
QD-5	0.093	0.031	0.110	28
QD-6	0.093	-	0.110	-
QD-7	0.094	-	0.110	-

* The yields were calculated based on one batch of the synthesis. However, each size of the PbTe QDs was synthesized at least times.

Table S2 EDS Results of PbTe QDs sample QD-2

Element	Weight %	Atomic %
TeL	20.2	29.2
PbL	79.8	70.8
Total	100.0	100.0

Table S3 EDS Results of PbTe QDs sample QD-3

Element	Weight %	Atomic %
TeL	38.0	49.9
PbL	62.0	50.1
Total	100.0	100.0

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Table S4 EDS Results of PbTe QDs sample QD-4

Element	Weight %	Atomic %
TeL	35.0	46.7
PbL	65.0	53.3
Total	100.0	100.0

Table S5 EDS Results of PbTe QDs sample QD-5

Element	Weight %	Atomic %
TeL	37.8	49.7
PbL	62.2	50.3
Total	100.0	100.0

Table S6 IR Peak Assignment for TOP (purity 90%)[1-3]

Wavenumber/cm^{-1}	Assignment [a]
2956 (2966) [b]	$\nu_{as}(CH_3)$ (strong)
2924 (2925)	vas(CH_2)
2871 (2872)	$\nu_s(CH_3)$ (strong)
2852 (2855)	$\nu_s(CH_2)$
1464 (1467)	$\delta(CH_2)$
722 (721)	$\gamma(CH_2)$

[a] Symbols ν, δ, and γ refer to stretching, in-plane deformation, and out-of-plane deformation, respectively.
[b] The numbers in bracket are from reference 1's IR database.

Table S7 IR Peak Assignment for OLA (purity 80-90%)

Wavenumber/cm^{-1}	Assignment [a]
3004 (3005) [b]	ν(CH) of -CH=CH-
2954	$\nu_{as}(CH_3)$ (weak)
2924 (2924)	$\nu_{as}(CH_2)$
2853 (2853)	$\nu_s(CH_2)$
1465 (1467)	$\delta(CH_2)$
1378 (1378)	$\delta_s(CH_3)$
967 (967)	ν(C-Cl) of -C=C-
796 (796)	$\delta_s(CH_3)$
722 (721)	$\gamma(CH_2)$

[a] Symbols ν, δ, and γ refer to stretching, in-plane deformation, and out-of-plane deformation, respectively.
[b] The numbers in bracket are from reference 1's IR database.

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Table S8 IR Peak Assignment for TCE

Wavenumber/cm^{-1}	Assignment [a]
911 (910) [b]	*v*(C-Cl) (strong)
802 (802)	*v*(C-Cl)
777 (778)	*v*(C-Cl)
757 (767)	*v*(C-Cl)

[a] Symbol *v* refers to stretching vibration.
[b] The numbers in bracket are from reference 1's IR database.

Table S9 PbTe QDs Stability Test Results of Sample QD-1

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-1 (QD-1a)	After synthesis	2.6	9.1%
QD-1b	Stored as thin films on TEM copper grid for 130 days	3.4	8.3%

Table S10 PbTe QDs Stability Test Results of Sample QD-2

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-2 (QD-2a)	After synthesis	3.3	7.3%
QD-2b	Stored as thin films on TEM copper grid for 130 days	3.4	6.9%
QD-2c	Stored in TCE solution for 130 days	3.3	5.9%

Table S11 PbTe QDs Stability Test Results of Sample QD-3

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-3 (QD-3a)	After synthesis	5.5	5.6%
QD-3b	Stored as thin films on TEM copper grid for 130 days	5.5	5.2%
QD-3c	Stored in TCE solution for 130 days	5.6	4.6%

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Table S12 PbTe QDs Stability Test Results of Sample QD-4

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-4 (QD-4a)	After synthesis	9.5	7.4%
QD-4b	Stored as thin films on TEM copper grid for 130 days	10.4	5.2%
QD-4c	Stored in solid form for 130 days	varies	uneven

Table S13 PbTe QDs Stability Test Results of Sample QD-5

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-5 (QD-5a)	After synthesis	10.5	8.2%
QD-5b	Stored as thin films on TEM copper grid for 130 days	11.8	6.5%
QD-5c	Stored in TCE solution for 130 days	11.3	8.2%

Table S14 PbTe QDs Stability Test Results of Sample QD-6

Sample #	Sample Measurement	Size (nm)	Size Distribution (σ)
QD-6 (QD-6a)	After synthesis	14.0	8.7%
Qd-6b	Stored as thin films on TEM copper grid for 130 days	14.9	9.4%

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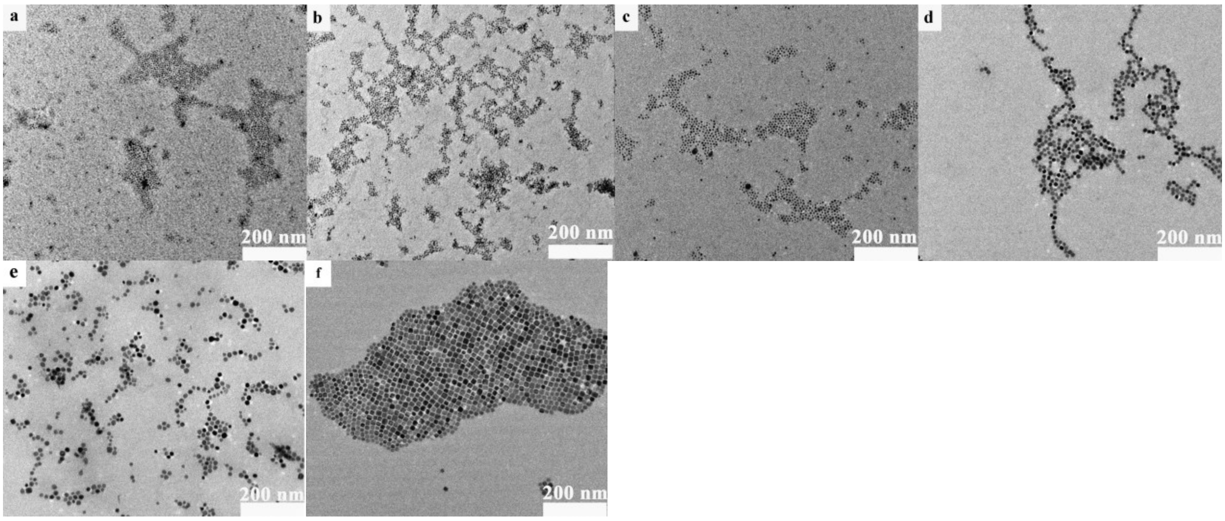
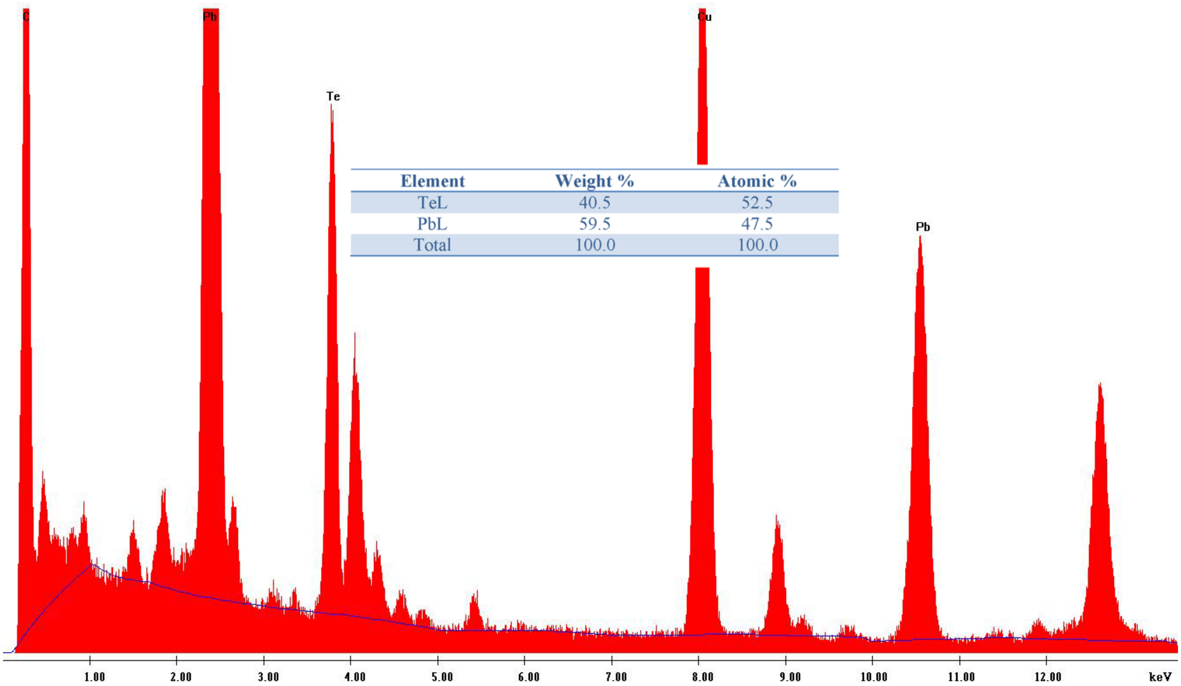


Fig. S1 TEM images showing large areas of the hydrophobic PbTe QDs. Fig. S1a-S1f corresponding to PbTe QDs sample QD-1 to QD-6.



Element	Weight %	Atomic %
TeL	40.5	52.5
PbL	59.5	47.5
Total	100.0	100.0

Fig. S2 EDS Result of PbTe QDs sample QD-6.

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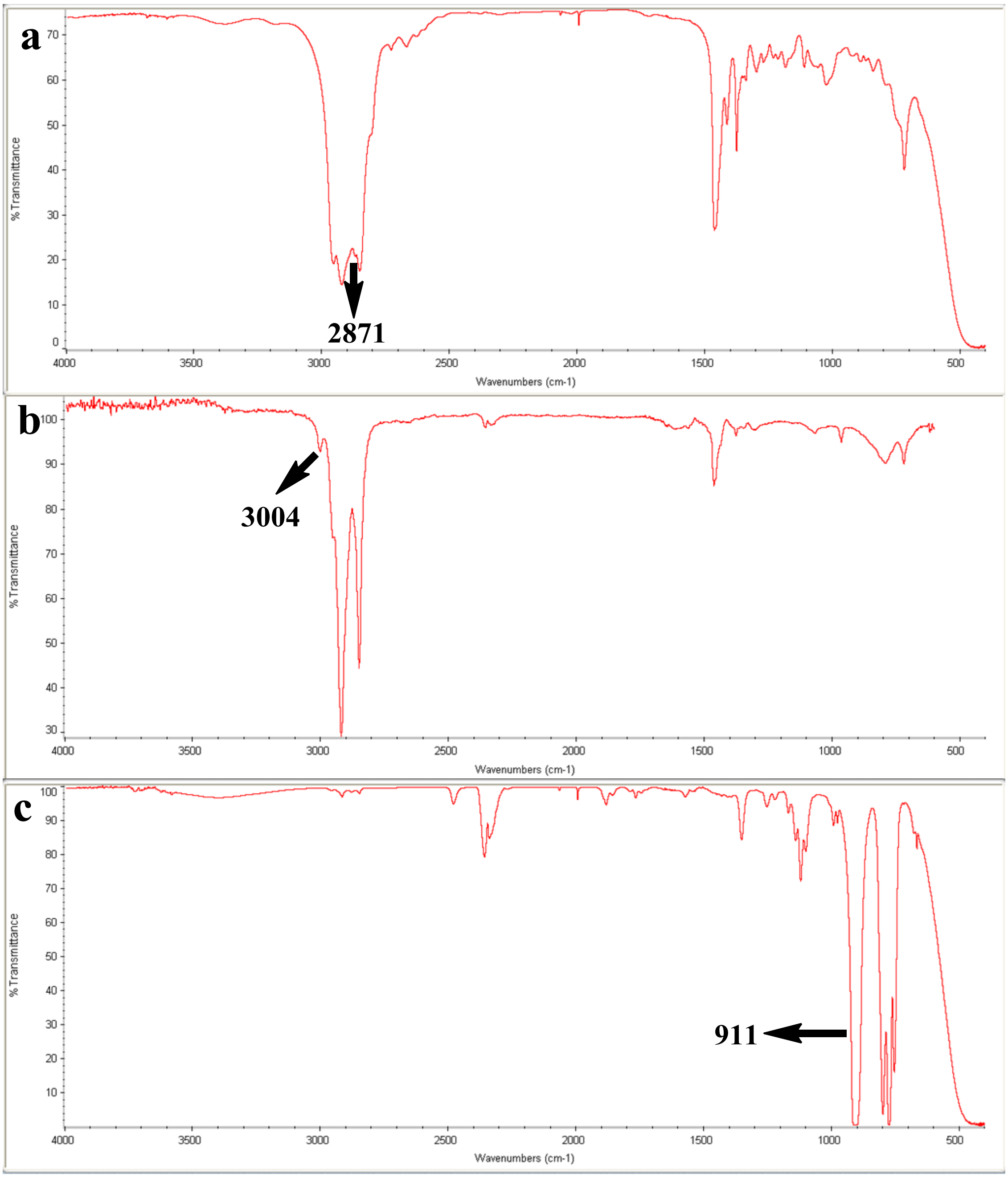

Fig. S3 IR spectra of TOP, OLA, and TCE. Fig. S3a is IR spectrum of TOP with typical $v_s(CH_3)$ stretching at 2871 cm-^{1}; Fig. S3b is IR spectrum of OLA with typical v(CH) of -CH=CH- stretching at 3004 cm-^{1}; Fig. S3c is IR spectrum of TCE with typical v(C-Cl) stretching at 911 cm-^{1}. Refer to Table S6-S8 for the IR peak assignment for TOP, OLA, and TCE.

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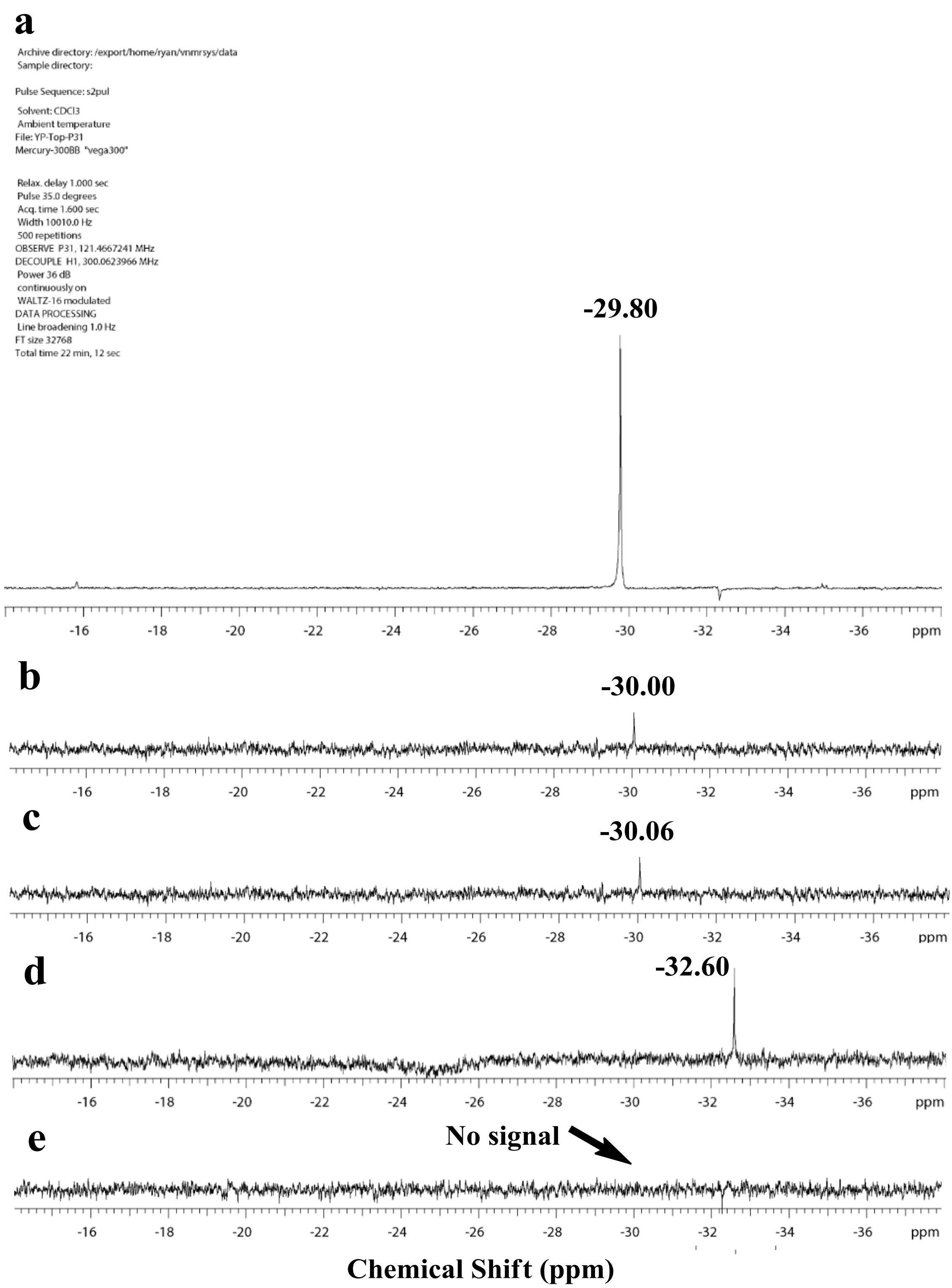

Fig.S4 ^{31}PNMR spectra of TOP, TOP-OLA containing 9.4% TOP, TOP-OLA containing 1.6% TOP, after reaction mixture from PbTe QD synthesis, and purified PbTe QDs. The analyses were performed on a Varian Mercury-300 300 MHz spectrometer at room temperature with $CDCl_3$ as solvent. Fig.S4a is the ^{31}P spectrum of TOP, δ = -29.80 ppm; Fig. S4b is the ^{31}P spectrum of TOP-OLA containing 9.4% TOP, δ = -30.00 ppm. Fig.S4c is the ^{31}P spectrum of TOP-OLA containing 1.6% TOP, δ = -30.06 ppm. Fig.S4d

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is the ^{31}P spectrum of the reaction mixture, δ = - 32.60 ppm. Fig. S4e is the ^{31}P spectrum of the purified PbTe QDs with no ^{31}P signal detected. It demonstrates that TOP is not attached to the surface of PbTe QDs and TOP is not a capping ligand of PbTe QDs.

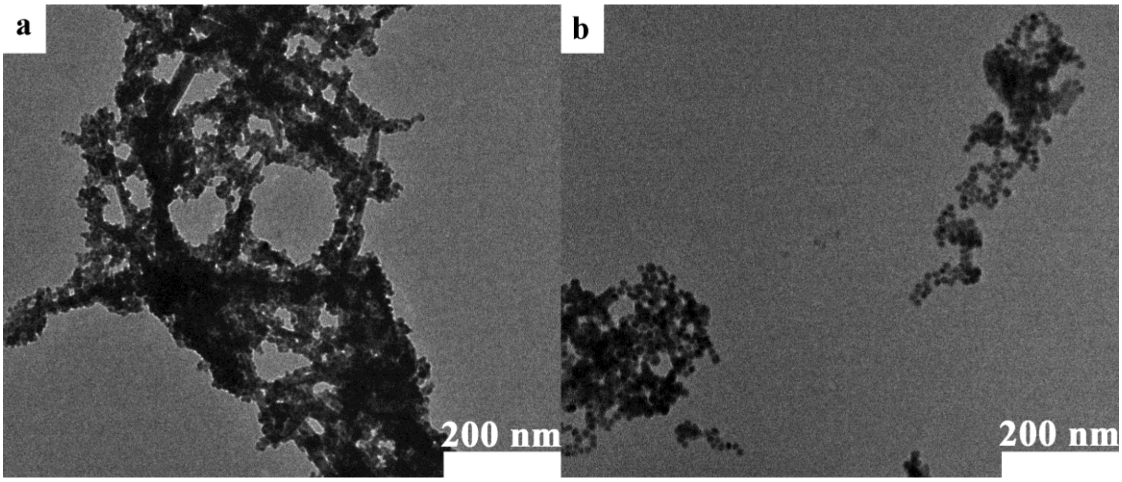

Fig. S5 TEM images showing large areas of the hydrophilic PbTe QDs samples. Fig. S5a-S5b corresponding to PbTe QDs sample QD-8 and QD-9.

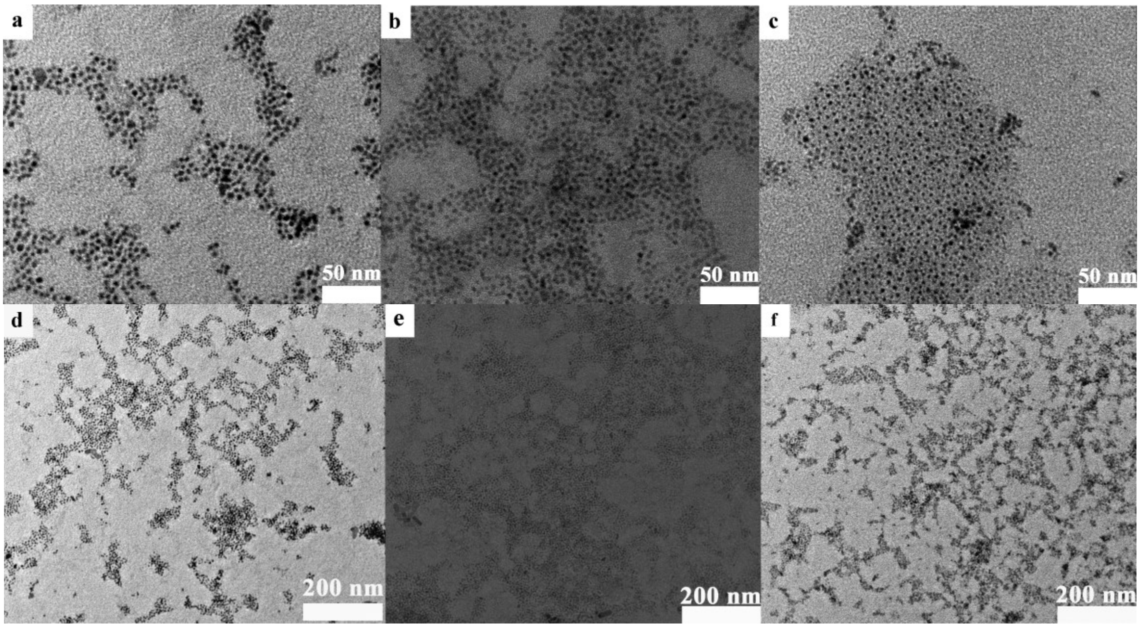

Fig. S6 The TEM images showing both small (50 nm scale bar) and large (200 nm scale bar) areas of the PbTe QDs stability test of sample QD-2. Fig. S6a and Fig. S6d, QD-2a of 3.3 nm with σ = 7.3%: samples measured after synthesis; Fig. S6b and Fig. S6e, QD-2b of 3.4 nm with σ = 6.9%: samples stored as thin film on TEM copper grid and measured after 130 days; Fig. S6c and Fig. S6f, QD-2c of 3.3 nm with σ = 5.9%: samples stored in TCE and measured after 130 days. There are no changes for QD-2. The PbTe QDs are air-stable as thin film and relatively air-stable (shape variations) in TCE.

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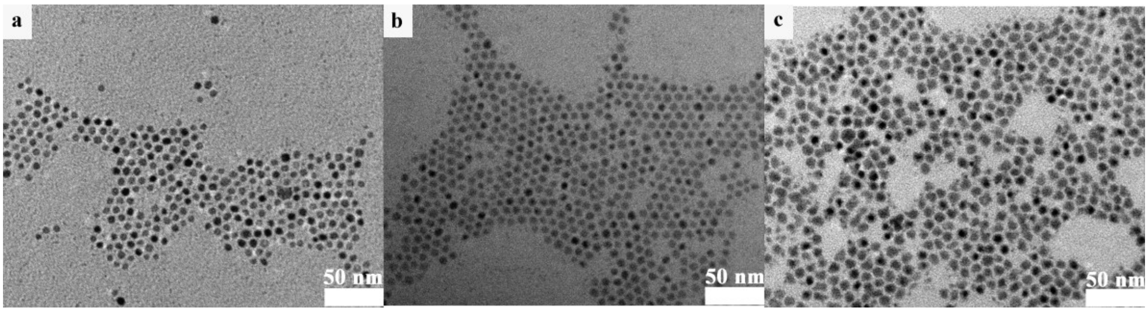

Fig. S7 The TEM images of the PbTe QDs stability test of sample QD-3 (Fig. S7a-7c). Fig. S7a, QD-3a of 5.5 nm with σ = 5.6%: samples measured after synthesis; Fig. S7b, QD-3b of 5.5 nm with σ = 5.2%: samples stored as thin films on TEM copper grid and measured after 130 days; Fig. S7c, QD-3c of 5.6 nm with σ = 4.6%: samples stored in TCE and measured after 130 days. The PbTe QDs are air-stable as thin film even tested from different batches of synthesis.

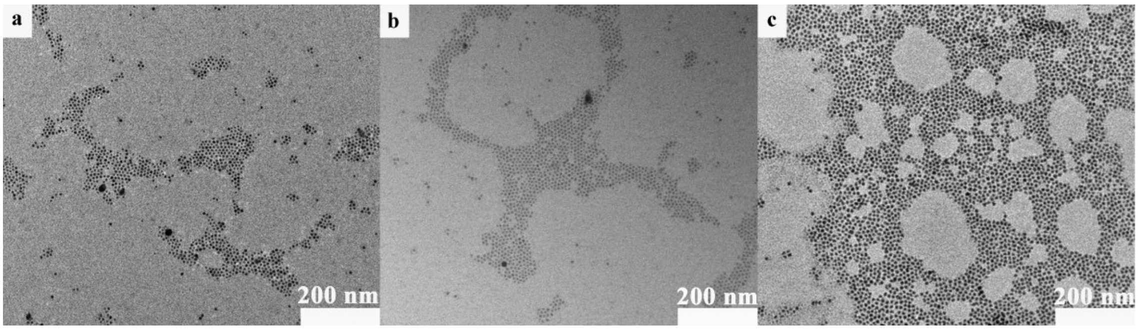

Fig. S8 The TEM images showing large area of the PbTe QDs stability test of sample QD-3. Fig. S8a, QD-3a of 5.5 nm with σ = 5.6%: samples measured after synthesis; Fig. S6b, QD-8b of 5.5 nm with σ = 5.2%: samples stored as thin films on TEM copper grid and measured after 130 days; Fig. S8c, QD-3c of 5.6 nm with σ = 4.6%: samples stored in TCE and measured after 130 days. There are also no changes for QD-3. The PbTe QDs are air-stable as thin film. It is also relatively air-stable (shape variations) in TCE.

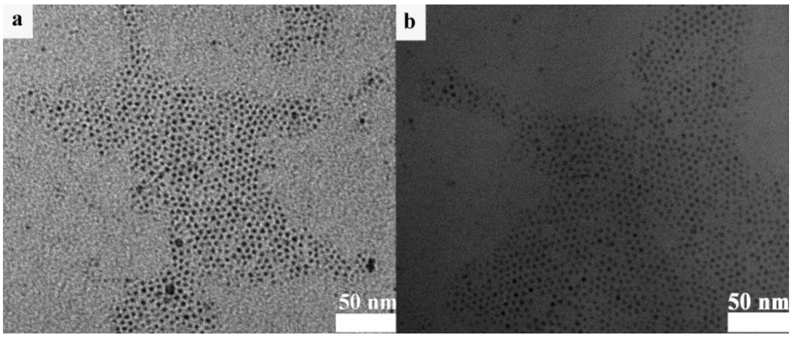

Fig. S9 The TEM images of the PbTe QDs stability test of sample QD-1. Fig. S9a, QD-1a of 2.6 nm with σ = 9.1%: samples measured after synthesis; Fig. S9b, QD-1b of 3.4 nm with σ = 8.3%: samples stored as thin films on TEM copper grid and measured after 130 days. The bigger size of 3.4 nm measured on TEM film is due to its σ > 9.1%

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and experimental measurement error.

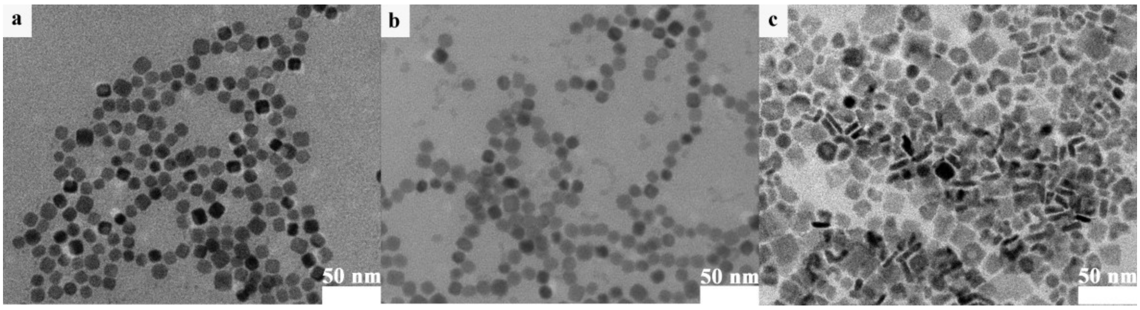

Fig. S10 The TEM images of the PbTe QDs stability test of sample QD-4. Fig. S10a, QD-4a of 9.5 nm with σ = 7.4%: samples measured after synthesis; Fig. S10b, QD-4b of 10.4 nm with σ = 7.5%: samples stored as thin films on TEM copper grid and measured after 130 days; Fig. S8c, QD-10c (decomposing or decomposed): stored in solid form and measured after 130 days. The PbTe QDs are air-stable as thin film. However, it is unstable in solid form.

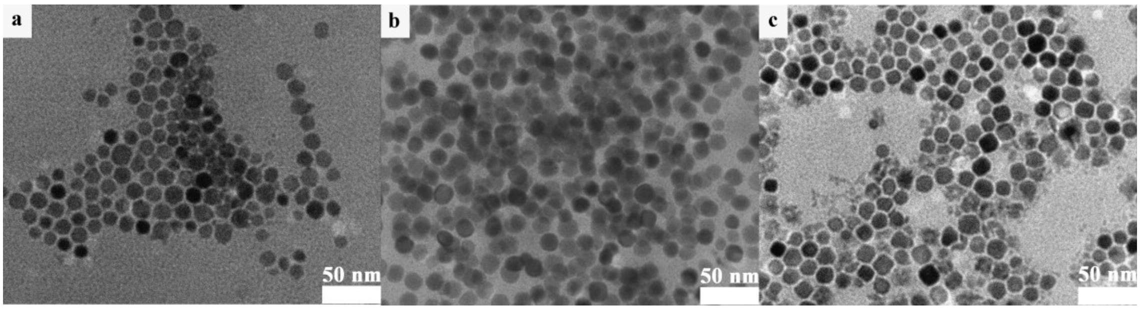

Fig. S11 The TEM images of the PbTe QDs stability test of sample QD-5. Fig. S11a, QD-5a of 10.5 nm with σ = 8.2%: samples measured after synthesis; Fig. S11b, QD-5b of 11.8 nm with σ = 6.5%: samples stored as thin films on TEM copper grid and measured after 130 days; Fig. S11c, QD-5c of 11.3 nm with σ = 8.2%: samples stored in TCE and measured after 130 days. The bigger size of 11.8 nm measured on TEM film is due to its σ > 8.2% but within experimental measurement error. Overall, the samples are air-stable as thin film. The samples are relatively air-stable (shape variations) in TCE.

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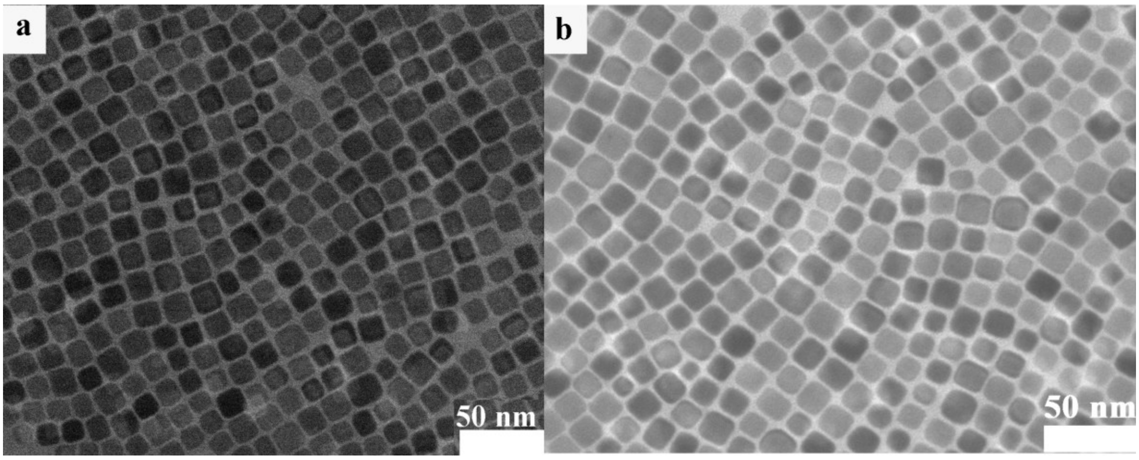

Fig. S12 The TEM images of the PbTe QDs stability test of sample QD-6. Fig. S12a, QD-6a of 14.0 nm with σ = 8.7%: samples measured after synthesis; Fig. S12b, QD-6b of 14.9 nm with σ = 9.4%: samples stored as thin films on TEM copper grid and measured after 130 days. The apparent enlargement of the sample in Fig. S12b is due to the moisture adsorption on the surface of PbTe QDs making the spacing distance between PbTe nanocrystals bigger. The samples are air-stable as thin film.

1. ASIT, in *Integrated Spectral Database System of Organic Compounds SDBD (the National Institute of Advanced Industrial Science and Technology, Japan).*
2. P. Torkington, *Transactions of the Faraday Society*, 1949, **45**, 445-447.
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