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Supplementary Information

Biomineralization of PbS and PbS-CdS Core-Shell Nanocrystals and their Application in Quantum Dot Sensitized Solar Cells

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Contents:

MSNATSQDRA LALATLAIHG GQSPDPSTGA VMPPIYATST YAQSSPGEHQ GFEYSRTHNP
TRFAYERCVA SLEGGTRGFA FASGMAASST VIELLDAGSH VVAMDDIYGG SFRLFERVRR
RTAGLDFSFV DLTDLAAFEA SITPKTKMVW IETPTNPMLK IVDIAAVAAI AKRHGLIVVV
DNTFASPMLQ RPLELGADLV LHSATKYLNG HSDMVGGMVV VGDNAELAEQ MAFLQNSVGG
VQGPFDSFLA LRGLKTLPLR MKAHCANALA LAQWLEKHPA VEKVIYPGLA SHPQHELAGK
QMAGYGGIVS IVLKGGFDAA KRFCEKTELF TLAESLGGVE SLVNHPAVMT HASIPVARRE
QLGISDALVR LSVGVEDLGD LQVDLGEALK

Figure S1: Sequence of the cystathionine γ-lyase that was derived from electrospray ionization mass spectrometry of a PbS QD solution synthesized using the *Stenotrophomonas maltophilia* strain SMCD1 (NCBI accession number WP_012509966). The QD containing supernatant was dialyzed against distilled water to reduce the free Pb salt and L-cysteine concentration, lyophilized and analyzed by electrospray ionization mass spectrometry (ESI-MS).

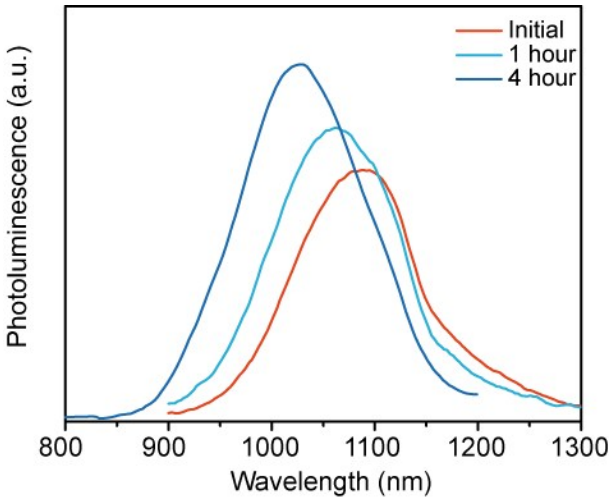

Figure S2: Photoluminescence characteristics of PbS-CdS core-shell nanoparticles, demonstrating a clear blue-shift as a function of the time that the PbS seed particles are in contact in the solution containing the Cd-precursor.

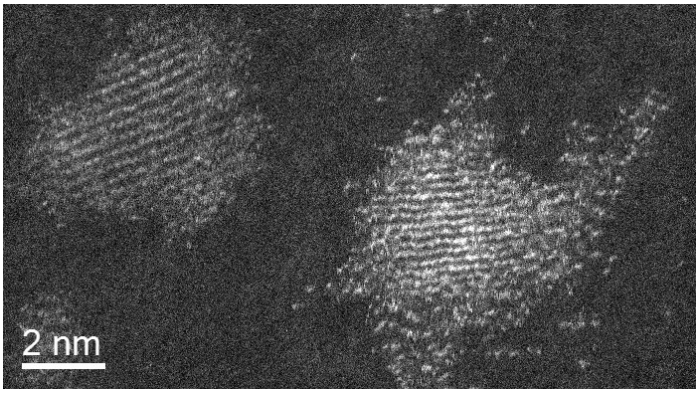

Figure S3. HAADF-STEM image of an intentionally grown PbS-CdS core-shell nanocrystal (*right*) and a pure CdS nanocrystal resulting from a secondary nucleation event (*left*).

Table S1. Lattice fitting of PbS nanocrystals shown in Figure 4 a) & c) and 4 b) & d) to the rock salt PbS structure. <x,y> denotes the angle between two intersecting planes x and y. Planes are identified in Figure 4 c).

Nanocrystal Identification as cubic PbS					
Figure 4a,c): $[1\bar{1}\bar{2}]$ projection			Figure 4b,d): $[1\bar{1}0]$ projection		
	Measurement	Matching		Measurement	Matching
Plane 1	d=1.79 Å	1.91 Å (311)	Plane 1	d=3.43 Å	3.49 Å (111)
Plane 2	d=2.10 Å	2.11 Å (220)	Plane 2	d=2.10 Å	2.13 Å (220)
Plane 3	d=3.43 Å	3.53 Å$(1\bar{1}1)$	Plane 3	d=3.43 Å	3.57 Å $(11\bar{1})$
<1, 2>	31.5˚	32.2˚	<1, 2>	35.3˚	36.0˚
<1, 3>	58.5˚	57.9˚	<1, 3>	70.5˚	71.9˚
<2, 3>	90.0˚	89.9˚	<2, 3>	35.3˚	35.9˚

Table S2 Lattice fitting of PbS-CdS nanocrystals shown in Figure 6 b) and 6 c) to the rock salt PbS structure. <x,y> denotes the angle between two intersecting planes x and y. Planes are identified in Figure 6 c).

Nanocrystal identification as cubic PbS		
Figure 6(c): [031] projection		
	Measurement	Matching
Plane 1	d=1.79 Å	1.76 Å $(11\bar{3})$
Plane 2	d=1.79 Å	1.77 Å $(1\bar{1}3)$
Plane 3	d=2.97 Å	2.98 Å (200)
<1, 2>	31.5˚	32.2˚
<1, 3>	58.5˚	57.9˚
<2, 3>	90.0˚	89.9˚