SUPPORTING INFORMATION PARAGRAPH

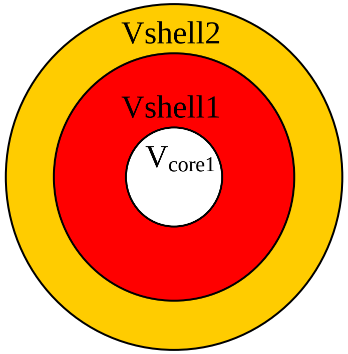
Tabelle 1: Analytic data for CdSe and CdSe/ZnS NPs. CdSe/ZnS NPs in the right part of the table were synthesized from the CdSe NPs on the left of the same column

CdSe						**CdSe/ZnS from ratio of zinc:sulfur precursor of 1: 1.3**													
λ_{em}	FWHM	λ_{abs}	QY	r_{TEM}	r_{abs}	λ_{em}	FWHM	λ_{abs}	QY	TPTest R_{f1}	R_{f2}	r_{abs}	r_{TEM}	$a_{Shell} = r_{TEM} - r_{abs}$	$a_{Shell} = \Delta r_{TEM}$	a_{Shell}= calc. from the amount of added ZnS precursor for 100 % yield.	$\Delta\lambda_{em}$	ΔFWHM	$\Delta\lambda_{abs}$
[nm]	[nm]	[nm]	[%]	[nm]	[nm]	[nm]	[nm]	[nm]	[%]	-	-	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]
582	26	572	4	1.91	1.79	602	29	596	5	x	x	2.21	2.47	0.3	0.6	0.38	20	3	24
581	25	573	3	1.64	1.8	578	27	565	12	x	x	1.69	2.21	0.5	0.6	0.76	-3	2	-8
572	26	561	4	1.83	1.64	582	26	569	23	0.0	0.0	1.75	1.89	0.1	0.1	1.14	10	0	8
576	26	563	5	1.97	1.67	582	26	570	30	0.0	0.0	1.76	2.12	0.4	0.1	1.52	6	0	7
574	30	561	4	x	1.64	595	35	595	37	0.2	0.7	2.19	2.72	0.5	x	1.71	21	5	34
576	25	566	2	1.78	1.71	582	33	578	30	0.0	0.2	1.88	2.12	0.2	0.3	1.9	6	8	12
571	27	559	4	1.93	1.62	587	30	574	43	0.4	1.2	1.82	2.37	0.6	0.4	2.28	16	3	15
575	31	566	4	x	1.71	594	36	576	44			1.85	2.58	0.7	x	2.28	19	5	10
564	36	547	4	x	1.49	580	32	565	49			1.69	2.6	0.9	x	2.28	16	-4	18
605	27	597	3	2.7	2.23	623	36	605	23	0.3	0.5	2.41	3.13	0.7	0.4	2.28	18	9	8
603	27	595	3	2	2.19	635	36	609	10	0.4	0.5	2.51	2.28	-0.2	0.3	2.28	32	9	14
572	28	562	x	x	1.66	595	37	576		0.4	0.6	1.85	2.33	0.5	2.3	2.28	23	9	14

CdSe						**CdSe/ZnS from ratio of zinc:sulfur precursor of 1: 3**													
λ_{em}	FWHM	λ_{abs}	QY	r_{TEM}	r_{abs}	λ_{em}	FWHM	λ_{abs}	QY	TPTest R_{f1}	R_{f2}	r_{abs}	r_{TEM}	$a_{Shell} = r_{TEM} - r_{abs}$	$a_{Shell} = \Delta r_{TEM}$	a_{Shell}= calc. from the amount of added ZnS precursor for 100 % yield.	$\Delta\lambda_{em}$	ΔFWHM	$\Delta\lambda_{abs}$
[nm]	[nm]	[nm]	[%]	[nm]	[nm]	[nm]	[nm]	[nm]	[%]	-	-	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]
579	29	567	x	1.93	1.72	603	29	590	41	0.1	0.0	2.09	2.16	0.1	0.2	0.76	24	0	23
581	30	567	x	x	1.72	590	31	577	x	x	x	1.86	x	-1.9	x	1.52	9	1	10
570	30	558	x	2.12	1.61	582	30	571	37	0.1	0.5	1.78	2.22	0.4	0.1	2.28	12	0	13

CdSe						**CdSe/ZnS from ratio of zinc:sulfur precursor of 3: 1**													
λ_{em}	FWHM	λ_{abs}	QY	r_{TEM}	r_{abs}	λ_{em}	FWHM	λ_{abs}	QY	TPTest R_{f1}	R_{f2}	r_{abs}	r_{TEM}	$a_{Shell} = r_{TEM} - r_{abs}$	$a_{Shell} = \Delta r_{TEM}$	a_{Shell}= calc. from the amount of added ZnS precursor for 100 % yield.	$\Delta\lambda_{em}$	ΔFWHM	$\Delta\lambda_{abs}$
[nm]	[nm]	[nm]	[%]	[nm]	[nm]	[nm]	[nm]	[nm]	[%]	-	-	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]	[nm]
577	27	563	x	x	1.67	582	27	576	15	0.0	0.0	1.85	x	x	x	0.76	5	0	13
573	29	557	x	2.08	1.6	589	30	571		0.0	0.0	1.78	x	x	x	1.52	16	1	14
566	32	554	x	2.09	1.56	576	29	561	24	0.0	0.0	1.64	2.37	0.7	0.3	2.28	10	-3	7

Precursor amounts depend on the initial core size and the ratio of the "Zn" and "S "precursor in each additional layer of the ZnS shell



The radius of the CdSe core r_{core1} (nm) can be obtained from the UV/VIS absorption wavelength λ (nm) of the first excitonic absorption peak..

(According to Lit. 37: W. W. Yu, L. Qu, W. Guo, X. Peng, *Chem. Mater*. **2003**,*15*,2854.)

For CdSe:

r_{core1} = 0.5* [(1.6122 *10-9)λ^4- (2.6575 *10-6) λ^3 + (1.6242 * 10-3) λ^2 - (0.4277) λ + (41.57)]

$$V_{core1} = \frac{4}{3} * \pi * r_{core1}^3$$

For a shell of thickness a_{shell} (e.g. 1 ML of ZnS)

$$V_{total1} = \frac{4}{3} * \pi * r_{total1}^3 = \frac{4}{3} * \pi * (r_{core1} + a_{shell1})^3 \Rightarrow V_{shell1} = V_{total1} - V_{core1}$$

With the density and the molar mass of the bulk shell material the amount of ZnS precursor can be calculated to grow a shell with the thickness a_{shell} around the core with the radius r_{core1}.

$$n_{shell1} = \frac{m_{shell1}}{M_{shell1}} = \frac{\varphi_{shell} * V_{shell}}{M_{shell}}$$

To estimate how much precursor is needed to shell all the CdSe cores with the size V_{core1} in the experiment a simplification is necessary to calculate how many cores are there.

From the amount of CdO and TOP/Se precursor we calculate the maximal volume V_{max} of one single CdSe particle that can theoretically be formed at 100 % yield and divide it by the actual CdSe particle size V_{core1}. This gives the number N of the CdSe cores in the experiment.

$$V_{\max} = 100\% * \frac{\varphi_{CdSe,bulk}}{m_{CdSe}} * = 100\% * \frac{n_{CdO\_precursor} * M_{CdO}}{\varphi_{CdSe,bulk}}$$

$$N = \frac{V_{\max}}{V_{core1}}$$

Therefore $N*n_{shell1}$ mol shell material ZnS are needed to form a layer of a_{shell} nm thickness.

To calculate the amount of precursor for a ZnS shell of a_{shell}=6*0.38 nm thickness the above calculation is calculated for each of the six layers a 0.38 nm. The amount of ZnS required in each layer can be formed from a 1:1 molar ratio of the “Zn” and “S” precursor or as in our best experiments with a slight excess of 1:1.3.

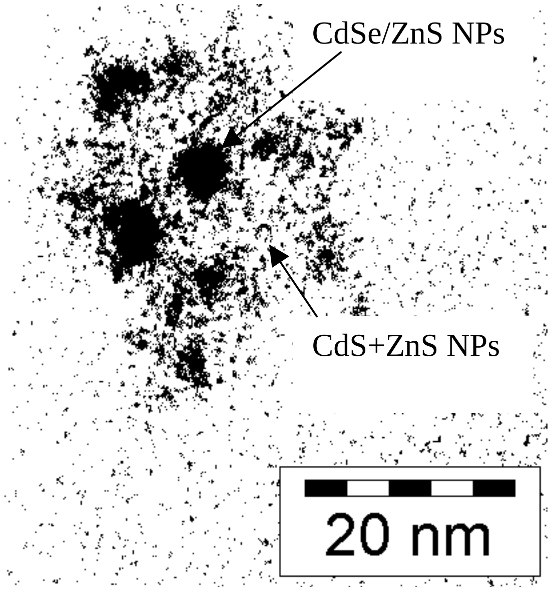


Figure 1. TEM picture of a CdSe/ZnS sample (lem = 595 nm, FWHM = 37 nm, Rf1 = 0.43, Rf2 = 0.60, QY = %). Most likely it shows the simultaneous formation of ZnS and CdS NPs during the synthesis of CdSe/ZnS core shell QDs. (The threshold in this picture was manually increased to enhance contrast).