Blue CdSe/CdS Core/Crown Nanoplatelet Light-Emitting Diodes Obtained via a Design-of-Experiments Approach – Supporting Information

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SECTION 1: CdSe/CdS NPL synthesis parameters

experiment	carboxylic acid chain length	carboxylic acid amount	propionic acid amount	reaction time	injection temperature	growth temperature
No.	#C	mmol	mmol	min	°C	°C
1	16	0.8	1.78	8	185	225
2	12	1.2	0.99	8	205	225
3	18	1	1.78	20	205	225
4	12	1.2	1.78	20	185	217.5
5	18	1.2	1.78	8	195	210
6	18	0.8	0.99	20	185	210
7	16	1	0.99	14	195	217.5
8	12	1	0.2	8	185	210
9	18	0.8	0.2	8	205	217.5
10	12	0.8	0.2	20	195	225
11	18	1.2	0.2	14	185	225
12	16	1.2	0.2	20	205	210
13	12	0.8	1.78	14	205	210

Table S1. *Experimental parameters for the Definitive Screening Design of the 3.5 ML blue-emitting CdSe nanoplatelet synthesis. Every input factor has been varied over three different levels.*

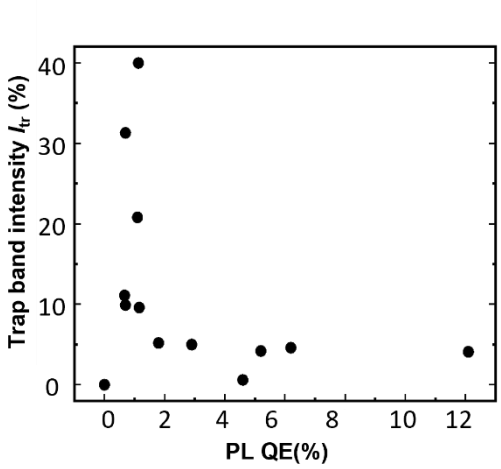

Figure S1. *Evolution of the trap band intensity I_{tr} as a function of PL QE. In samples with high PL QE, I_{tr} is minimized accordingly.*

	PL QE	f_{QD}	I_{tr}
b_0	-0.1	17.7	35.1
b_1	1.4	17.4	-3.7
b_2	0.5	8.1	3.5
b_3	1.9	-33.4	-4.9
b_4	-0.4	0.8	2.7
b_5	0.3	5.9	0.0
b_6	-1.5	7.0	-4.2
b_{11}	3.3	-20.9	-23.4
b_{22}	0.8	30.0	-5.5
b_{33}	-0.9	**32.7**	0.5
b_{44}	0.1	-24.4	0.6
b_{55}	-2.8	17.1	-2.4
b_{66}	3.2	-16.7	0.3

Table S2. *Model coefficients for each response (PL QE, QD fraction f_{QD}, trap band intensity I_{tr}). They are obtained through a multilinear regression of the responses, according to* ***equation 1*** *(see main text).*

experiment	carboxylic acid chain length	carboxylic acid amount	propionic acid amount	reaction time	injection temperature	growth temperature
No.	#C	mmol	mmol	min	°C	°C
14	18	1.2	2.67	13	215	250
15	18	1.4	1.67	16	215	220
16	18	1.2	1.80	13	215	250
17	18	1.4	0.94	13	215	250
18	18	1.2	0.94	13	185	220
19	18	1.2	2.67	16.5	185	250
20	18	1	2.67	20	185	220
21	18	1	0.94	20	200	250
22	18	1.2	1.80	16.5	200	235
23	18	1.38	1.67	16	215	220
24	18	1.36	1.67	16	215	220

Table S3. *Experimental parameters for the second synthesis run of the 3.5 ML blue-emitting CdSe nanoplatelet synthesis. Every input factor has been varied over three different levels.*

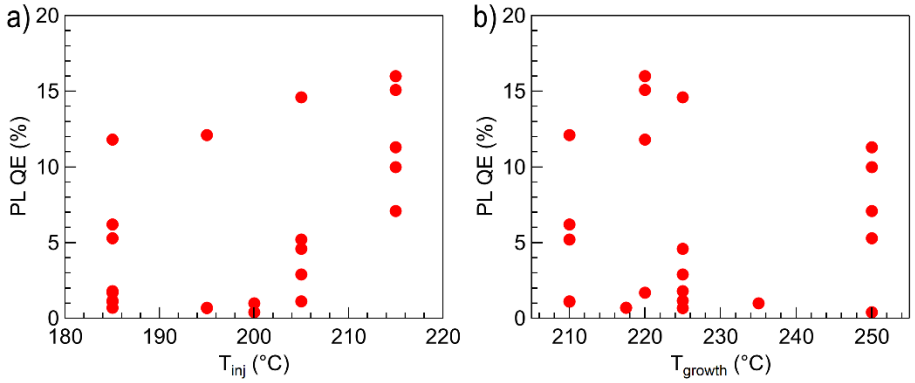

Figure S2. *PL QE as a function of injection and growth temperature for the combined results of first and second run. An increase in PL QE is observed for higher injection temperature, while there is no clear dependency on the growth temperature.*

	PL QE	f_{QD}	I_{tr}
b_0	16.0	2.2	0.5
b_2	-2.6	-3.9	0.7
b_3	-1.6	-6.6	0.5
b_{23}	1.1	6.5	0.2
b_{22}	-2.3	0.6	0.4
b_{33}	-5.7	6.8	1.5

Table S4. *Model coefficients of multilinear regression model for each response (PL QE, QD fraction f_{QD}, trap band intensity I_{tr}), for the central composite face-centered design.*

SECTION 2: LED fabrication

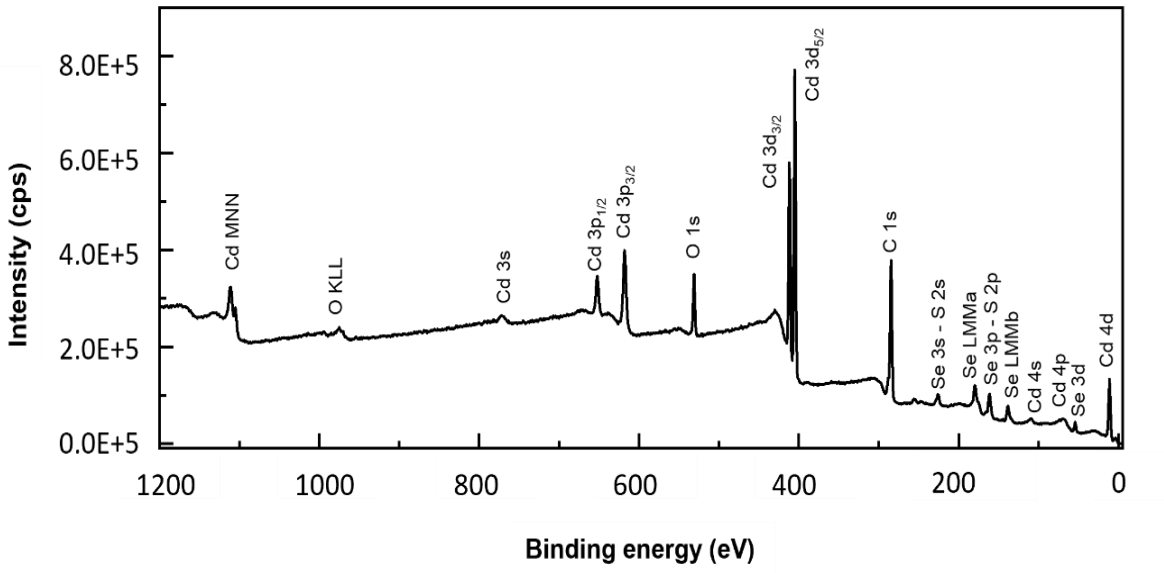

***Figure S3**. Low-resolution XPS spectrum, where peaks for Cd, Se, C, O are evident.*

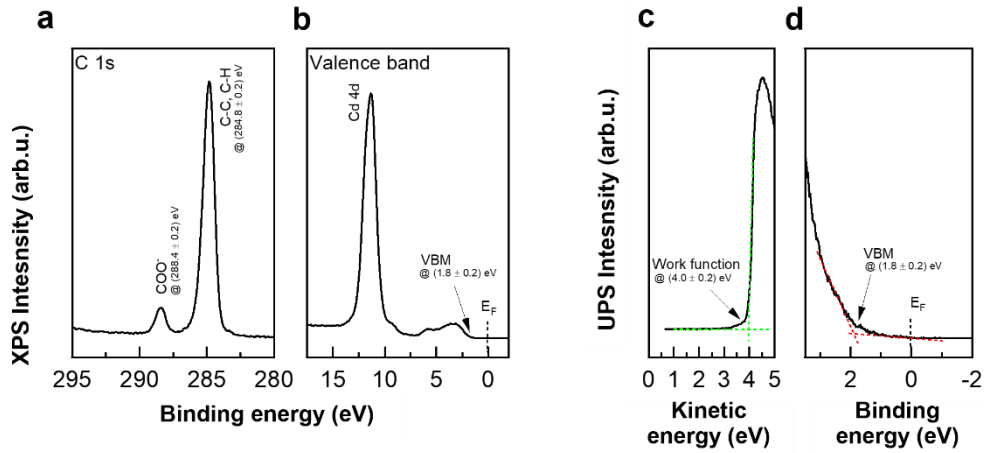

***Figure S4.** (Left) high-resolution XPS spectra, (right) high-resolution UPS spectra.*

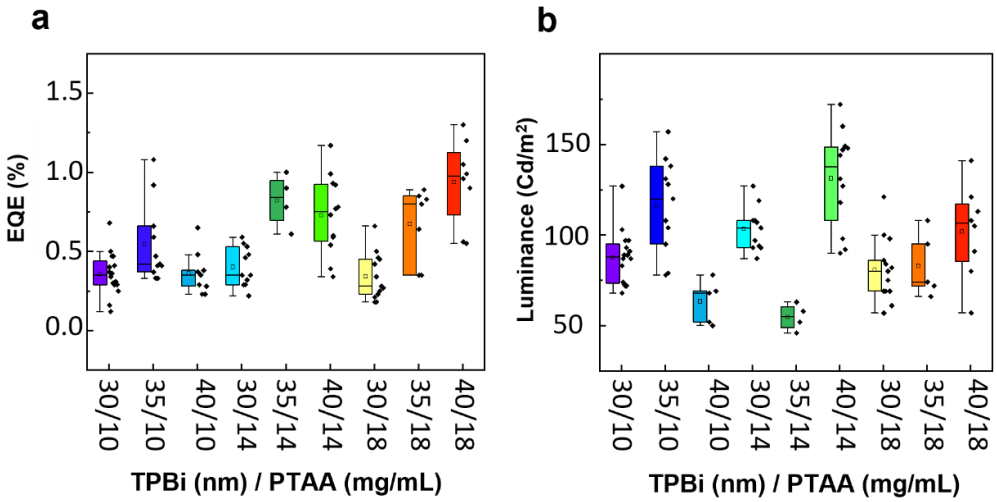

Figure S5: *EQE (left) and luminance (right) for 8 LED samples prepared via the central composite face-centered design. Device 30-14 device is omitted because the luminance was an outlier. We report on the individual values of measurable pixels (maximum 6) in each device, together with the average value (□), median line and standard deviation (box).*

Term	EQE (%)
d_0	1.60
d_1	0.21
d_2	0.04
d_{12}	0.46
d_{11}	-0.52
d_{22}	-0.03
Explained Variance [%]	57
SD of the residuals	0.34

$$y = d_0 + d_1X_2 + d_2X_3 + d_{12}X_2X_3 + d_{11}{X_2}^2 + d_{22}{X_3}^2$$

***Table* S5.** *List of coefficients for the CCF model, explained variance of EQE response and standard deviation (SD) of the residuals. We also report the model equation below.*

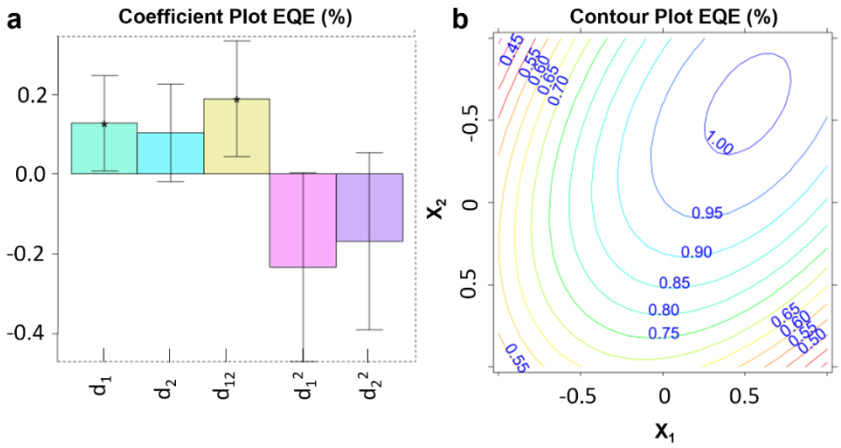

Figure S6. *Coefficient plot (left) for EQE of CCF (Face-centered Central Composite Design) of LED fabrication: cross term TPBi*PTAA (d_{12}) shows significance. Contour plot for EQE% of CCF showing an optimum zone located at high level of PTAA (mg/mL) and TPBi (nm).*

Emissive material	PL peak position (nm)	FWHM of PL (nm)	EL peak position (nm)	FWHM of EL (nm)	PL → EL broadening (nm)	Ref.
CdSe/CdxZn1-xS/ZnS QRs	465	26	472	30	4	1
$Zn_xCd_{1-x}S$/ZnS core/shell QDs	442	21	445	25	4	2
CdSe/CdS core/shell NPLs	556	12	560	14	2	3
CdSe/CdS core/crown NPLs	515	8	516	10	2	4
CdSe/CdS core/crown NPLs	461	10	467	11	1	5
CdSe/CdS core/crown NPLs	**465**	**14**	**467**	**16**	**2**	**This Work**

Table S6. *Photoluminescence and electroluminescence peak position and full-width-at-half-maximum for different literature sources on quantum rods (QRs), quantum dots (QDs) and nanoplatelets (NPLs).*

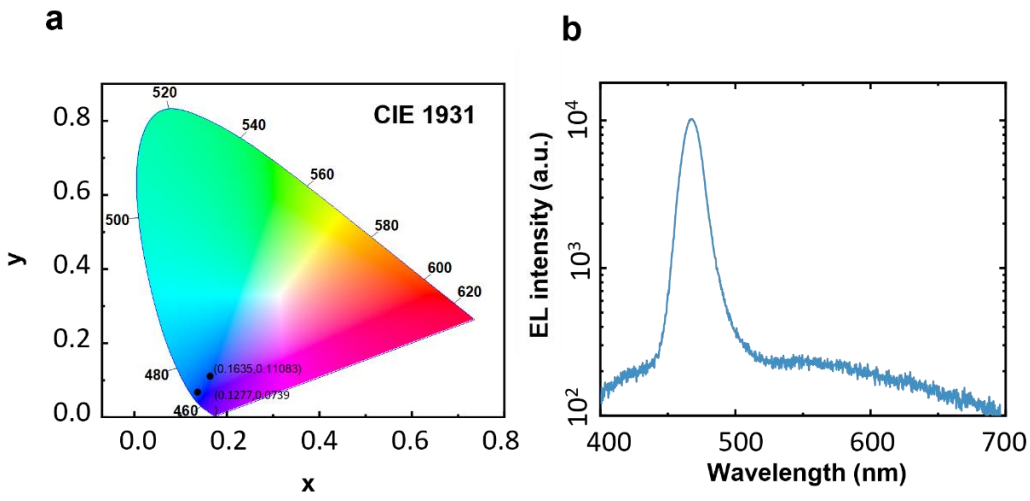

Figure S7. *(a) CIE diagram of the electroluminescence of a typical blue-emitting CdSe/CdS LED without 525 nm short-pass filter (0.1635,0.11083) and with a (simulated) 525 nm short-pass filter (0.1277,0.0739). (b) EL of CdSe/CdS LED at 6V in logarithmic scale with a residual weak trap band centered at 550 nm.*

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