Supplementary Materials

Ytterbium-Doped Lead–Halide Perovskite Nanocrystals: Synthesis, Near-Infrared Emission, and Open-Source Machine Learning Model for Prediction of Optical Properties

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Table S1. Experimental parameters for the synthesis of Yb-doped $CsPbCl_3$ pNCs taken from Refs. [15,23,26,45,46,56–58] (see main text).

Chemical formula	DOI	Pb_mmol	Yb_mmol	OlAm_mL	OlAc_mL	temperature_°C	time_sec
Yb:$CsPbCl_3$	10.1039/c8tc03957g	0.12	0.38	2	2	260	5
Yb:$CsPbCl_3$	10.1021/acs.nanolett.8b05104	0.2	0.08	0.5	1	240	1
Yb:$CsPbCl_3$	10.1021/acs.nanolett.8b01066	0.2	0.16	0.5	1	240	1
Yb:$CsPbCl_3$	10.1021/acs.nanolett.7b04575	0.38	0.19	1	1	240	30
Yb:$CsPbCl_3$:Mn(2.17%)	10.1002/advs.202001317	0.2	0.02	1	0.5	200	10
Yb:$CsPbCl_3$:Mn(1.45%)	10.1002/advs.202001317	0.2	0.04	1	0.5	200	10
Yb:$CsPbCl_3$:Mn(1.3%)	10.1002/advs.202001317	0.2	0.06	1	0.5	200	10
Yb:$CsPbCl_3$:Mn(1.14%)	10.1002/advs.202001317	0.2	0.08	1	0.5	200	10
Yb:$CsPbCl_3$	10.1021/acs.jpcc.9b01296	0.4	0.32	1	2	240	1
Yb:$CsPbCl_3$	10.1021/acsami.1c09421	0.2	0.09	1	3	240	1

Table S2. Comparison of the predicted and experimental quantum yields Yb-doped CsPbCl₃ in the NIR spectral region reported in Refs. [15,23,26,45,46,56–58] (see main text).

Chemical formula	DOI	Prediction of NIR QY_%	Experimental NIR QY_%	Absolute difference_%
Yb:CsPbCl₃	10.1039/c8tc03957g	124.3	120.1	4.2
Yb:CsPbCl₃	10.1021/acs.nanolett.8b05104	132.6	114	18.6
Yb:CsPbCl₃	10.1021/acs.nanolett.8b01066	155.7	170	14.3
Yb:CsPbCl₃	10.1021/acs.nanolett.7b04575	145.4	142.7	2.7
Yb:CsPbCl₃:Mn(2.17%)	10.1002/advs.202001317	55.4	32.5	22.9
Yb:CsPbCl₃:Mn(1.45%)	10.1002/advs.202001317	61.2	64.6	3.4
Yb:CsPbCl₃:Mn(1.3%)	10.1002/advs.202001317	67	103.3	36.3
Yb:CsPbCl₃:Mn(1.14%)	10.1002/advs.202001317	72.8	66.3	6.5
Yb:CsPbCl₃	10.1021/acs.jpcc.9b01296	147.3	146	1.3
Yb:CsPbCl₃	10.1021/acsami.1c09421	105.7	110	4.3

Table S3. Linear regression coefficients for variables used in the model equation:.

$$\text{NIR PL QY (\%)} = \beta_1 \cdot Pb_{mmol} + \beta_2 \cdot Yb_{mmol} + \beta_3 \cdot OlAm_{mL} + \beta_4 \cdot OlAc_{mL} + \beta_5 \cdot temperature_{°C} + \beta_6 \cdot time_{sec}$$

Coefficient	Variables	Value
β_1	Pb_mmol	−93.47
β_2	Yb_mmol	289.10
β_3	OlAm_mL	−84.18
β_4	OlAc_mL	6.14
β_5	temperature_°C	0.68
β_6	time_sec	1.38