## Supporting Information for

## Origin of Luminescence Spectra Width in Perovskite Nanocrystal with Surface Passivation

Yung Jin Yoon<sup>†</sup><sup>a</sup>, Yun Seop Shin<sup>†</sup><sup>a</sup>, Chan Beom Park<sup>a</sup>, Jung Geon Son<sup>a</sup>, Jae Won Kim<sup>a</sup>, Hyeon Seo Kim<sup>a</sup>, Woo Jin Lee<sup>a</sup>, Jungwoo Heo<sup>a</sup>, Gi-Hwan Kim<sup>\*</sup><sup>b</sup>, and Jin Young Kim<sup>\*</sup><sup>a</sup>

<sup>a</sup>Perovtronics Research Center, Department of Energy Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, South Korea. E-mail: jykim@unist.ac.kr

<sup>b</sup>School of Materials Science and Engineering, Gyeongsang National University, Jinju 52828,

Korea, Republic of Korea E-mail: <a href="mailto:ghkim@gnu.ac.kr">ghkim@gnu.ac.kr</a>



**Fig. S1.** TEM images of the blue emissive PeNCs synthesized with (a) 140°C injection (b) 160°C injection and (c) 180°C injection conditions.



**Fig. S2.** PL spectra from the green emissive PeNCs synthesized with different injection temperature. (FWHM: 25.36nm for 140°C, 22.72nm for 160°C, and 20.96nm for 180°C injection temperature condition)



**Fig. S3.** Size distribution of the green emissive PeNCs synthesized with different injection temperature. (mean size: 10.67nm for 140°C, 12.55nm for 160°C, and 13.24nm for 180°C; standard deviation: 1.54nm for 140°C, 1.90nm for 160°C, and 1.57nm for 180°C)



Fig. S4. PL spectra from the PeNCs synthesized with different growth time conditions.



**Fig S5**. TEM images of the PeNCs synthesized with (a) 5 seconds (b) 5 minutes and (c) 30 minutes growth time condition.



Fig. S6. Size distribution of the PeNCs synthesized with different growth time.



**Fig. S7.** PL spectra from the PeNCs synthesized with different ratio of precursor halides at same injection temperature (160 °C).



**Fig. S8.** XPS Survey spectra of the pristine (PR) PeNCs and the surface passivated (SP) PeNCs with assist of ligands with different alkyl chain lengths, (i.e., SP-TOP sample was passivated with assist of TOP).



**Fig. S9.** FT-IR spectra around P-C bond region from surface passivated PeNCs assist of different nucleophiles with varying alkyl chain lengths.



**Fig. S10.** XPS Survey spectra of the pristine (PR) and the surface passivated (SP) PeNCs with different injection temperature conditions (i.e., PR-140 samples were synthesized at 140°C and SP-140 samples were surface passivated result of PR-140).



Fig. S11. XRD pattern of the pristine (PR) and surface passivated (SP) PeNCs.



Fig S12. TEM images of the (a) pristine (PR) and (b) surface passivated (SP) PeNCs.



Fig. S13. Size distribution of the pristine (PR) and surface passivated (SP) PeNCs.



**Fig. S14.** FT-IR spectra around C-H bond region from surface passivated PeNCs assist of different nucleophiles with varying alkyl chain lengths.



**Fig. S15.** Absorption spectra from the pristine (PR) and surface passivated (SP) PeNCs. (inset. lower intensity region of the absorption spectra.)



**Fig. S16.** AFM topographical images of the (a) pristine (PR) and (b) surface passivated (SP) PeNCs.



**Fig. S17.** Operational spectra stability of the PeLEDs based on the pristine (PR) and surface passivated (SP) PeNCs.

**Table S1.** Summarized peak positions, full width at half maximum of spectra (FWHM), photoluminescence quantum yield (PLQY) and statistics of size distribution of PeNCs synthesized with different injection temperatures.

Injection Condition	Peak (nm)	FWHM (nm)	FWHM (eV)	PLQY (%)	Mean Size (nm)	SD (nm)
140°C	471.89	27.06	0.151	7.80	7.78	0.94
160°C	471.20	23.80	0.133	6.90	9.51	0.69
180°C	471.86	20.22	0.113	11.26	12.39	2.08

**Table S2.** Summarized peak positions, full width at half maximum of spectra (FWHM), photoluminescence quantum yield (PLQY) and statistics of size distribution of PeNCs synthesized with different growth time.

Growth Time	Peak (nm)	FWHM (nm)	FWHM (eV)	PLQY (%)	Mean Size (nm)	SD (nm)
5s	471.20	23.80	0.133	6.9	9.52	0.69
1m	473.21	22.25	0.123	10.73	-	-
5m	471.48	22.13	0.124	8.6	9.30	0.73
10m	471.90	22.52	0.125	6.9	-	-
30m	471.59	23.23	0.130	6.7	9.18	0.72

**Table S3.** Summarized peak positions and full width at half maximum of spectra (FWHM) ofPeNCs synthesized with different precursor halide ratio.

Halide Ratio (Br %)	Peak (nm)	FWHM (nm)	FWHM (eV)
55%	456.94	20.28	0.120
60%	464.28	21.07	0.121
62%	471.20	23.80	0.133
65%	471.60	20.79	0.116
70%	480.45	21.17	0.114

**Table S4.** Summarized peak positions and full width at half maximum of spectra (FWHM) of PeNCs with surface passivation assist of nucleophiles with different alkyl chain lengths.

	Peak (nm)	FWHM (nm)	FWHM (eV)	PLQY (%)
PR-160	471.20	23.80	0.133	6.90
SP-TOP	469.86	21.54	0.121	86.57
SP-THP	468.52	20.67	0.117	85.12
SP-TBP	472.42	19.27	0.107	90.66

**Table S5.** Summarized atomic ratio of PeNCs with surface passivation assist of nucleophiles with different alkyl chain lengths calculated from the XPS measurement. Normalized with the Cs peak.

	Cs	Pb	Br	Cl
PR-160	1	0.810	1.87	1.39
SP-TOP	1	0.757	2.15	1.57
SP-THP	1	0.791	2.01	1.51
SP-TBP	1	0.780	2.13	1.56

**Table S6.** Summarized peak positions and full width at half maximum of spectra (FWHM) of PeNCs before (PR) and after surface passivation (SP) with different injection temperatures.

	Peak (nm)	FWHM (nm)	FWHM (eV)	PLQY (%)
PR-140	471.89	27.06	0.151	7.80
SP-140	469.79	18.69	0.105	78.83
PR-160	471.20	23.80	0.133	6.90
SP-160	472.42	19.27	0.107	90.66
PR-180	471.86	20.22	0.113	11.26
SP-180	469.88	19.38	0.109	86.35

**Table S7.** Summarized atomic ratio of PeNCs before (PR) and after surface passivation (SP) with different injection temperatures calculated from the XPS measurement. Normalized with the Cs peak.

	Cs	Pb	Br	Cl
PR-140	1	0.771	2.03	1.38
SP-140	1	0.723	2.19	1.61
PR-160	1	0.810	1.87	1.39
SP-160	1	0.780	2.13	1.56
PR-180	1	0.937	2.02	1.49
SP-180	1	0.851	2.00	1.45

**Table S8.** Parameters of biexponential fitting for time-resolved PL lifetime of pristine (PR) and surface passivated (SP) PeNCs synthesized with different injection temperatures.  $f_1$  and  $f_2$  are percent contributions of lifetimes, fast-decay  $\tau_1$  and slow-decay  $\tau_2$  respectively.

	τ <sub>1</sub> (ns)	f <sub>1</sub> (%)	τ <sub>2</sub> (ns)	f <sub>2</sub> (%)	τ <sub>ave</sub> (ns)	$\chi^2$
PR-140	1.31	83.24	10.80	16.76	2.90	1.79
SP-140	1.40	69.31	4.88	30.69	2.47	1.27
PR-160	1.39	83.25	9.87	16.75	2.81	1.63
SP-160	1.42	55.95	3.72	44.05	2.44	1.10
PR-180	2.21	88.75	8.34	11.25	2.90	1.54
SP-180	1.79	61.14	4.04	38.86	2.66	1.13