Electronic Supplementary Information

Dynamically Tunable Multicolor Emissions from Zero-Dimensional Cs_3LnCl_6 (Ln: Europium and Terbium) Nanocrystals with Wide Color Gamut

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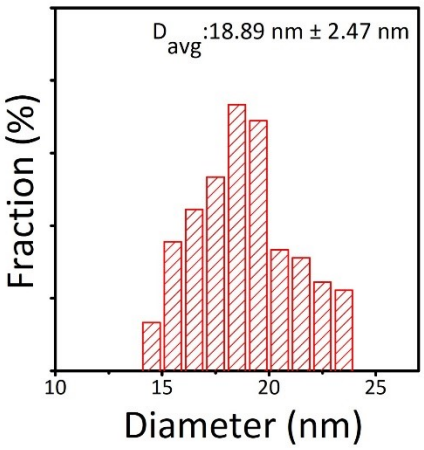

Figure S1. Size distribution of the Cs_3EuCl_6 NCs. Average size was 18.89 ± 2.47 nm.

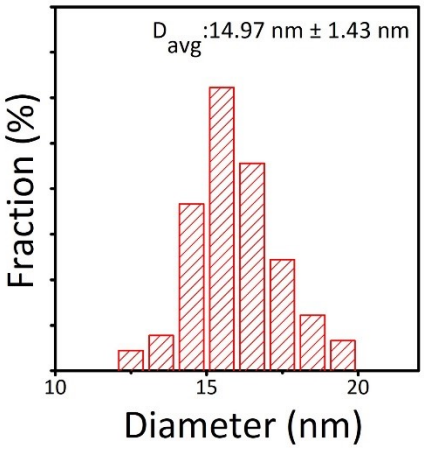

Figure S2. Size distribution of the Cs_3TbCl_6 NCs. Average size was 14.97 ± 1.43 nm.

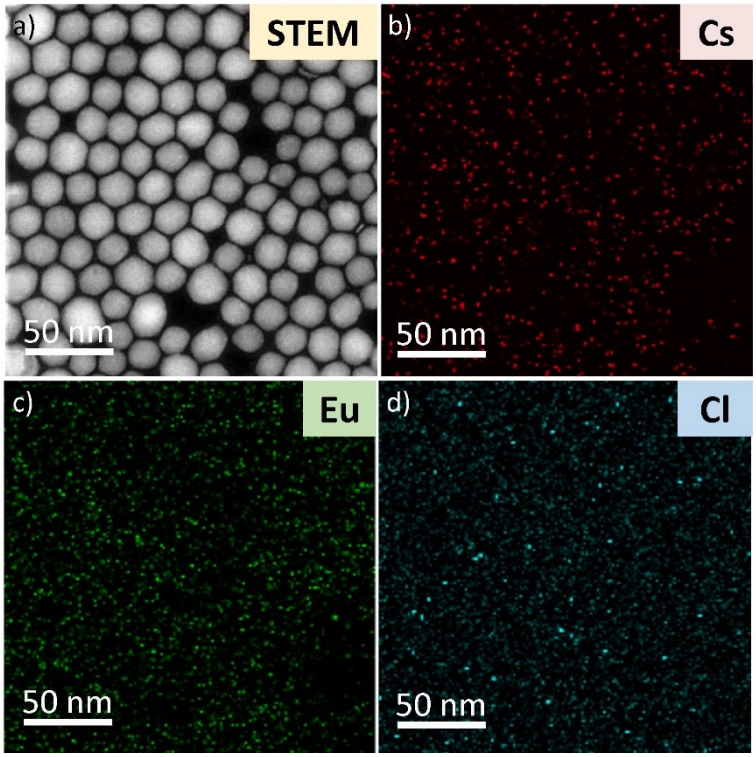

Figure S3. a) STEM image of Cs_3EuCl_6 and EDS elemental mappings of b) Cs, c) Eu, and d) Cl.

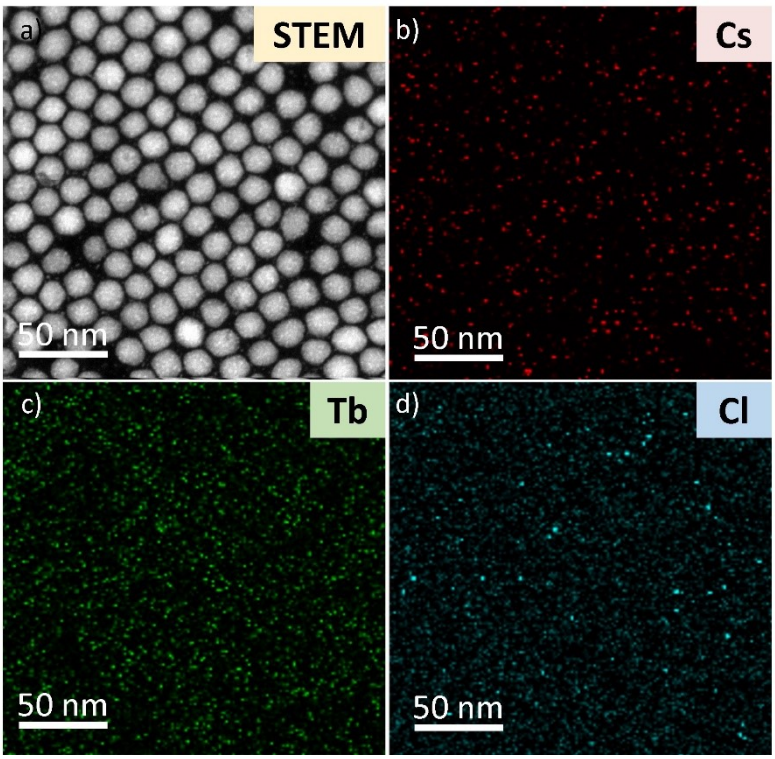

Figure S4. a) STEM image of Cs_3TbCl_6 and EDS elemental mappings of b) Cs, c) Tb, and d) Cl.

Table S1. Lattice parameters of the Cs_3LnCl_6 (Ln =Eu, Tb) crystal structure (space group: C2/c, #15)[1, 2]

Compound	*a*/Å	*b*/Å	*c*/Å	*ß*/degree
Cs_3EuCl_6	27.065	8.192	13.203	99.93
Cs_3TbCl_6	26.990	8.180	13.171	99.97

Table S2. Atomic coordinates and equivalent isotropic displacement parameters of Cs_3EuCl_6 (space group: C2/c)[2]

Atom	*x*/a	*y*/b	*z*/c	U_{11}
Eu1	0.25000	0.25000	0.50000	0.012
Eu2	0.00000	0.789(7)	0.25000	
Cs1	0.050(1)	0.726(6)	0.930(3)	0.025
Cs2	0.162(1)	0.815(6)	0.305(3)	
Cs3	0.346(1)	0.187(5)	0.851(3)	
Cl1	0.247(5)	0.389(1)	0.693(10)	0.026
Cl2	0.322(5)	0.491(16)	0.482(9)	
Cl3	0.324(6)	0.068(16)	0.579(11)	
Cl4	0.045(5)	0.544(17)	0.173(10)	
Cl5	−0.060(4)	0.798(16)	0.060(10)	
Cl6	0.063(5)	0.050(16)	0.197(10)	

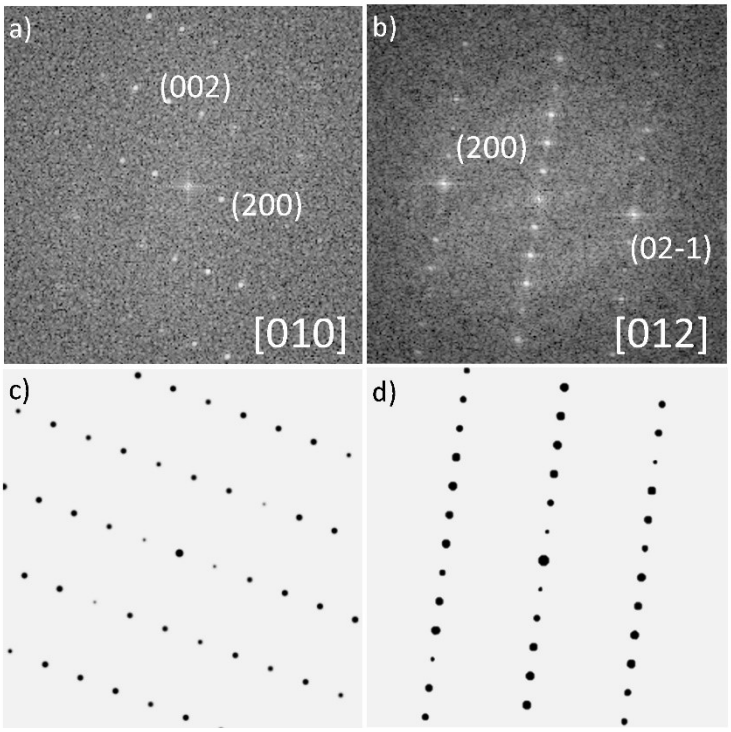

Figure S5. FFT of the high-resolution TEM image of an isolated a) Cs_3EuCl_6 NC and b) Cs_3TbCl_6 NC and a simulated ED pattern projected from the c) [010] zone axis of Cs_3EuCl_6 NC and d) [012] zone axis of Cs_3TbCl_6 NC.

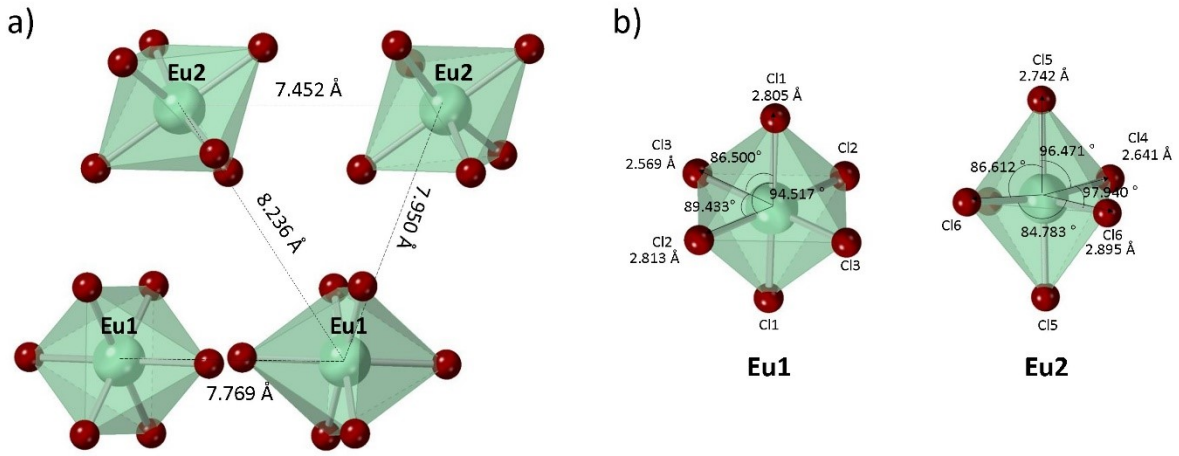

Figure S6. Distances between the Eu centers (left) and distances and degrees of Eu–Cl bonds of the $[EuCl_6]^{3-}$ octahedrons.

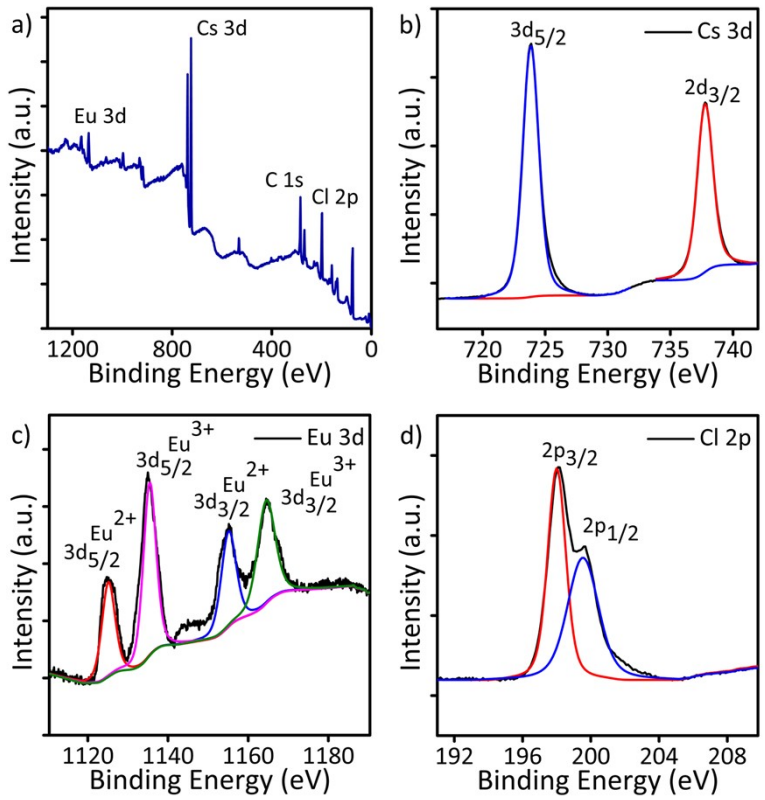

Figure S7. a) XPS survey spectra of Cs_3EuCl_6 NCs. High-resolution XPS spectra of b) Cs 3d, c) Eu 3d, and d) Cl 2p.

Table S3. Results of the fitting of the TRPL spectra of the Cs_3EuCl_6 NCs to a biexponential function. The TRPL measurements were conducted at room temperature, and the decay was monitored.

Excitation Wavelength (nm)	Emission Wavelength (nm)	τ_1 (ns)	Proportion(%)	τ_2 (ns)	Proportion(%)	τ_3 (ns)	Proportion(%)
374	430	21.3	40	64.1	25	2.51	35

Excitation Wavelength (nm)	Emission Wavelength (nm)	τ_1 (ms)	Proportion(%)	τ_2 (ms)	Proportion(%)
264	590	2.10	10	4.2	90

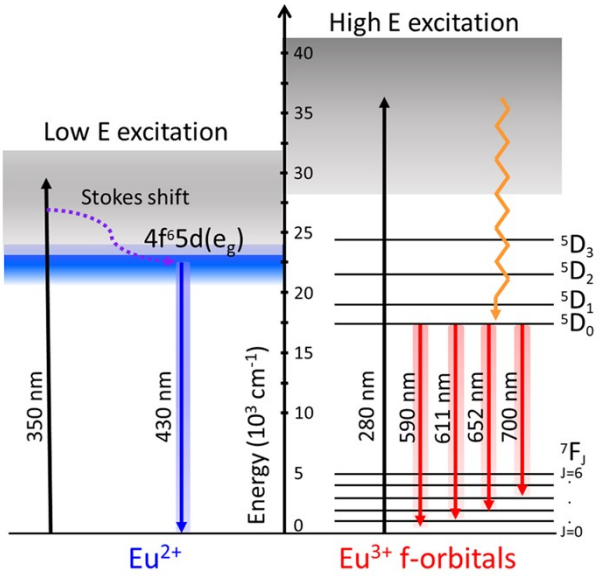

Figure S8. Schematic of the energy diagram of Cs_3EuCl_6 NCs under high and low energy excitations.

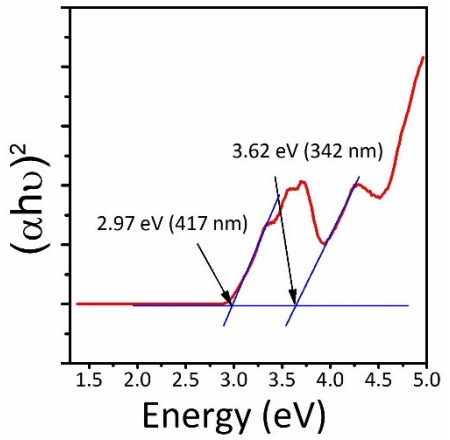

Figure S9. Diffuse reflectance spectrum of the Cs_3EuCl_6 NCs.

Table S4. Results of PL, PLE, PLQY, and lifetime of Cs_3EuCl_6 NCs under high and low energy excitations.

PL color	PLE l_{max} (nm)	PL l_{max} (nm)	PLQY (%)	Lifetime
Red PL	280	590 (max), 611, 652, 700	48.78	3.99 ms
Blue PL	350	430	5.38	25.79 ns

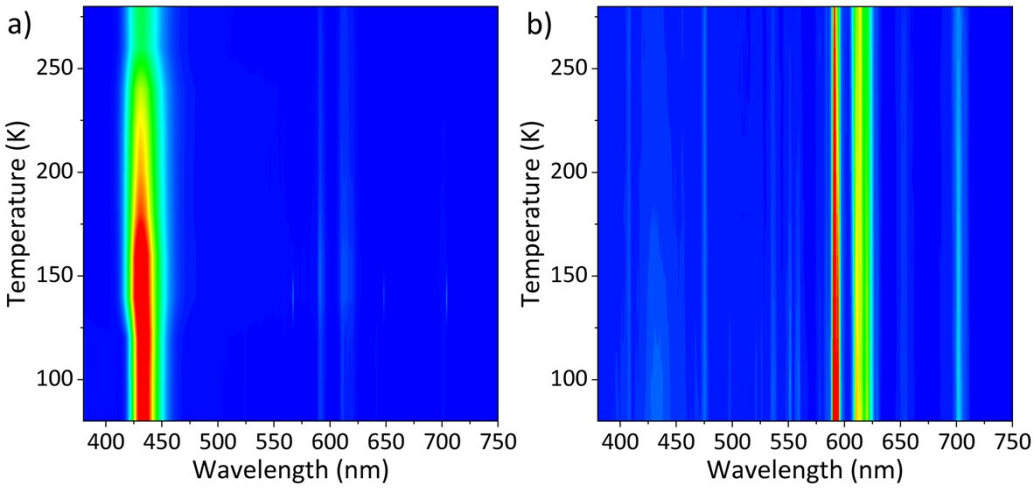

Figure S10. Temperature-dependent PL spectra of the Cs_3EuCl_6 NCs under a) 350 nm and b) 280 nm excitation.

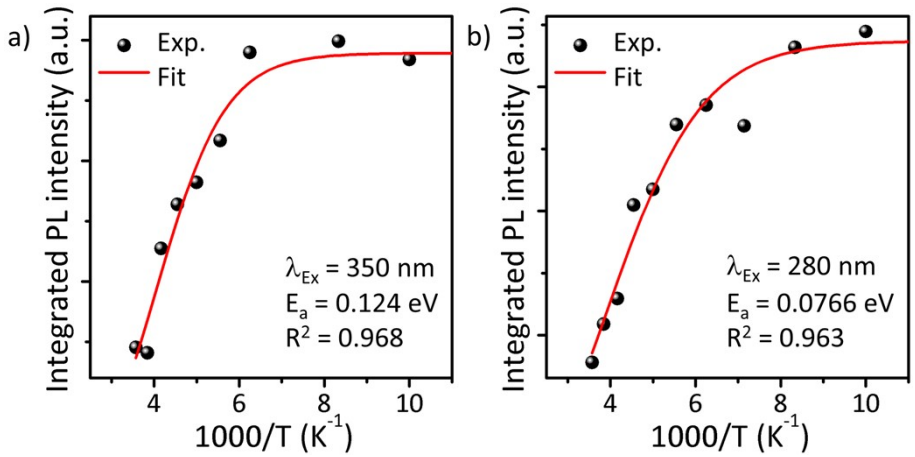

Figure S11. Temperature dependence of the integrated PL intensity of Cs_3EuCl_6 NCs under a) 350 nm and b) 280 nm excitation.

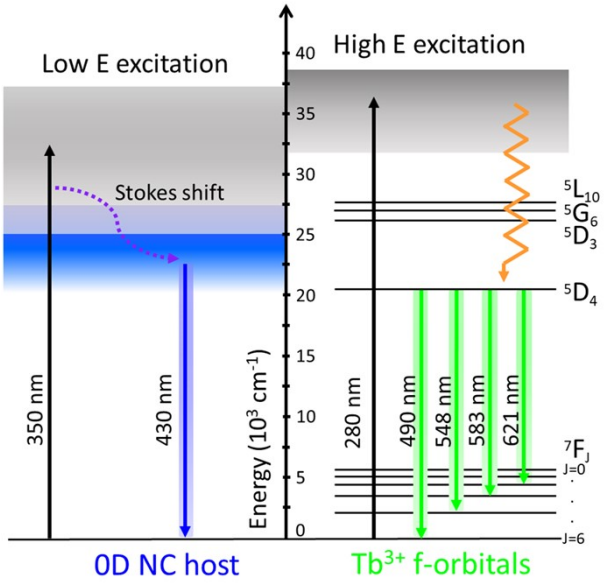

Figure S12. Schematic of the energy diagram of Cs_3TbCl_6 NCs under high and low energy excitations.

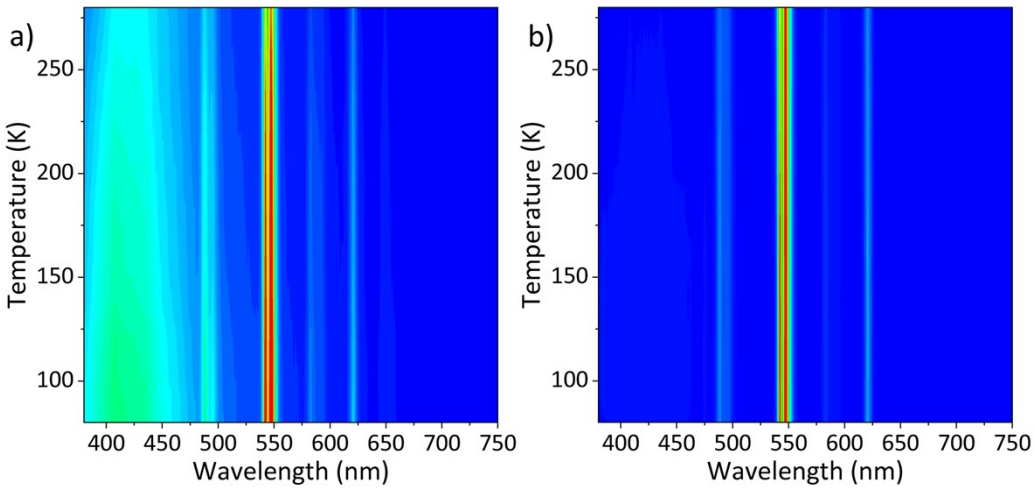

Figure S13. Temperature-dependent PL spectra of the Cs_3TbCl_6 NCs under a) 350 nm and b) 280 nm excitation.

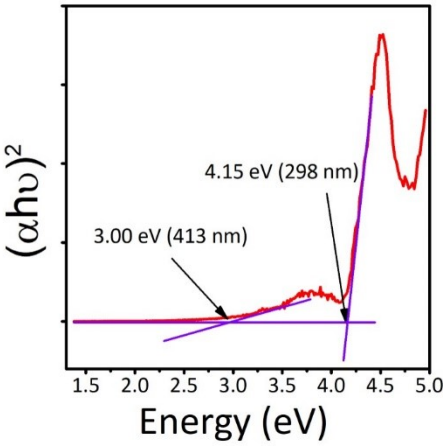

Figure S14. Diffuse reflectance spectrum of the Cs_3TbCl_6 NCs.

Table S5. Results of the fitting of the TRPL spectra of the Cs_3TbCl_6 NCs to a biexponential function. The TRPL measurements were conducted at room temperature, and the decay was monitored.

Excitation wavelength (nm)	Emission Wavelength (nm)	τ_1 (ns)	Proportion(%)	τ_2 (ns)	Proportion(%)	τ_3 (ns)	Proportion(%)
374	**430**	1.31	84	5.16	12	12.05	3

Excitation wavelength (nm)	Emission Wavelength (nm)	τ_1 (ms)	Proportion(%)	τ_2 (ms)	Proportion(%)
264	**550**	0.62	19	6.71	81

Table S6. Results of PL, PLE, PLQY, and lifetime of Cs_3TbCl_6 NCs under high and low energy excitations.

PL color	PLE l_{max} (nm)	PL l_{max} (nm)	PLQY (%)	Lifetime
Green PL	280	490, 548 (max), 583, 621	36.85	5.53 ms
Blue PL	355	430	3.49	2.16 ns

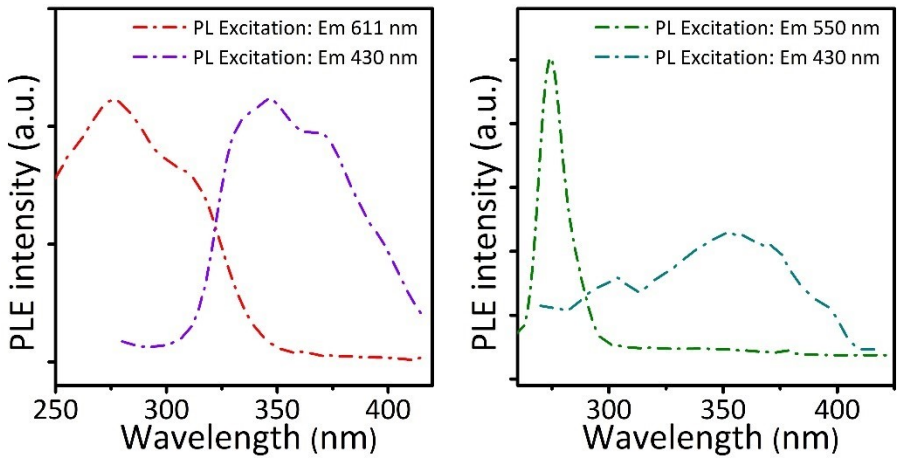

Figure S15. a) PLE spectra of Cs_3EuCl_6 NCs monitored at 611 and 430 nm. b) PLE spectra of Cs_3TbCl_6 NCs monitored at 550 and 430 nm.

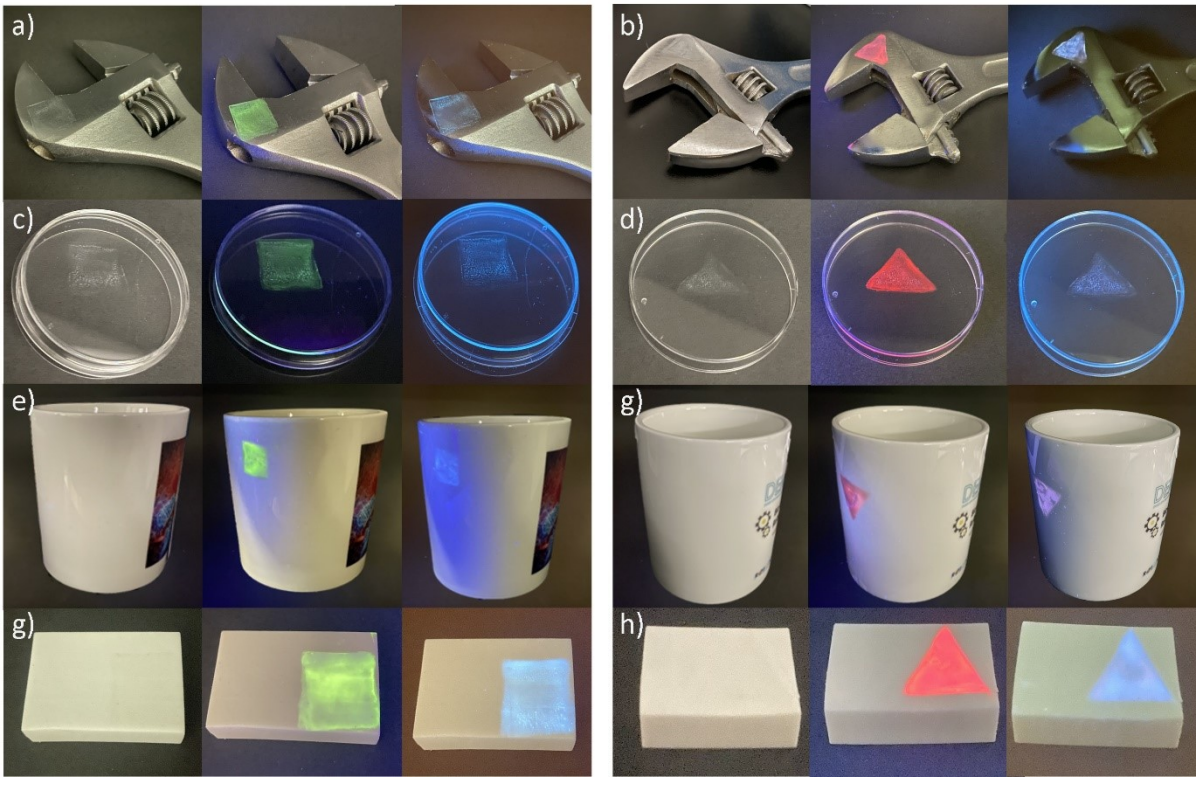

Figure S16. Photographs of transfer-printed NC films using a, c, e, g) Cs_3EuCl_6 NCs and b, d, g, h) Cs_3TbCl_6 NCs on steel, plastic, porcelain, and rubber substrates, respectively. Left) under daylight, middle) under 254 nm, and right) under 365 nm excitation.

References

1. a) H. J. Seifert, *J. Therm. Anal. Calorim.*, 2006, **83**, 479-505.
b) H. J. Seifert, H. Fink and B. Baumgartner, *J. Solid State Chem.*, 1993, **107**, 19-26.