

Supporting Information

Crystal structure and Photoluminescence tuning of novel single-phase phosphors $\text{Ca}_8\text{ZnLu}(\text{PO}_4)_7$: Eu^{2+} , Mn^{2+} for near-UV converted white light-emitting diodes

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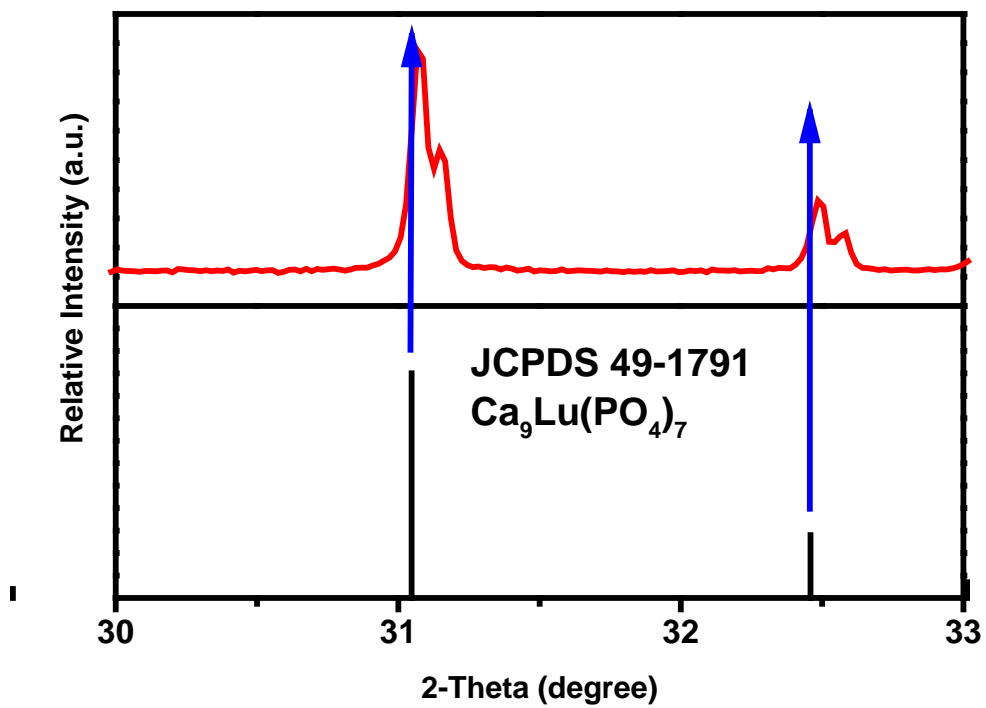


Figure S1. The magnified XRD pattern of CZLP host in the 2-theta range from 30° to 33°.

Table S1. Rietveld refinement data of the crystal structure of CZLP host.

atom	symmetry	Wyckoff	<i>x</i>	<i>y</i>	<i>z</i>	occu.	U (Å ²)
Ca1	18	b	0.142(1)	0.2874(6)	0.16667	0.7284	0.0462(9)
Ca2	18	b	0.2764(8)	0.149(1)	0.30000(2)	0.9578	0.0462(9)
Ca3	18	b	0.146(1)	0.2801(6)	0.0606(2)	0.9808	0.0462(9)
Zn1	18	b	0.142(1)	0.2874(7)	0.16667	0.1489	0.0462(9)
Zn5	6	a	0	0	0.2342(2)	0.552	0.0462(9)
Lu1	18	b	0.142(1)	0.2874(6)	0.16667	0.1227	0.0462(9)
Lu2	18	b	0.2764(8)	0.149(1)	0.30000(2)	0.0422	0.0462(9)
Lu3	18	b	0.146(1)	0.2801(6)	0.0606(2)	0.0192	0.0462(9)
Lu5	6	a	0	0	0.2342(2)	0.448	0.0462(9)
P1	6	a	0	0	0	1	0.036(2)
P2	18	b	0.350(1)	0.190(2)	0.2012(4)	1	0.036(2)
P3	18	b	0.318(1)	0.181(2)	0.0992(3)	1	0.036(2)
O1	18	b	0.351(2)	0.212(3)	0.2477(7)	1	0.020(2)
O2	18	b	0.010(3)	0.275(3)	0.3501(9)	1	0.020(2)
O3	18	b	0.432(2)	0.129(3)	0.1842(7)	1	0.020(2)
O4	18	b	0.202(2)	0.119(3)	0.1947(5)	1	0.020(2)
O5	18	b	-0.013(3)	0.269(3)	0.1143(7)	1	0.020(2)
O6	18	b	0.246(2)	0.250(3)	0.1177(8)	1	0.020(2)
O7	18	b	0.088(4)	0.157(2)	0.2722(5)	1	0.020(2)
O8	18	b	0.277(2)	0.165(2)	0.0593(5)	1	0.020(2)
O9	18	b	0.146(2)	-0.003(2)	0.4912(7)	1	0.020(2)
O10	6	a	0	0	0.0464(7)	1	0.020(2)

Table S2. Calculated and experimental crystal structural data of CZLP host. Coordinates of the crystallographic positions (in units of the lattice constants, (x, y, z) from left to right in one row) of all ions are given. The symbol “Z” stands for the number of chemical formula units in one conventional unit cell.

<i>R3c</i>		<i>CZLP</i>				
(No. 161)		<i>Calc.</i>	<i>Exp.</i>			
<i>a</i> , Å		10.20127				10.4195
<i>b</i> , Å		10.22330				10.4195
<i>c</i> , Å		36.74220				37.2880
α , °		89.62				90
β , °		90.15				90
γ , °		120.09				120
<i>V</i> , Å ³		3315.26				3505.9
<i>Z</i>		6				6
<i>M1</i> (18b)	0.12066	0.27053	0.16198	0.142	0.2874	0.16667
	-0.27361	-0.14358	0.16781	-0.2874	-0.1454	0.16667
	0.14388	-0.13386	0.16473	0.1454	-0.142	0.16667
	-0.18423	-0.39253	0.00246	-0.18793	-0.37927	3.33333E ⁻⁶
	-0.20147	0.19183	8.48445E ⁻⁴	-0.19133	0.18793	3.33333E ⁻⁶
	0.39521	0.20537	0.00146	0.37927	0.19133	3.33333E ⁻⁶
<i>M2</i> (18b)	-0.37672	-0.17505	-0.03122	-0.39027	-0.18433	-0.03333
	0.17573	-0.1988	-0.0335	0.18433	-0.20593	-0.03333
	0.20361	0.37818	-0.03455	0.20593	0.39027	-0.03333
	-0.45982	0.49027	0.13355	-0.46073	0.48233	0.13333
	-0.04795	0.4614	0.1331	-0.05693	0.46073	0.13333
	-0.49457	0.03881	0.1315	-0.48233	0.05693	0.13333
<i>M3</i> (18b)	0.13362	0.28436	0.06162	0.146	0.2801	0.0606
	-0.26971	-0.14226	0.06114	-0.2801	-0.1341	0.0606
	0.15433	-0.12262	0.06103	0.1341	-0.146	0.0606
	-0.19597	-0.3971	-0.10766	-0.19923	-0.38657	-0.10607
	-0.19838	0.20369	-0.1081	-0.18733	0.19923	-0.10607
	0.37542	0.2006	-0.10527	0.38657	0.18733	-0.10607
<i>M5</i> (6a)	0.37353	-0.29036	-0.1001	0.33333	-0.33333	-0.09913
	-0.33492	0.33002	0.06938	-0.33333	0.33333	0.06753
<i>P1</i> (6a)	-0.0012	-0.00141	0.00314	0	0	0
	-0.34577	0.31302	-0.16208	0	0	-0.5
<i>P2</i> (18b)	-0.32812	-0.15106	-0.13541	-0.31667	-0.14333	-0.13213
	0.13325	-0.17235	-0.1313	0.14333	-0.17333	-0.13213
	0.18282	0.32737	-0.13031	0.17333	0.31667	-0.13213
	-0.48496	-0.47098	0.03627	-0.49333	-0.47667	0.03453
	0.01841	0.49401	0.03621	0.01667	0.49333	0.03453
	0.47527	-0.01603	0.03622	0.47667	-0.01667	0.03453
<i>P3</i> (18b)	0.32412	0.18269	0.1004	0.318	0.181	0.0992
	-0.17725	0.14459	0.10037	-0.181	0.137	0.0992

	-0.14188	-0.32488	0.09891	-0.137	-0.318	0.0992
	-0.4757	-0.488	-0.0653	-0.47033	-0.48567	-0.06747
	-0.00557	0.48406	-0.06666	-0.01533	0.47033	-0.06747
	0.49141	0.01078	-0.06637	0.48567	0.01533	-0.06747
O1(18b)	-0.35982	-0.16838	-0.09417	-0.31567	-0.12133	-0.08563
	0.09033	-0.18874	-0.09103	0.12133	-0.19433	-0.08563
	0.18377	0.27322	-0.09161	0.19433	0.31567	-0.08563
	-0.47957	-0.4245	0.07565	-0.47233	-0.45467	0.08103
	0.05955	0.48409	0.0755	0.01767	0.47233	0.08103
	0.42207	-0.06458	0.0752	0.45467	-0.01767	0.08103
O2(18b)	0.33097	-0.05196	0.01384	0.34333	-0.05833	0.01677
	0.06079	0.39287	0.01362	0.05833	0.40167	0.01677
	-0.37179	-0.32468	0.01446	-0.40167	-0.34333	0.01677
	0.28386	0.28625	-0.15359	0.265	0.275	-0.1499
	-0.01261	-0.28187	-0.15277	0.01	-0.265	-0.1499
	-0.23742	0.01354	-0.14723	-0.275	-0.01	-0.1499
O3(18b)	-0.26388	-0.25025	-0.14808	-0.23467	-0.20433	-0.14913
	0.21217	-0.00832	-0.14448	0.20433	-0.03033	-0.14913
	0.02389	0.27101	-0.14577	0.03033	0.23467	-0.14913
	0.3548	0.44046	0.02061	0.36367	0.46233	0.01753
	0.08109	-0.34335	0.02153	0.09867	-0.36367	0.01753
	-0.43019	-0.08314	0.02147	-0.46233	-0.09867	0.01753
O4(18b)	0.17324	0.11181	0.18116	-0.46467	-0.21433	-0.13863
	0.24186	-0.23763	-0.1394	0.21433	-0.25033	-0.13863
	0.26238	-0.49527	-0.13333	0.25033	0.46467	-0.13863
	-0.40722	0.43045	0.02965	-0.41633	0.45233	0.02803
	-0.15829	0.42223	0.03012	-0.13133	0.41633	0.02803
	-0.42154	0.15996	0.03155	-0.45233	0.13133	0.02803
O5(18b)	-0.02171	0.2233	0.11968	-0.013	0.269	0.1143
	-0.21253	-0.24075	0.11736	-0.269	-0.282	0.1143
	0.24664	0.02143	0.11595	0.282	0.013	0.1143
	-0.08227	-0.44478	-0.0444	-0.05133	-0.39767	-0.05237
	-0.3457	0.09599	-0.05186	-0.34633	0.05133	-0.05237
	0.44078	0.35398	-0.04827	0.39767	0.34633	-0.05237
O6(18b)	0.27045	0.28873	0.1161	0.246	0.25	0.1177
	-0.28598	-0.01903	0.11307	-0.25	-0.004	0.1177
	0.02187	-0.27241	0.11085	0.004	-0.246	0.1177
	-0.31112	-0.39127	-0.05089	-0.32933	-0.41667	-0.04897
	-0.05428	0.32139	-0.05462	-0.08733	0.32933	-0.04897
	0.38915	0.07318	-0.05471	0.41667	0.08733	-0.04897
O7(18b)	0.41519	-0.15458	-0.05099	0.42133	-0.17633	-0.06113
	0.16818	-0.41679	-0.06204	0.17633	-0.40233	-0.06113
	0.43141	-0.40984	-0.05588	0.40233	-0.42133	-0.06113
	-0.23907	-0.49582	0.10749	-0.26433	0.49033	0.10553

	-0.25551	0.23793	0.10803	-0.24533	0.26433	0.10553
	0.49594	0.25664	0.1086	-0.49033	0.24533	0.10553
O8(18b)	0.29394	0.17012	0.05927	0.277	0.165	0.0593
	-0.14669	0.14103	0.05958	-0.165	0.112	0.0593
	-0.13834	-0.29634	0.05744	-0.112	-0.277	0.0593
	-0.4688	0.49789	-0.10674	-0.44533	0.49833	-0.10737
	-0.05202	0.47717	-0.10681	-0.05633	0.44533	-0.10737
	0.49142	-0.00339	-0.1081	-0.49833	0.05633	-0.10737
O9(18b)	0.46891	-0.35203	0.16145	0.47933	-0.33633	0.15787
	0.32461	-0.20981	0.1568	0.33633	-0.18433	0.15787
	0.18047	0.49772	0.15757	0.18433	-0.47933	0.15787
	-0.14478	1.05355E-4	-0.00955	-0.149	-0.003	-0.0088
	0.14298	0.13879	-0.01104	0.146	0.149	-0.0088
	-0.01117	-0.15157	-0.0101	0.003	-0.146	-0.0088
O10(6a)	0.00227	-0.00275	0.0451	0	0	0.0464
	-0.35616	0.31181	-0.11986	-0.33333	0.33333	-0.12027

Notes: The Zn and Lu atoms in *M1* site for the calculated structural configuration are located in the crystallographic general positions 1 and 4, respectively, whereas those in *M5* site stay in the positions 2 and 1.

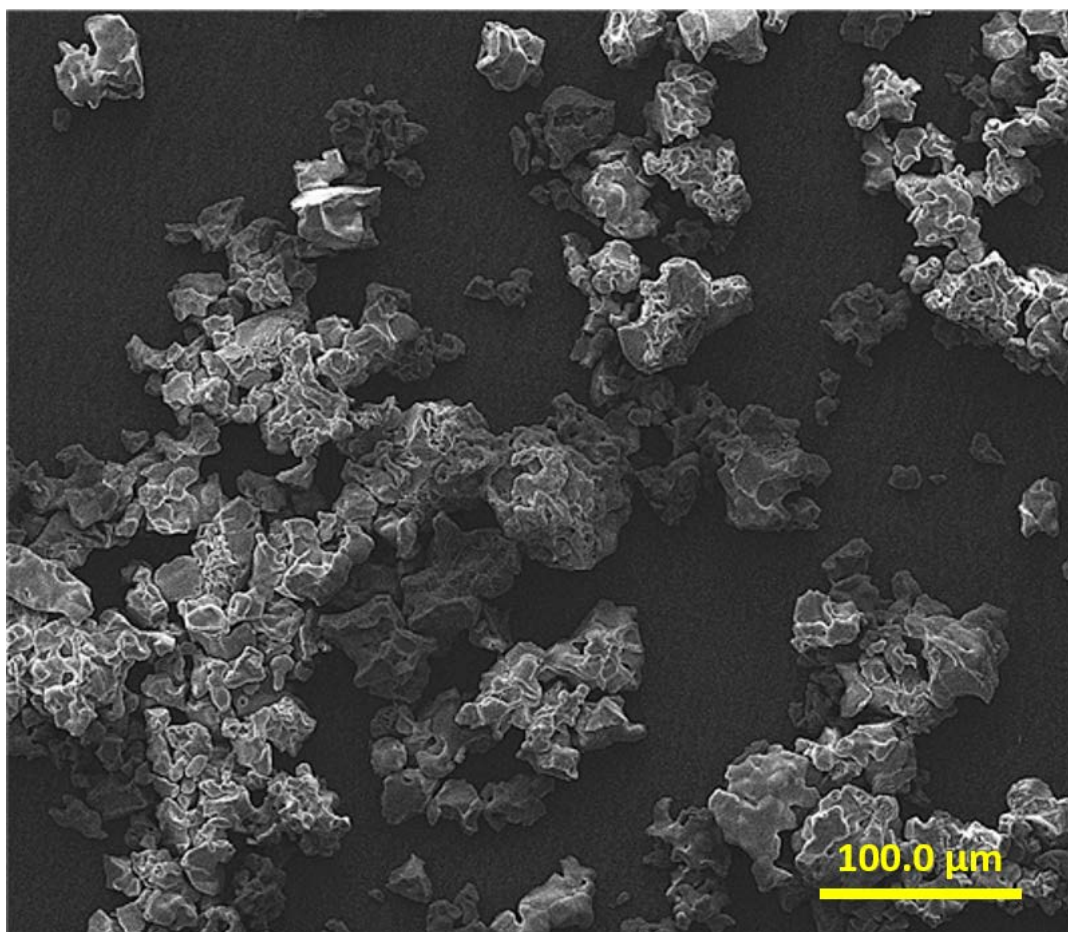


Figure S2. SEM image of CZLP: 0.03Eu²⁺.

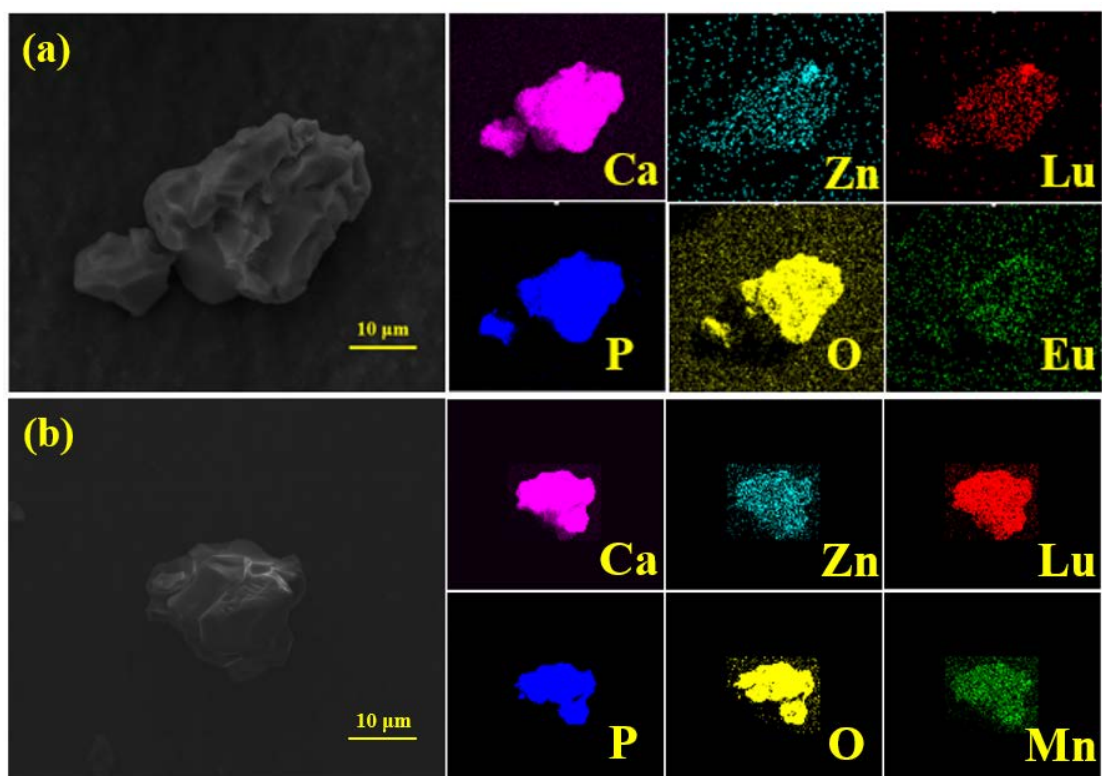


Figure S3. Element mappings of (a) CZLP: 0.03Eu²⁺ and (b) CZLP: 0.20Mn²⁺.

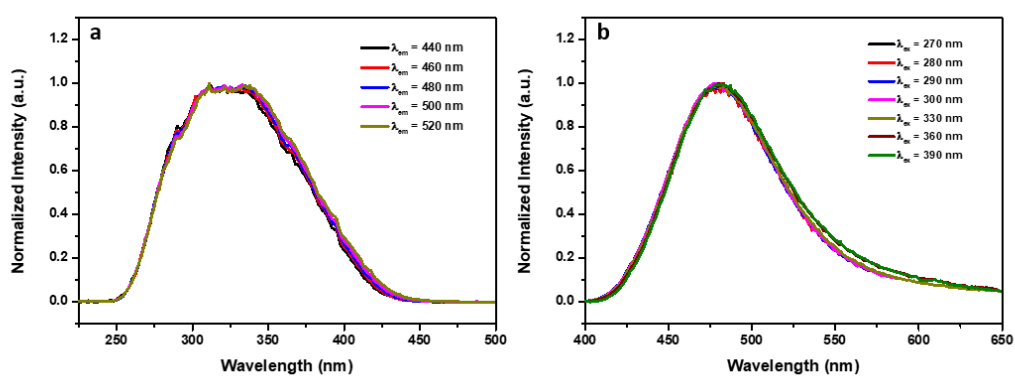


Figure S4. (a) Excitation (λ_{em} = 440, 460, 480, 500 and 520 nm) and (b) emission spectra (λ_{ex} = 270, 280, 290, 300, 330, 360 and 390 nm) of CZLP: 0.03Eu²⁺ at RT.

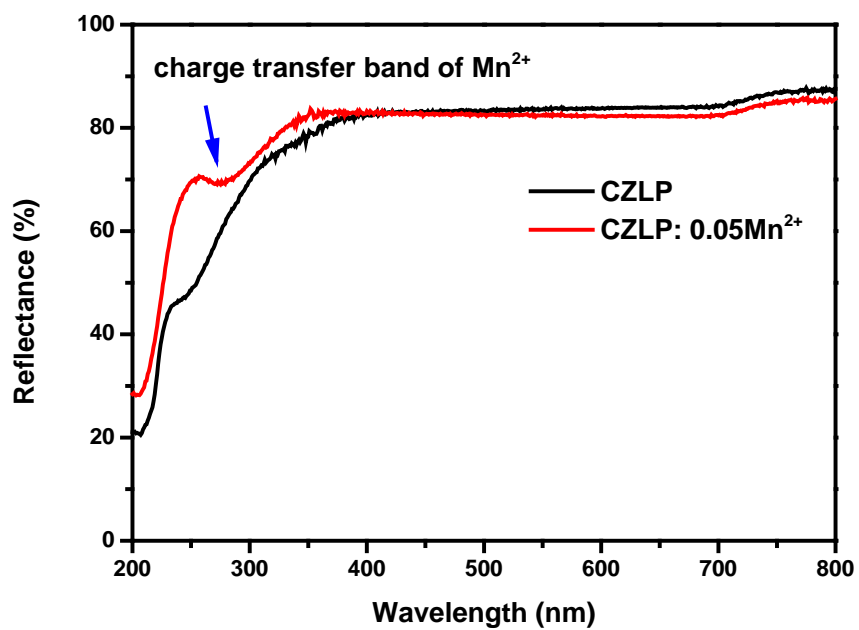


Figure S5. Diffuse reflectance spectra of CZLP and CZLP: 0.05Mn²⁺

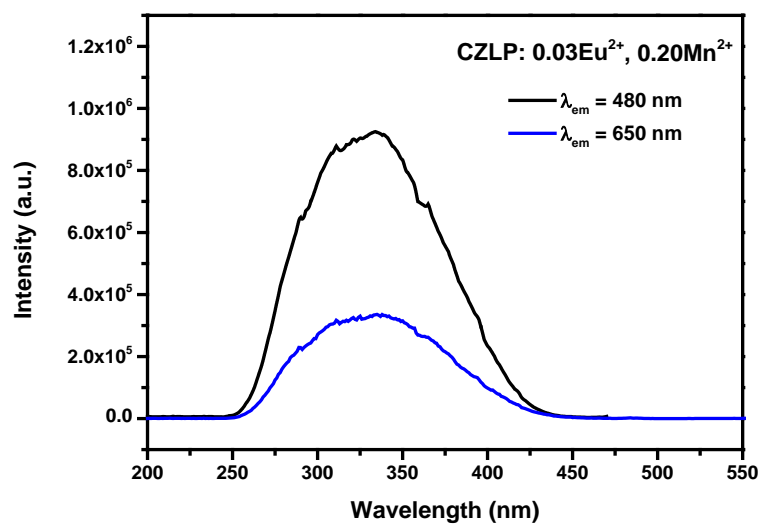


Figure S6. Excitation spectra of CZLP: 0.03Eu²⁺, 0.20Mn²⁺ monitored at 480 nm and 650 nm.

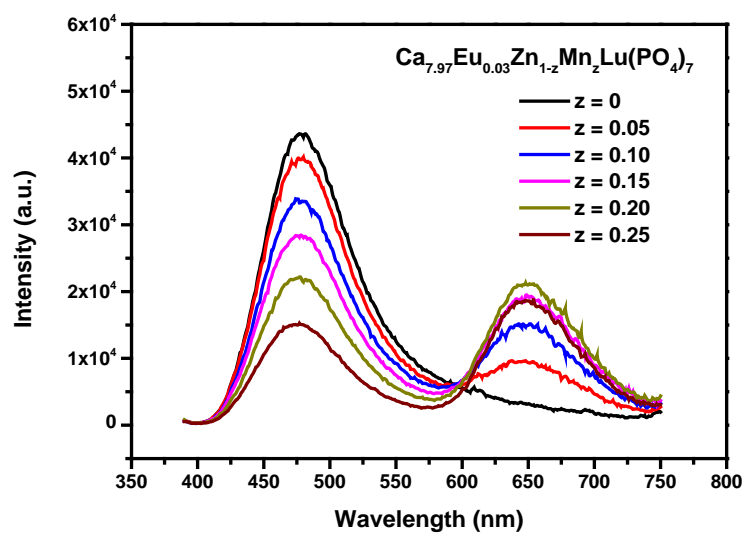


Figure S7. Emission spectra of CZLP: 0.03Eu²⁺, zMn²⁺ (z = 0, 0.05, 0.10, 0.15, 0.20 and 0.25) measured at RT.

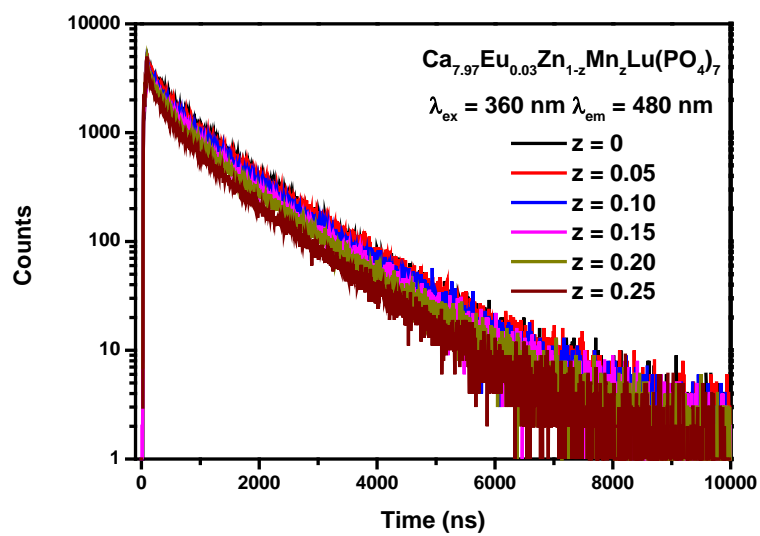


Figure S8. Luminescence decay curves of CZLP: 0.03Eu²⁺, zMn²⁺ (z = 0, 0.05, 0.10, 0.15, 0.20 and 0.25) measured at RT.

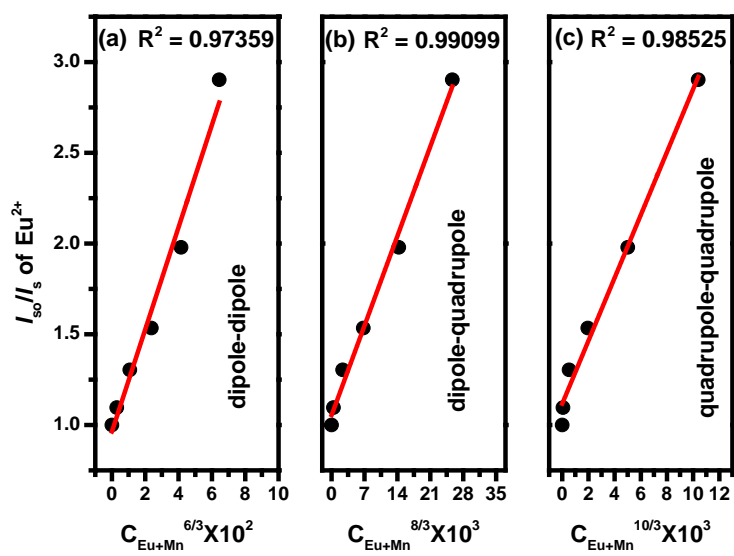


Figure S9. Dependence I_{so}/I_s of Eu^{2+} on $C^{n/3}$ ($n = 6, 8$ and 10).

Table S3. Chromatic coordinates (x, y) of $\text{Eu}^{2+}/\text{Mn}^{2+}$ singly-doped and co-doped CZLP.

Point	sample	Chromaticity coordinates
1	CZLP: 0.03Eu^{2+}	(0.186, 0.292)
2	CZLP: 0.20Mn^{2+}	(0.677, 0.323)
3	CZLP: $0.03\text{Eu}^{2+}, 0.05\text{Mn}^{2+}$	(0.215, 0.272)
4	CZLP: $0.03\text{Eu}^{2+}, 0.10\text{Mn}^{2+}$	(0.247, 0.275)
5	CZLP: $0.03\text{Eu}^{2+}, 0.15\text{Mn}^{2+}$	(0.272, 0.273)
6	CZLP: $0.03\text{Eu}^{2+}, 0.20\text{Mn}^{2+}$	(0.302, 0.273)
7	CZLP: $0.03\text{Eu}^{2+}, 0.25\text{Mn}^{2+}$	(0.327, 0.267)