Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

SUPPORTING INFORMATION

Tuning Luminescence from NIR-I to NIR-II in Cr^{3+}-doped Olivine Phosphors for Nondestructive Analysis

Hao Cai, Shengqiang Liu, Zhen Song*, Quanlin Liu*

The Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Science & Engineering, University of Science and Technology Beijing, Beijing 100083, China.

* Corresponding Author: E-mail address: qlliu@ustb.edu.cn (Quanlin Liu)

* Corresponding Author: E-mail address: zsong@ustb.edu.cn (Zhen Song)

Table S1. The refined structural parameters of Mg_2GeO_4:1% Cr^{3+}.

Space group		Pnma	**Symmetry**		orthorhombic
Cell parameters		a = 10.3049 Å, b = 6.0261 Å, c = 4.9097 Å, V = 304.887 Å^3			
Reliability factors		R_p = 8.47 %, R_{wp} = 14.0 %, R_{exp} = 8.83 %, χ^2 = 2.50			
Atom	**Site**	**x**	**y**	**z**	**Occ.**
Mg1	4a	0.000(0)	0.000(0)	0.000(0)	1.000
Mg2	4c	0.275(5)	0.250(0)	0.992(9)	1.000
Ge	4c	0.094(7)	0.250(0)	0.436(2)	1.000
O1	4c	0.093(5)	0.250(0)	0.789(3)	1.000
O2	4c	0.438(2)	0.250(0)	0.230(2)	1.000
O3	8d	0.164(7)	0.020(9)	0.268(5)	1.000

Table S2. The refined structural parameters of $LiScGeO_4$:1% Cr^{3+}.

Space group		Pnma	**Symmetry**		orthorhombic
Cell parameters		a = 10.6662 Å, b = 5.9874 Å, c = 4.9674 Å, V = 317.235 $Å^3$			
Reliability factors		R_p = 12.9 %, R_{wp} = 18.6 %, R_{exp} = 11.17 %, χ^2 = 2.77			
Atom	**Site**	**x**	**y**	**z**	**Occ.**
Li	4a	0.000(0)	0.000(0)	0.000(0)	1.000
Sc	4c	0.269(9)	0.250(0)	0.002(5)	1.000
Ge	4c	0.090(7)	0.250(0)	0.448(5)	1.000
O1	4c	0.097(8)	0.250(0)	0.801(8)	1.000
O2	4c	0.441(5)	0.250(0)	0.197(8)	1.000
O3	8d	0.170(2)	0.033(5)	0.285(1)	1.000

Table S3. Detailed bond length information of Mg_2GeO_4 (ICSD-41415).

	Bond length (Å)	Average (Å)		Bond length (Å)	Average (Å)		Bond length (Å)	Average (Å)
Mg1-O1	2.053		Mg2-O1	2.16		Ge-O1	1.74	
Mg1-O1	2.053		Mg2-O2	2.08				
Mg1-O2	2.08		Mg2-O3	2.05		Ge-O2	1.77	
		2.094			2.150			1.742
Mg1-O2	2.08		Mg2-O3	2.05		Ge-O3	1.73	
Mg1-O3	2.15		Mg2-O3	2.29				
Mg1-O3	2.15		Mg2-O3	2.29		Ge-O3	1.73	

Table S4. Detailed bond length information of $LiScGeO_4$ (ICSD-62481).

	Bond length (Å)	Average (Å)		Bond length (Å)	Average (Å)		Bond length (Å)	Average (Å)
Li-O1	2.086		Sc-O1	2.125		Ge-O1	1.732	
Li-O1	2.086		Sc-O2	2.069				
Li-O2	2.204		Sc-O3	2.08		Ge-O2	1.734	
		2.209			2.124			1.756
Li-O2	2.204		Sc-O3	2.08		Ge-O3	1.779	
Li-O3	2.337		Sc-O3	2.196				
Li-O3	2.337		Sc-O3	2.196		Ge-O3	1.779	

Table S5. The FWHM information of 600-1000 nm band in excitation spectra.

x	$\lambda_{I\text{-}0.5(left)}$ (nm)	$\lambda_{I\text{-}0.5(right)}$ (nm)	ΔE (eV)
0	578	756	0.51
0.1	584	766	0.50
0.2	588	774	0.51
0.3	593	785	0.51
0.4	599	794	0.51
0.5	602	803	0.52
0.6	607	811	0.51
0.7	611	814	0.51
0.8	622	832	0.50
0.9	625	848	0.52
1.0	634	858	0.51

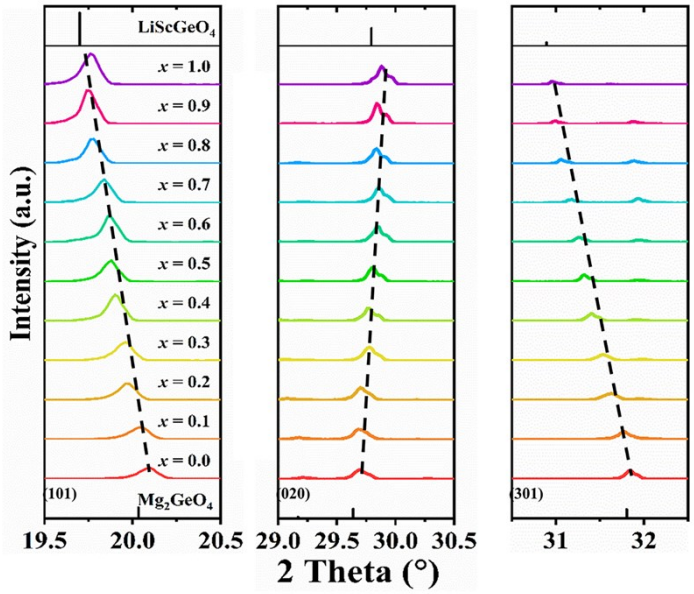

Fig. S1. 2 theta value of (101), (020) and (301) planes with the x value changing from 0 to 1.

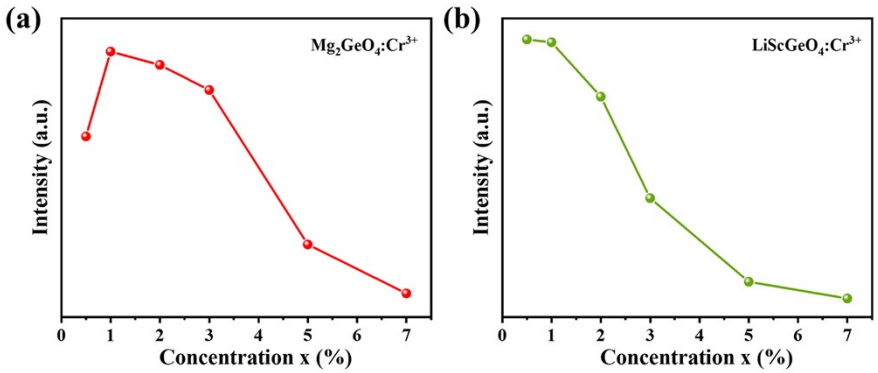

Fig. S2. The concentration dependent experiment of Mg_2GeO_4 and $LiScGeO_4$ (λ_{ex} = 465 nm).

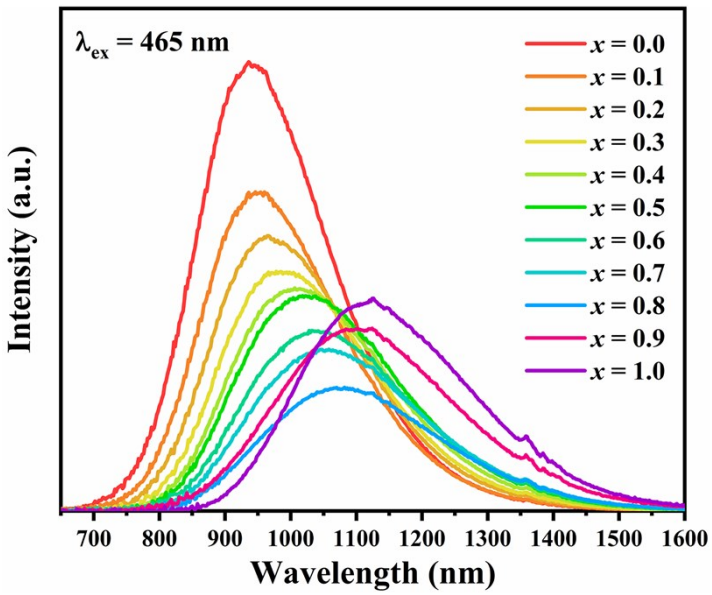

Fig. S3. PL spectra of $(Mg_{1-x}Li_x)(Mg_{1-x}Sc_x)GeO_4$:1%$Cr^{3+}$ with different compositions.

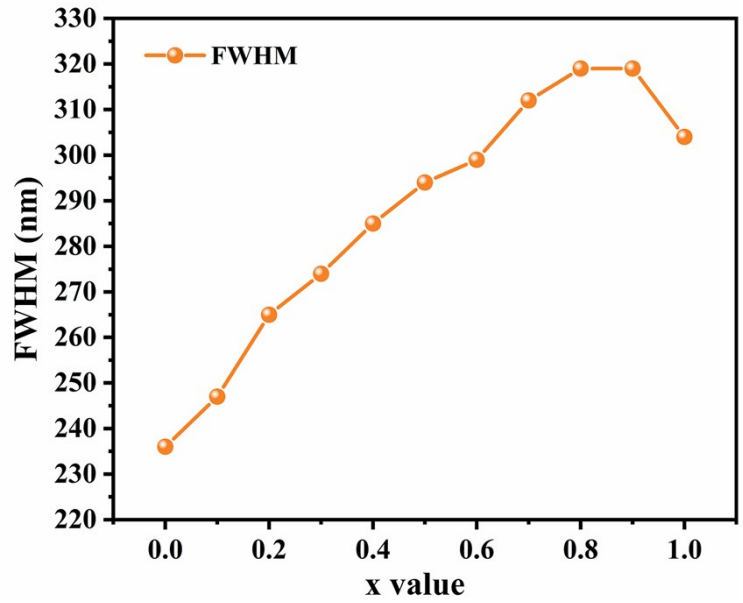

Fig. S4. FWHM of $(Mg_{1-x}Li_x)(Mg_{1-x}Sc_x)GeO_4$:1%$Cr^{3+}$ with different compositions.

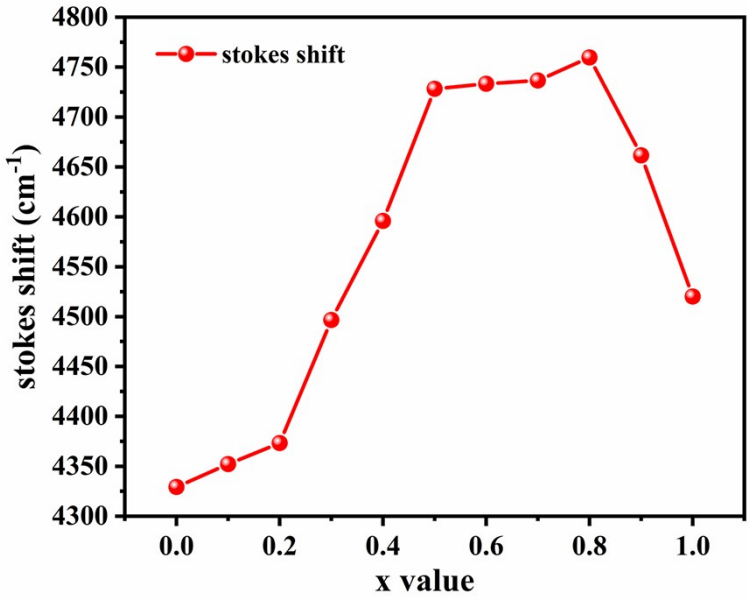

Fig. S5. Stokes shift of $(Mg_{1-x}Li_x)(Mg_{1-x}Sc_x)GeO_4$:1%$Cr^{3+}$ with different compositions.

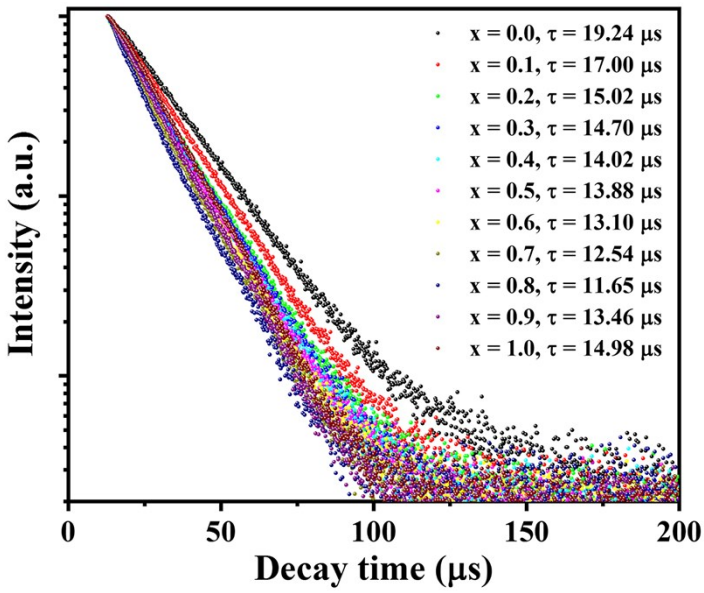

Fig. S6. Lifetimes of series of $(Mg_{1-x}Li_x)(Mg_{1-x}Sc_x)GeO_4$:1% Cr^{3+} phosphors (Monitored under their optimal excitation and emission wavelength).