

Supporting information

Ab Initio Two-sites Occupancy and Broadband Near-Infrared

Emission of Cr³⁺ in Li₂MgZrO₄

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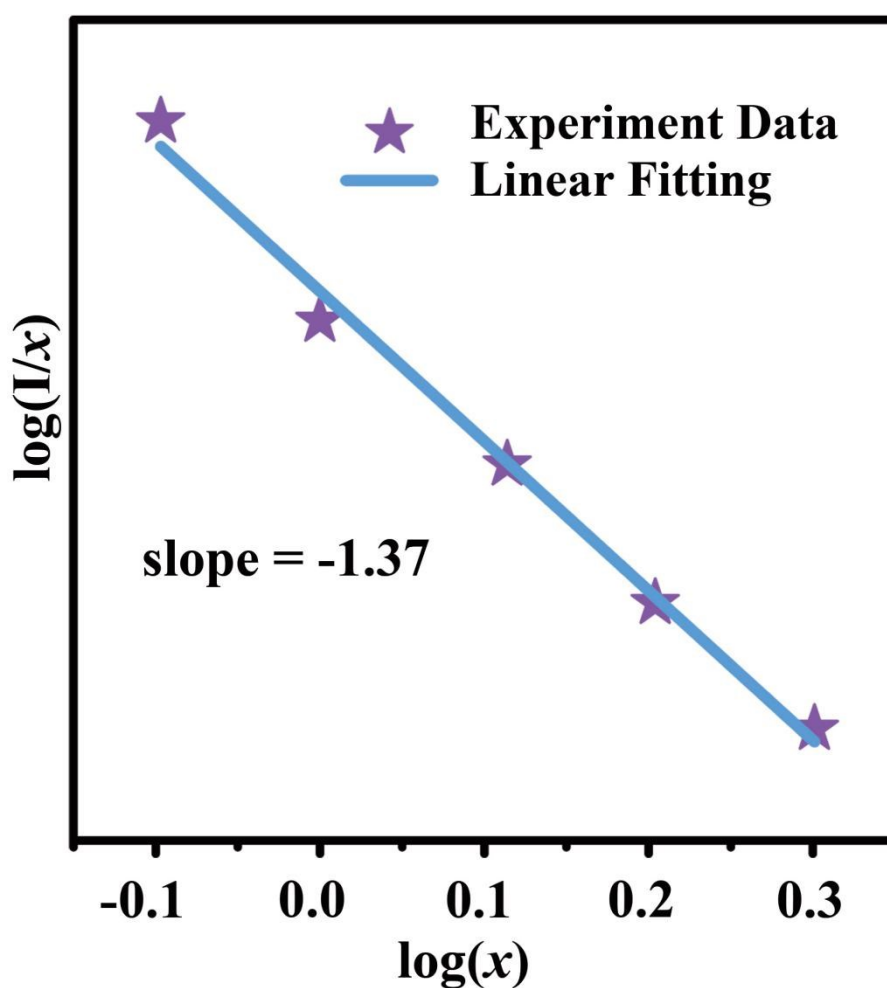


Figure S1. The dependence of $\log(I/x)$ on $\log(x)$ of the LMZ: $x\text{Cr}^{3+}$ phosphors.

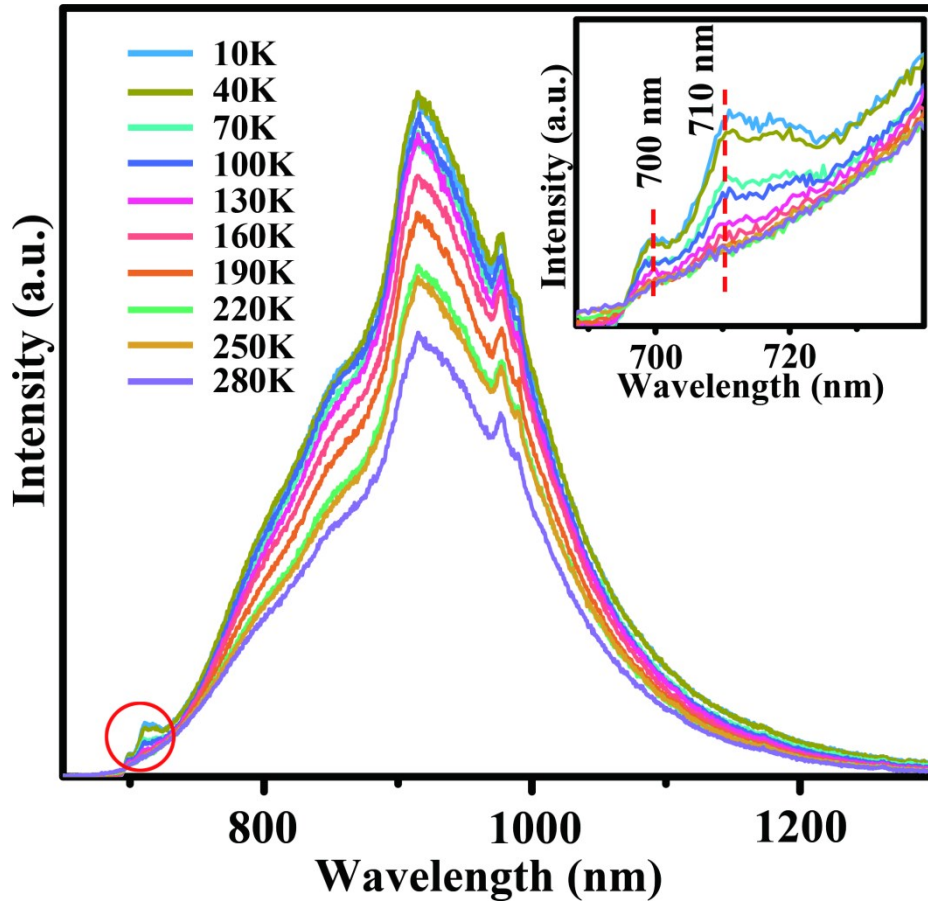


Figure S2. Temperature-dependent PL spectra of LMZ: 0.8%Cr³⁺ upon 470 nm excitation.

Table S1. Structure Parameters of Li₂MgZrO₄ from Crystallographic Information File (CIF).

			<i>x</i>	<i>y</i>	<i>z</i>	<i>Occ.</i>	<i>U</i>	<i>Site</i>	<i>Sym.</i>
1	<i>O</i>	<i>O1</i>	0.00000	0.25000	0.10800	1.000	0.015	8e	2mm
2	<i>Zr</i>	<i>Zr1</i>	0.00000	0.75000	0.12500	0.500	0.023	4a	-4m2
3	<i>Mg</i>	<i>Mg1</i>	0.00000	0.75000	0.12500	0.500	0.023	4a	-4m2
4	<i>Li</i>	<i>Li1</i>	0.00000	0.25000	0.37500	1.000	0.000	4b	-4m2