

SUPPORTING INFORMATION

Consequence of Optimal Bonding on Cation Ordering and Enhanced Near-Infrared Luminescence in Cr³⁺-doped Pyroxene Oxides

Hongzhen Liu, Fangyi Zhao, Hao Cai, Zhen Song*, and 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: qliu@ustb.edu.cn (Quanlin Liu)

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

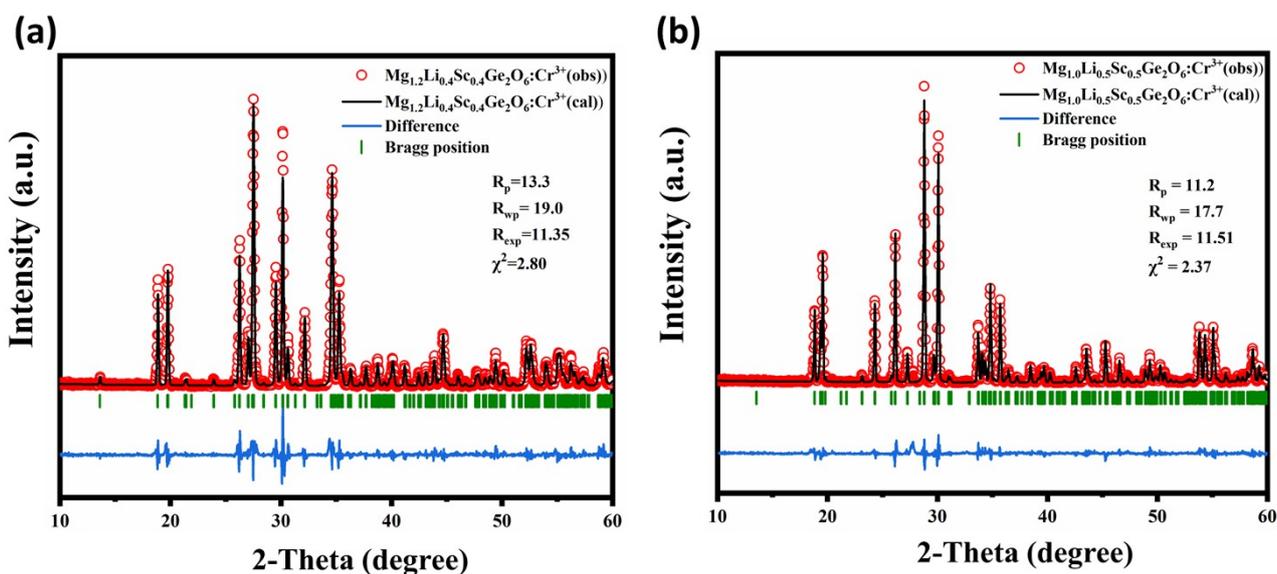


Fig. S1. (a)-(b) Rietveld refinement results of the synthesized $(\text{Mg}_{0.6}\text{Li}_{0.4})(\text{Mg}_{0.6}\text{Sc}_{0.4})\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$ and $(\text{Mg}_{0.5}\text{Li}_{0.5})(\text{Mg}_{0.5}\text{Sc}_{0.5})\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$, respectively.

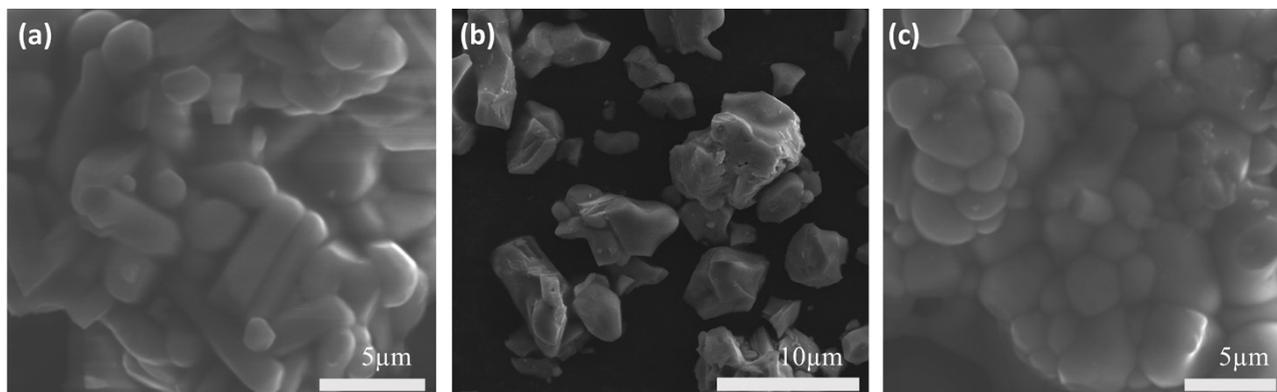


Fig. S2. (a)-(c) SEM images of the synthesized $\text{Mg}_2\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}, 4\%\text{Li}^+$, $\text{LiScGe}_2\text{O}_6:4\%\text{Cr}^{3+}$ and $(\text{Mg}_{0.6}\text{Li}_{0.4})(\text{Mg}_{0.6}\text{Sc}_{0.4})\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$, respectively.

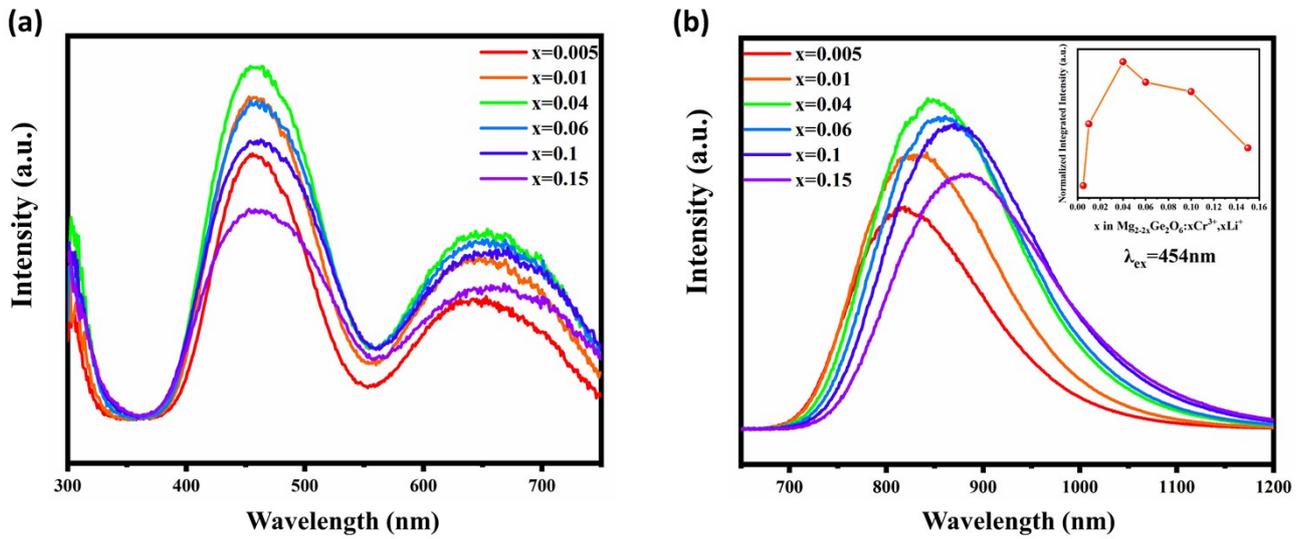


Fig. S3. (a) PLE spectra of $\text{Mg}_{2-2x}\text{Ge}_2\text{O}_6:x\text{Cr}^{3+},x\text{Li}^+$ ($x = 0.005-0.15$) samples under the optimum emission wavelength of each sample. (b) PL spectra of $\text{Mg}_{2-2x}\text{Ge}_2\text{O}_6:x\text{Cr}^{3+},x\text{Li}^+$ ($x = 0.005-0.15$) samples under the 454 nm excitation.

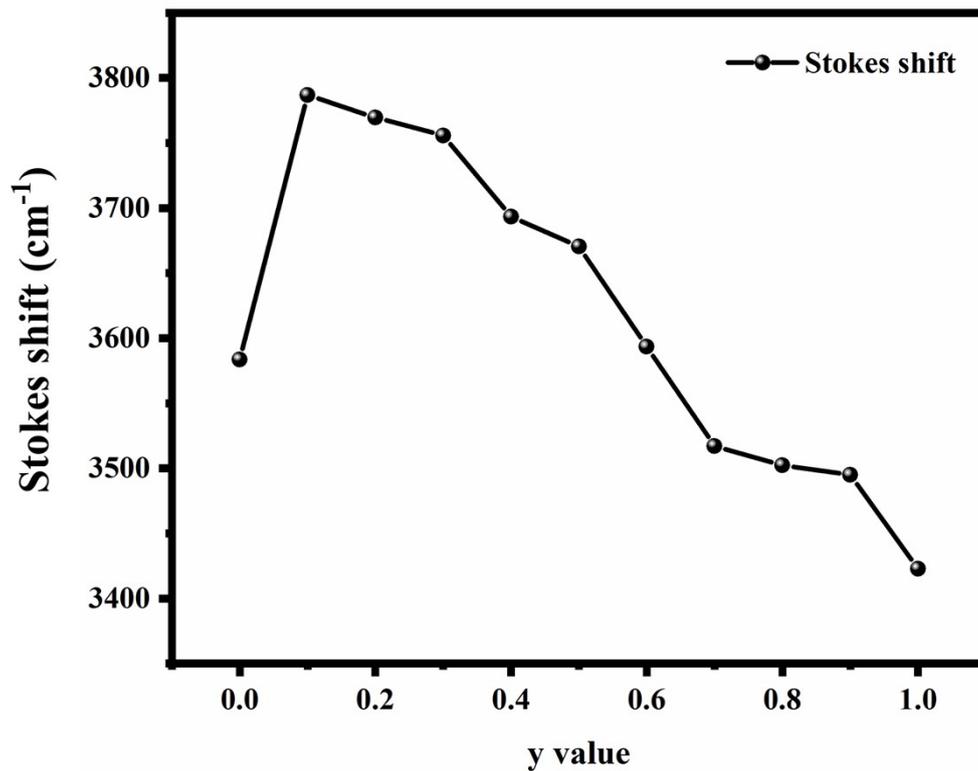


Fig. S4. Stokes shift of $(\text{Mg}_{1-y}\text{Li}_y)(\text{Mg}_{1-y}\text{Sc}_y)\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$ ($y = 0-1$) samples with different compositions.

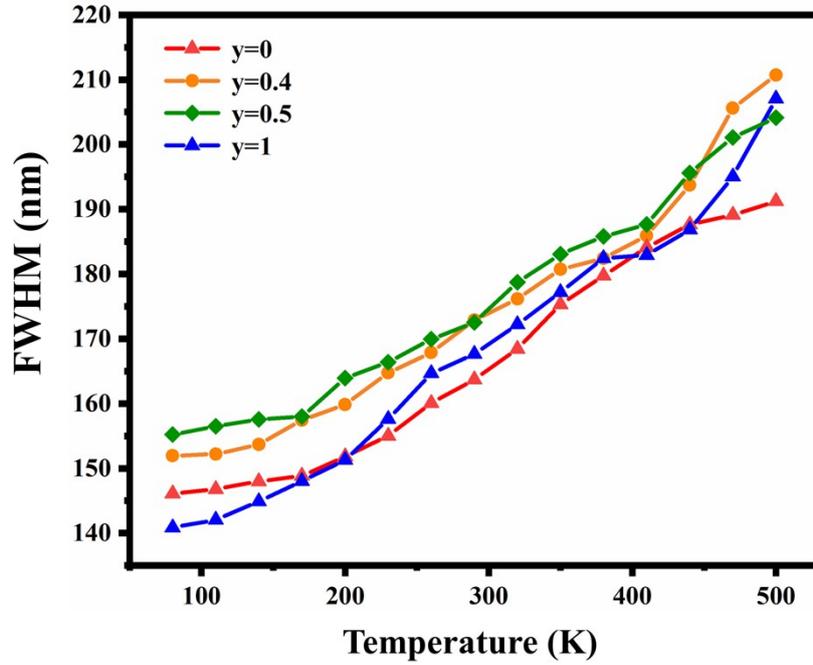


Fig. S5. FWHM vs temperature of the $(\text{Mg}_{1-y}\text{Li}_y)(\text{Mg}_{1-y}\text{Sc}_y)\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$ ($y = 0, 0.4, 0.5, 1$) samples.

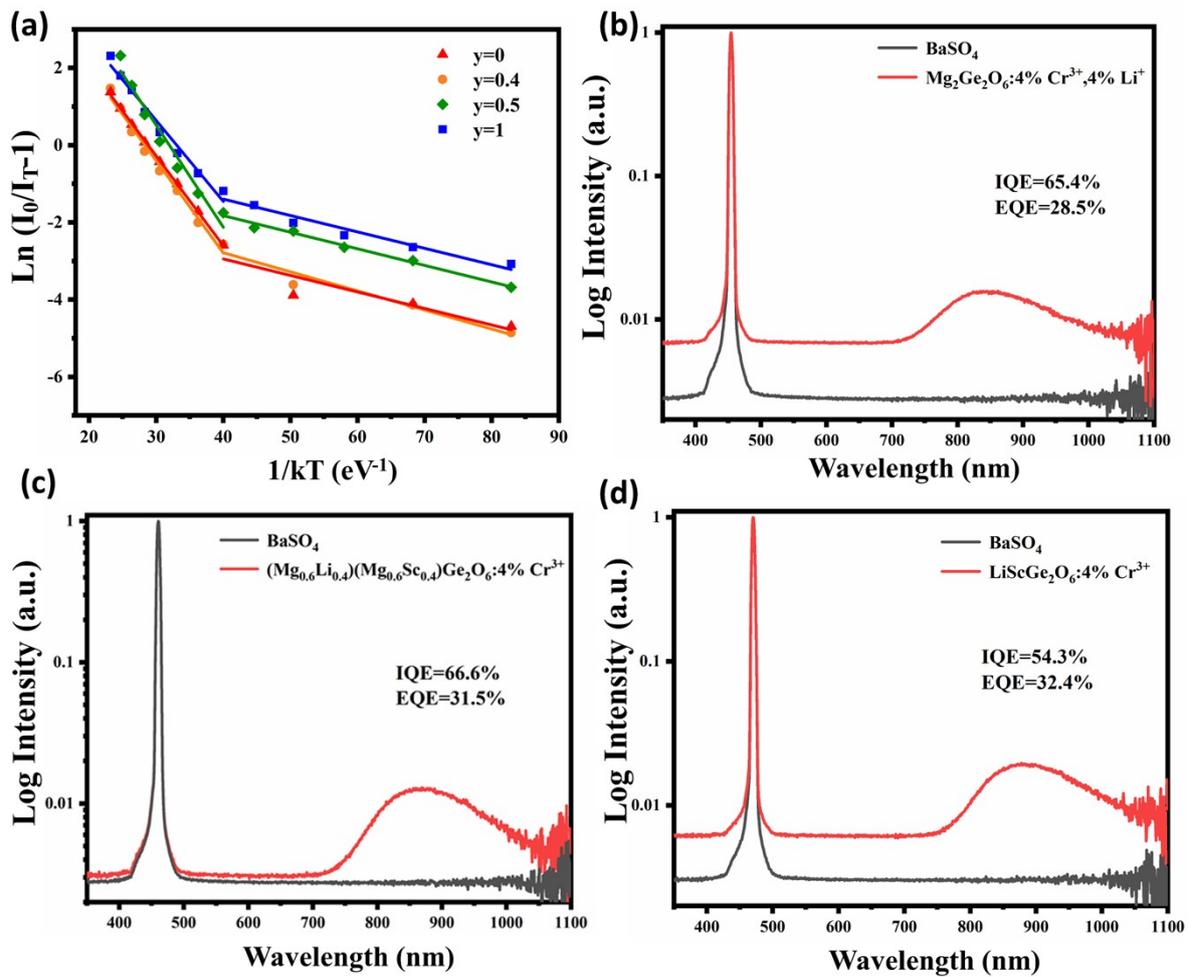


Fig. S6. (a) Plots of $\ln(I_0/I_T - 1)$ versus $1/kT$ of the $(\text{Mg}_{1-y}\text{Li}_y)(\text{Mg}_{1-y}\text{Sc}_y)\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$ ($y = 0, 0.4, 0.5, 1$) samples. (b)-(d) Normalized PL spectra with BaSO_4 as the reference under the 454, 470 and 460 nm excitation for quantum efficiency measurements of $\text{Mg}_2\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}, 4\%\text{Li}^+$, $(\text{Mg}_{0.6}\text{Li}_{0.4})(\text{Mg}_{0.6}\text{Sc}_{0.4})\text{Ge}_2\text{O}_6:4\%\text{Cr}^{3+}$ and $\text{LiScGe}_2\text{O}_6:4\%\text{Cr}^{3+}$ respectively.