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Distorted–octahedral site–occupation induced high efficiency broadband near infrared emission in $LiScGe_2O_6:Cr^{3+}$ phosphor

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The Supporting information contains 5 pages, including 3 Figures (Figure S1, S2 and S3) , 1 Table (Table S1) and Reference.

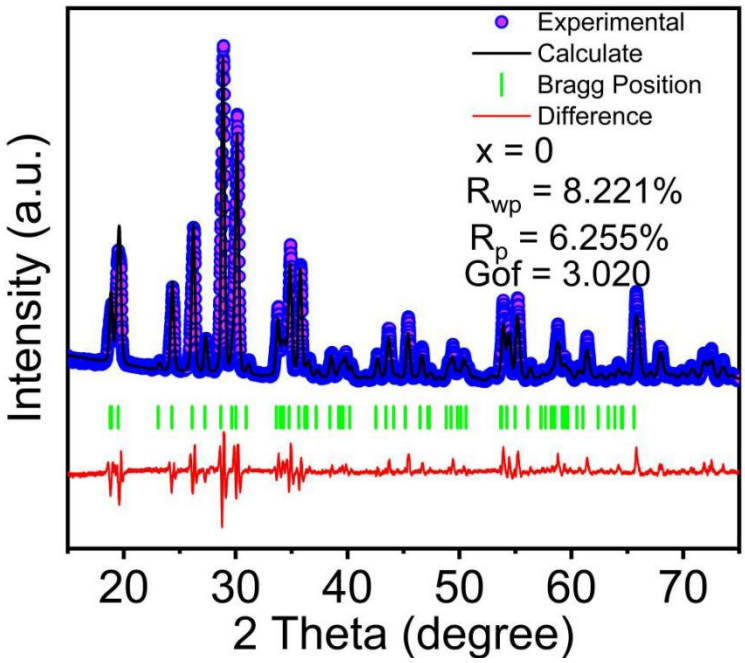

Figure S1. Rietveld refinement and experimental XRD pattern of $LiScGe_2O_6$.

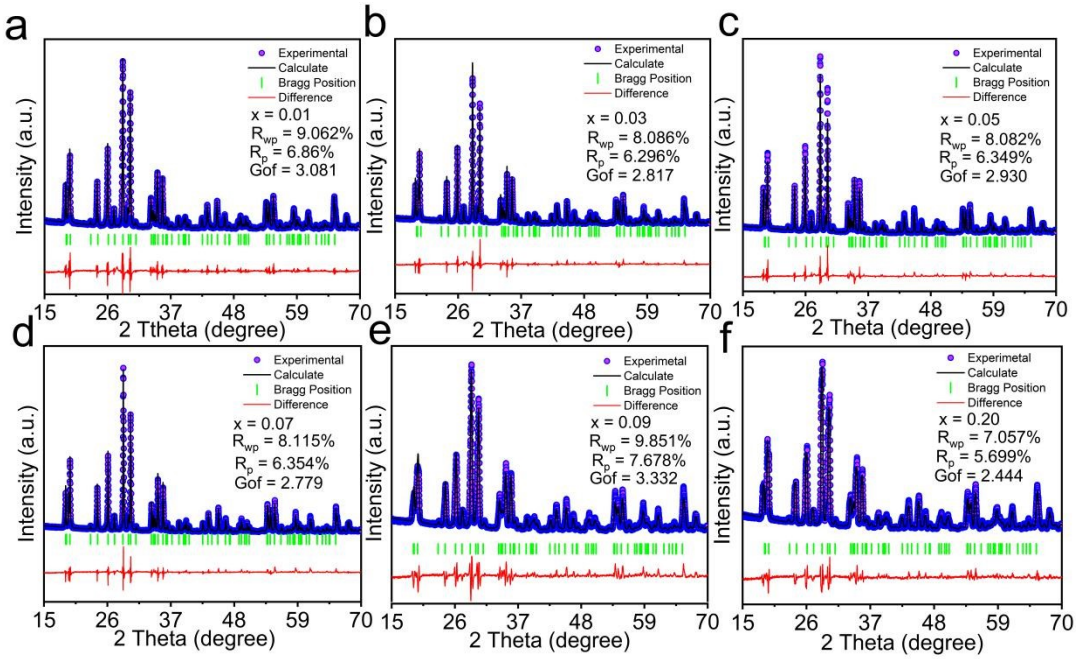

Figure S2. Rietveld refinement and experimental XRD patterns of $LiSc_{1-x}Ge_2O_6$:xCr^{3+}(x = 0.01-0.2).

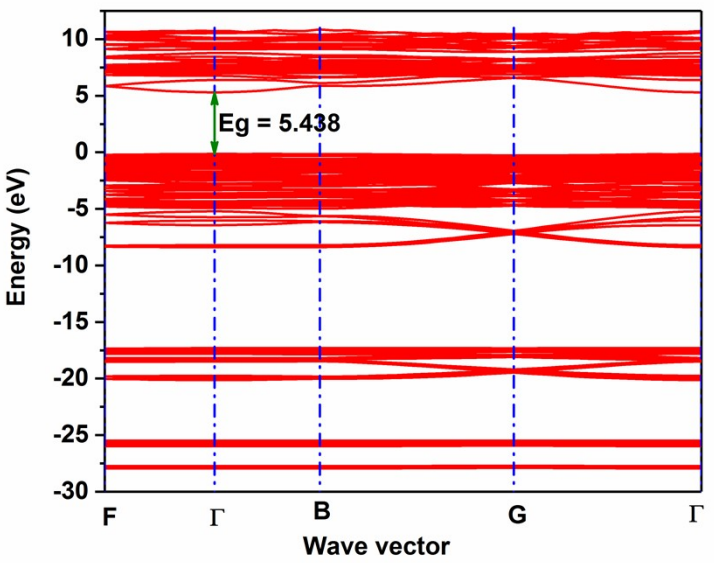

Figure S3. Band structure of $LiScGe_2O_6$.

Computational Methodology: The band structure of this compound in this study were performed using the projector augmented-wave (PAW) method [1, 2] as implemented in the Vienna ab initio simulation package (VASP) code.[3] The cutoff energy Ecut and k-point mesh were set as 499.034 eV and the 1 × 1 × 1 Monkhorst-Pack grid, respectively. The convergence criterion for the electronic energy was 10-5 eV, whereas the structures were relaxed until the Hellmann-Feynman forces were smaller than 0.02 eV Å−1. The HSE06 hybrid functional was applied in all the calculations.[4]

Reference:

[1] G.Kresse, J. Furthmüller, *Phys. Rev. B* 1999, **59**, 1758.

[2] G. Kresse, J. Furthmüller, *Phys. Rev. B* 1996, **54**, 11169.

[3] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.

[4] Y.-I. Matsushita, K. Nakamura, and A. Oshiyama, *Phys. Rev. B* 2011, 84, 075205.

Table S1. Structural parameters of the $LiScGe_2O_6$:xCr^{3+} (x = 0-0.20) samples based on the Rietveld refinement of the XRD patterns**.**

Parameter / x	a (Å)	b (Å)	c (Å)	α/γ(°)	β(°)	V (Å^3)
0	5.4637	9.1017	9.6890	90	102.9345	469.5944
0.01	5.4620	9.0963	9.6863	90	102.9452	469.0198
0.03	5.4563	9.0822	9.6776	90	102.9564	467.3659
0.05	5.4520	9.0692	9.6700	90	102.9654	465.9469
0.07	5.4562	9.0733	9.6786	90	102.9716	466.9172
0.09	5.4548	9.0648	9.6771	90	102.9784	466.2728
0.20	5.4773	9.0084	9.6473	90	103.0239	460.3812