

## Electronic Supplementary Information

# Disentangling Site Occupancy, Cation Regulation, and Oxidation State Regulation of the Near Infrared Emission in Chromium Doped SrGa<sub>4</sub>O<sub>7</sub> Phosphor

Jun'an Lai<sup>1</sup>, Jianbei Qiu<sup>1,2\*</sup>, Qi Wang<sup>1</sup>, Dacheng Zhou<sup>1,2</sup>, Zhangwen Long<sup>1</sup>, Yong

Yang<sup>1,2</sup>, Songhan Hu<sup>1</sup>, Xizheng Li<sup>1</sup>, Jiacheng Pi<sup>1</sup>, Jing Wang<sup>3\*</sup>

<sup>1</sup> College of Materials Science and Engineering, Kunming University of Science and  
Technology, Kunming 650093, China

<sup>2</sup> Key Lab. of Advanced Materials of Yunnan Province, Kunming 650093, China

<sup>3</sup> Sun Yat Sen Univ, Sch Chem, Sch Mat Sci & Engn, Guangzhou 510275, China

\*Corresponding author: Jianbei Qiu, E-mail address: [qiu@kmust.edu.cn](mailto:qiu@kmust.edu.cn)

Jing Wang, E-mail address: [ceswj@mail.sysu.edu.cn](mailto:ceswj@mail.sysu.edu.cn)

Tel:+86-871-5188856; Fax: +86-875-5188856

Table S1 1. Structural parameters for LZSO refined by Rietveld analysis of powder XRD at room temperature

Atom	Wyck	g	x	y	z
Ga1	8f	1	0.43975	0.24144	0.43975
Ga2	8f	1	0.0887	0.20044	0.0887
O1	8f	1	0.06243	0.092	0.06243
O2	8f	1	0.44824	0.05579	0.44824
O3	8f	1	0.25	0.35114	0.25
O4	4e	1	0	0.03518	0.25
Sr	4e	1	0	0.31172	0.25

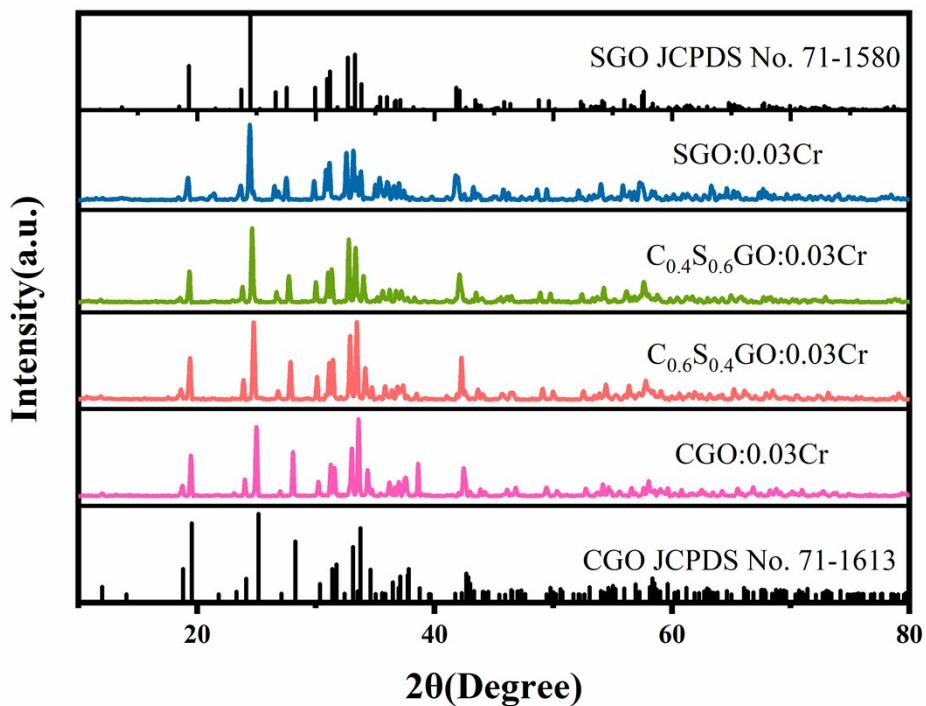


Figure S1 The XRD patterns of  $\text{Sr}(1-y)\text{Ca}(y)\text{Ga}_4\text{O}_7: 0.03\text{Cr}$  ( $y = 0, 0.2, 0.4, 0.6, 0.8, 1$ ) samples.

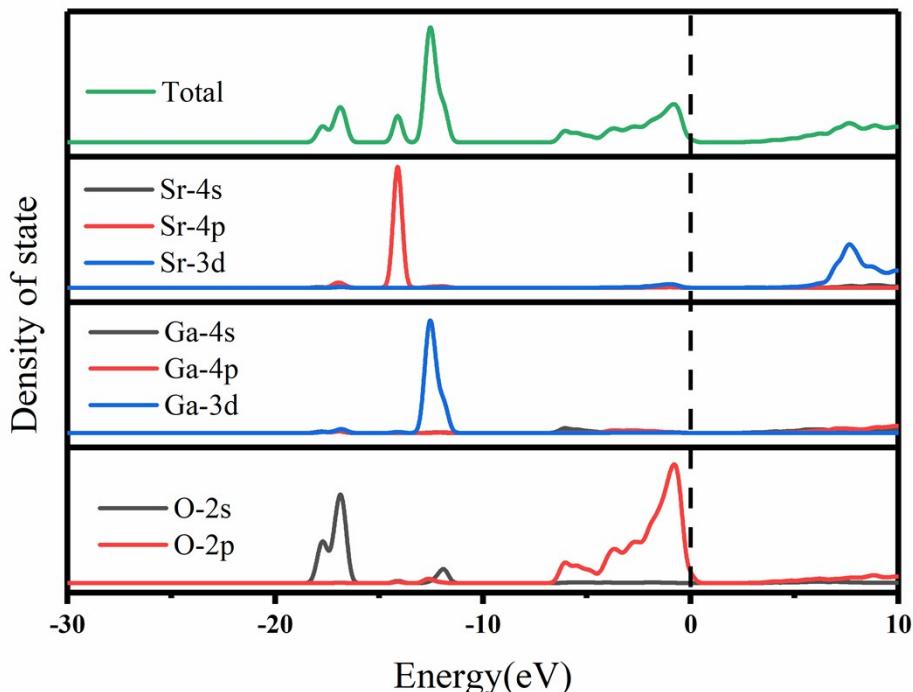


Figure S2 The total and partial DOSs of SGO.

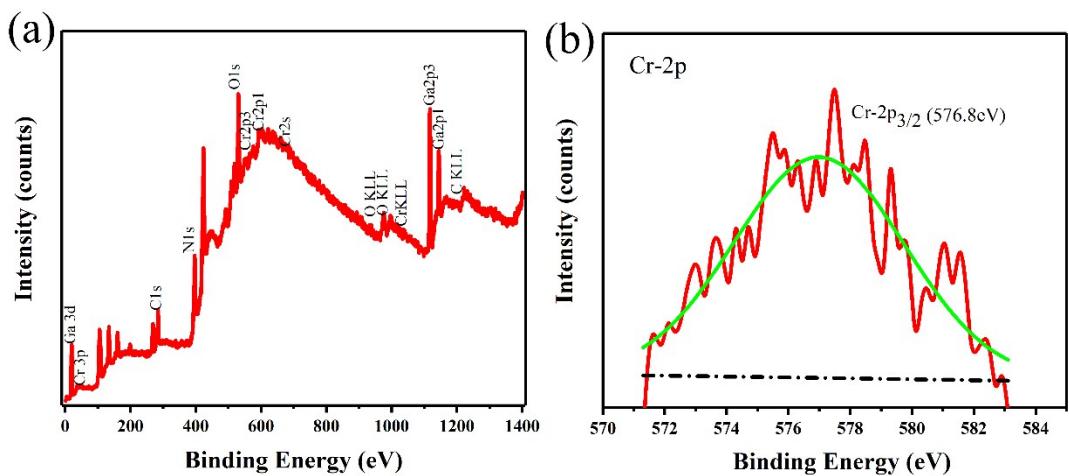


Figure S3 (a) XPS survey spectra of SGO:0.05Cr. (b)The Cr 2p levels of XPS spectra in SGO:0.05Cr.

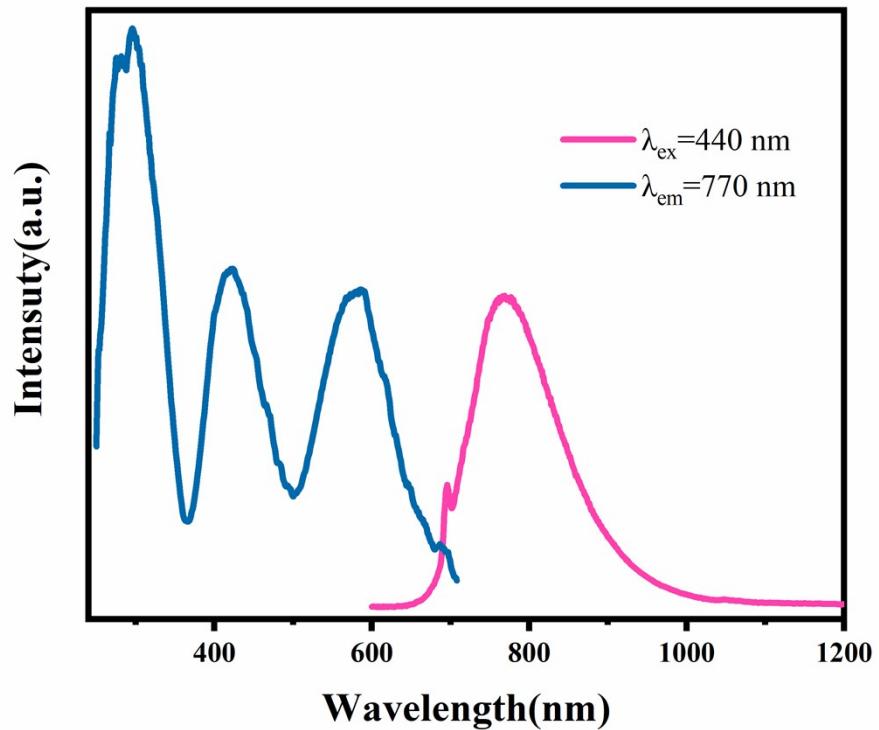


Figure S4 The full view PLE and PL spectra of SGO: 0.01Cr phosphor.

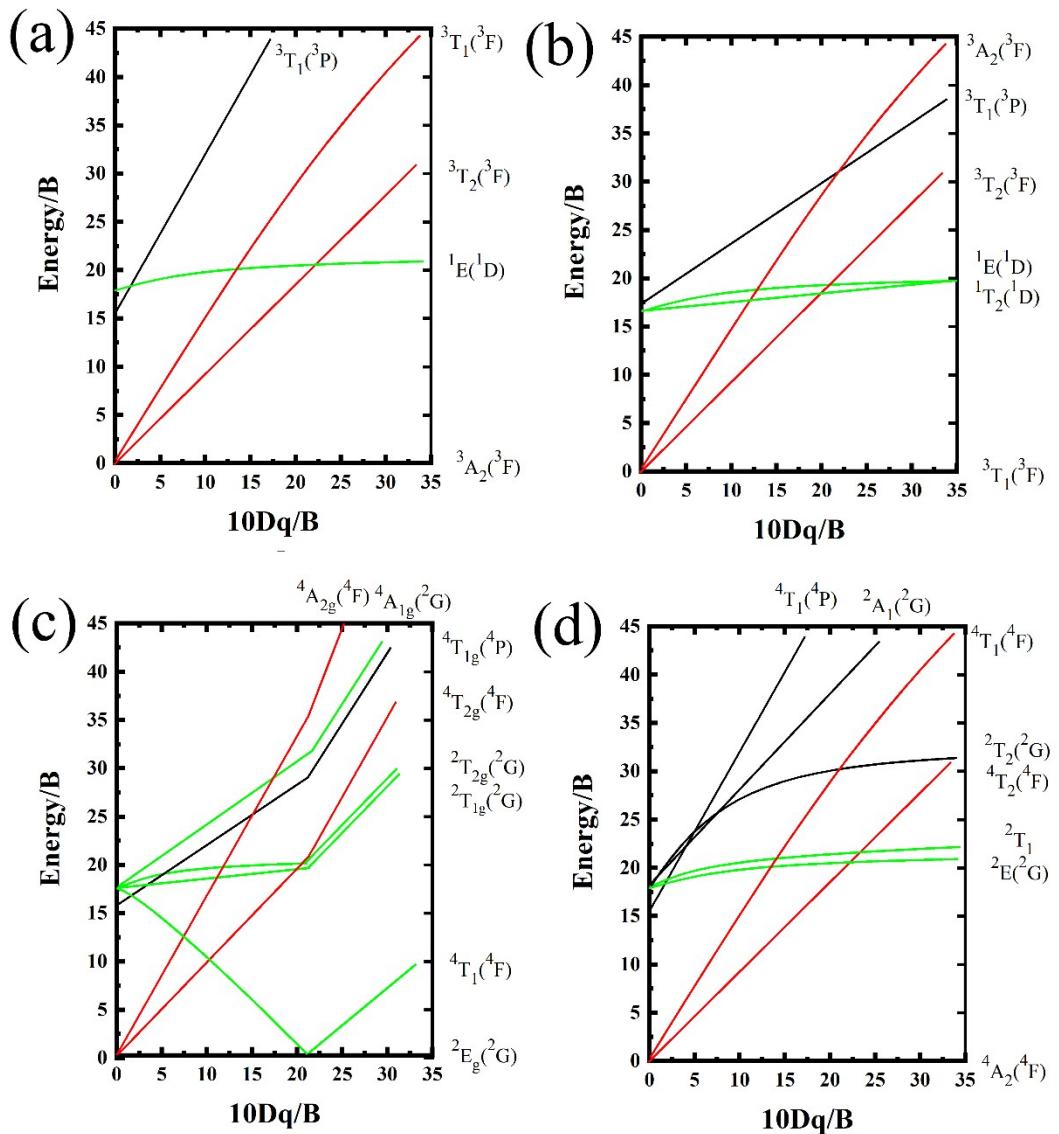


Figure S5. The Tanabe-Sugano diagram of (a) Cr<sup>4+</sup> ions in tetrahedron, (b) Cr<sup>4+</sup> ions in octahedron, (c) Cr<sup>3+</sup> ions in tetrahedron, (d) Cr<sup>3+</sup> ions in octahedron.

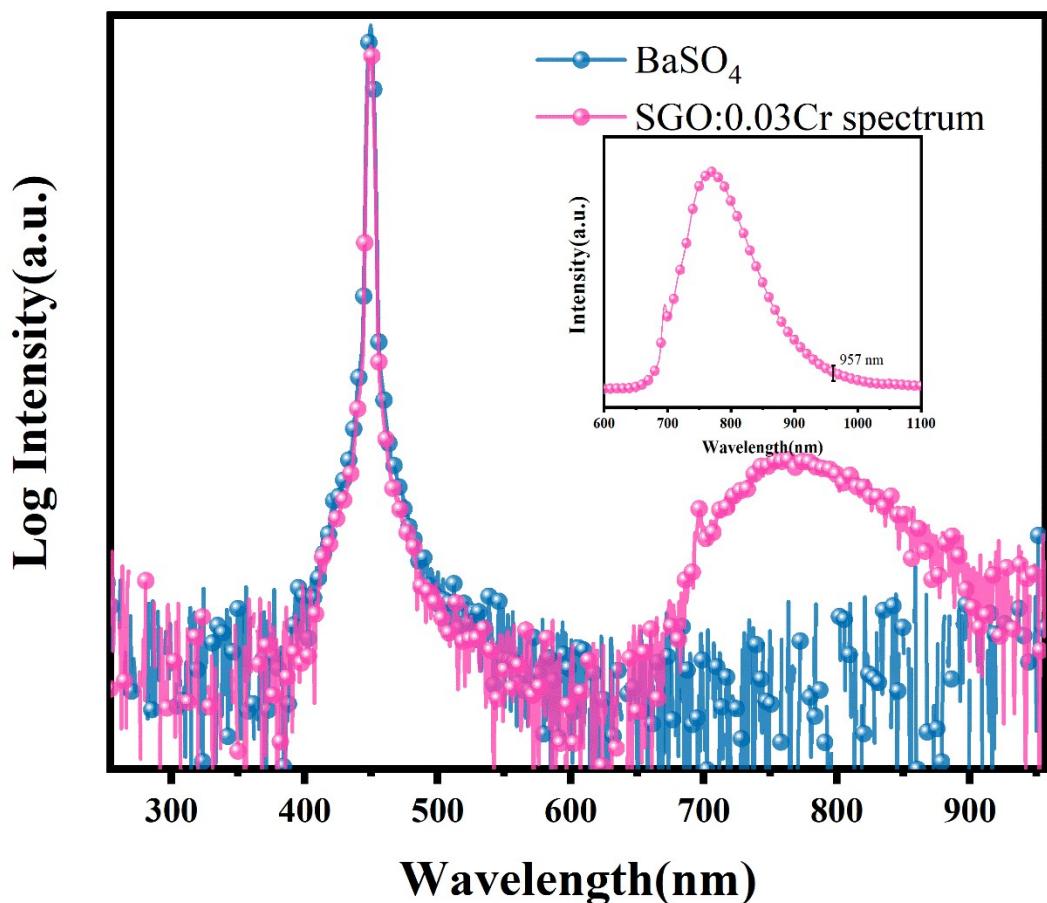


Figure S6 The IQE of SGO:0.03 Cr phosphor.

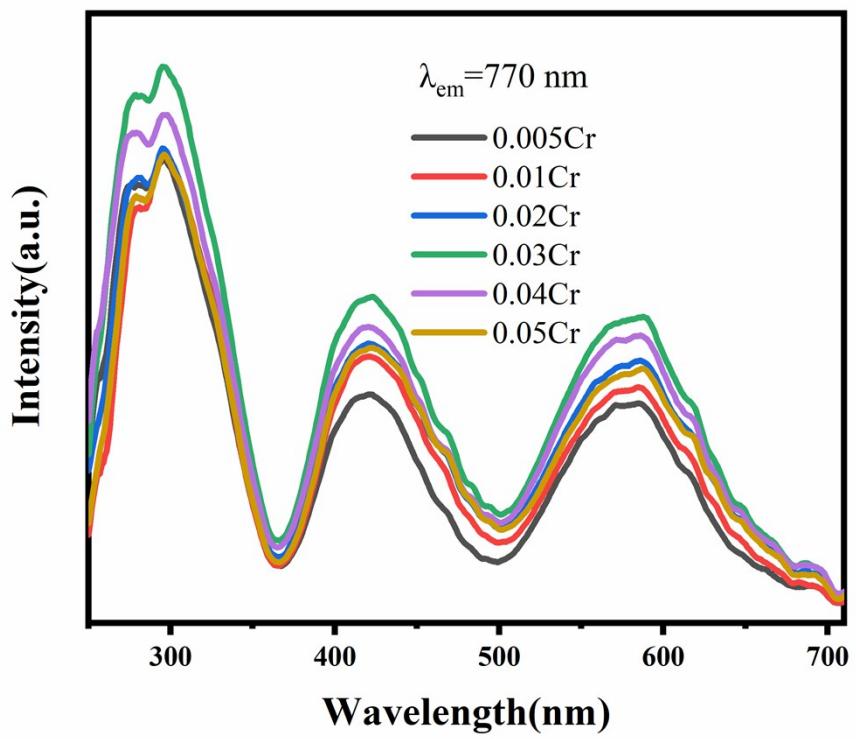


Figure S7. The PLE spectra of SGO:xCr ( $x=0.005, 0.01, 0.02, 0.03, 0.04$ , and  $0.05$ ).