

Supporting Information

for

**Self-trapped holes, oxygen vacancies and electrocatalytic  
performance of Zn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> microspindles**

Shuting Cui <sup>1</sup>, Yuchao Du <sup>1</sup>, Guoping Li <sup>2</sup>, Qiyong Chen <sup>1</sup>, Ning Tang <sup>2</sup>, Weikun Ge <sup>2</sup>,

Lili Xi <sup>1</sup>, Bo Shen <sup>2</sup>, Lijuan Zhao <sup>1,\*</sup>

<sup>1</sup>Materials Genome Institute, Shanghai University, Shanghai 200444, P. R. China

<sup>2</sup>School of Physics, Peking University, Beijing 100871, P. R. China

\*Corresponding Authors

Dr. Lijuan Zhao, Email address: [zhaolijuan@t.shu.edu.cn](mailto:zhaolijuan@t.shu.edu.cn)

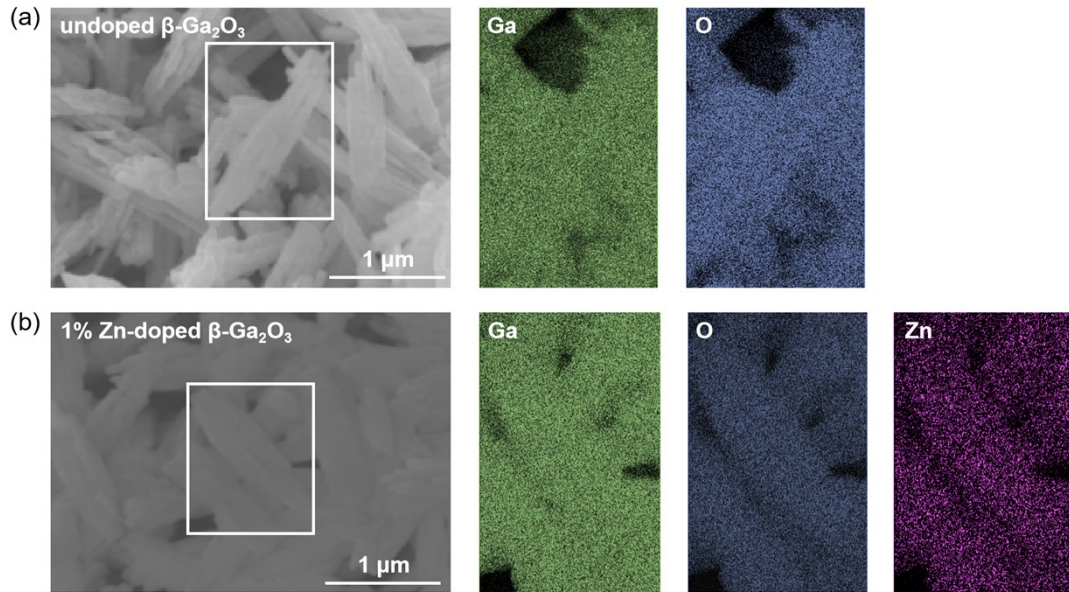


Fig. S1 The EDS mappings of elements in (a) undoped and (b) 1% Zn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> microspindles.

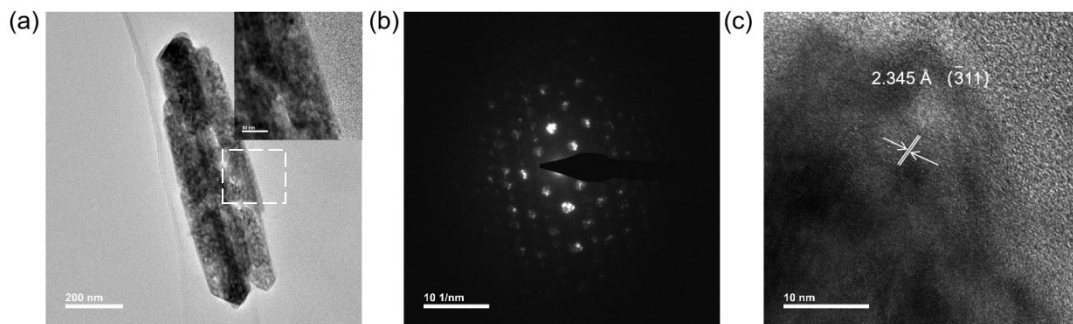


Fig. S2 (a) TEM image, (b) the corresponding SAED pattern and (c) HRTEM image of the 1% Zn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> spindles.

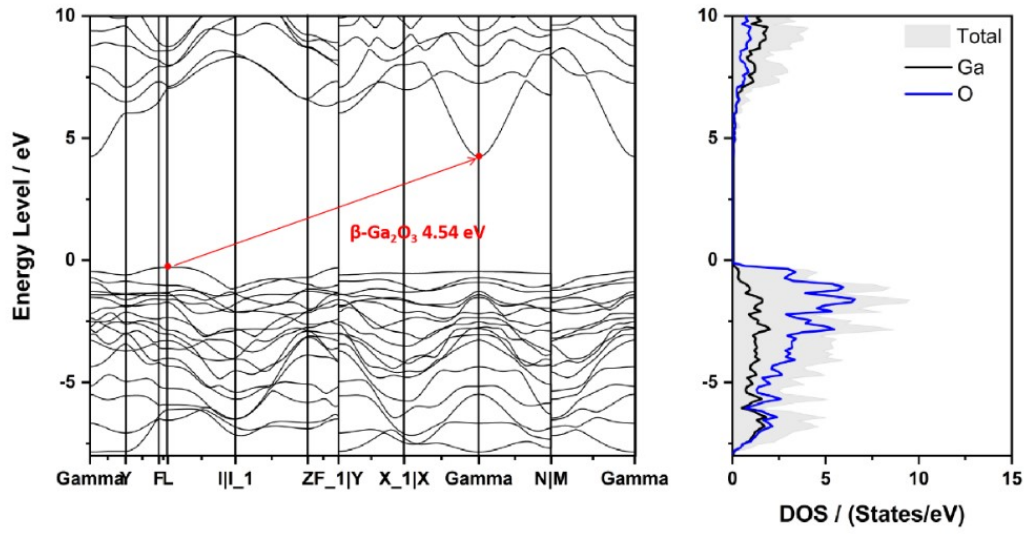


Fig. S3 The bandgap and DOS of the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> microspindles.

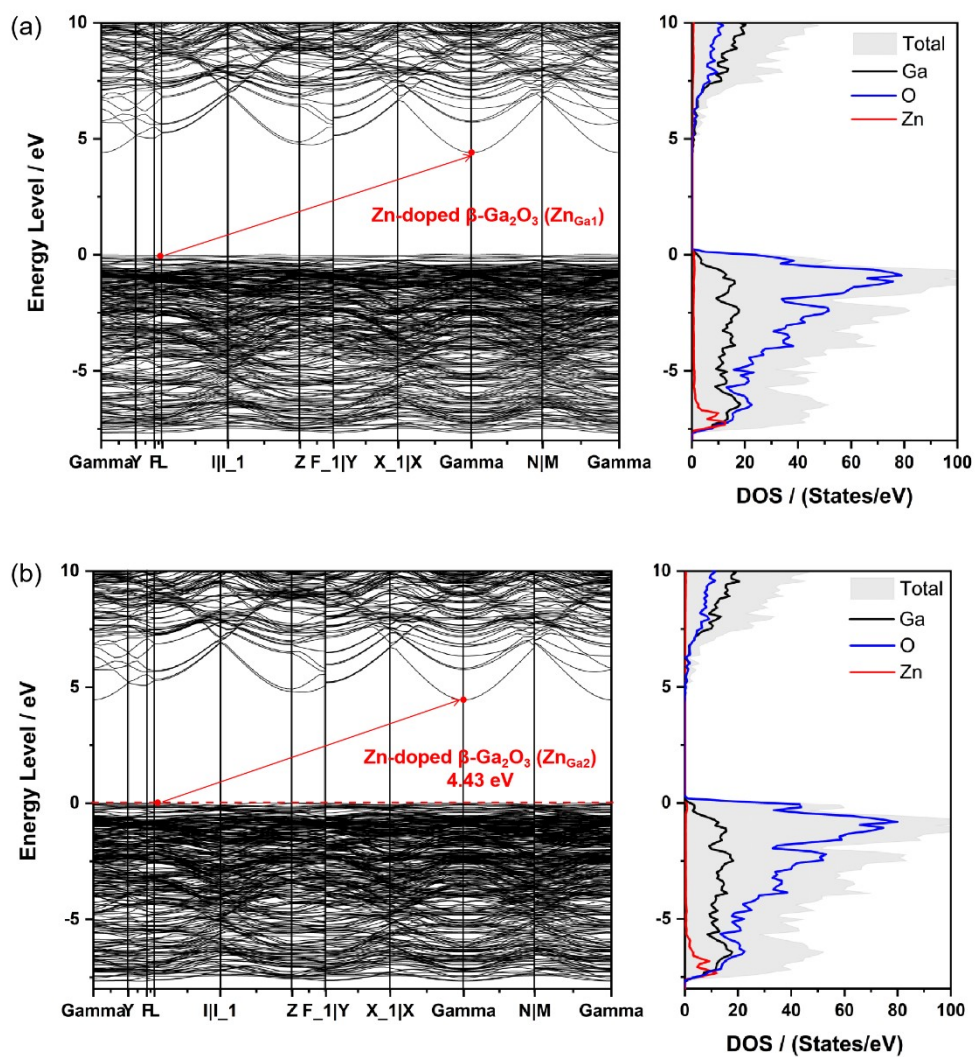


Fig. S4 The bandgap and DOS of the Zn-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> microspindles where (a) Zn replacing Ga<sub>1</sub> site and (b) Zn replacing Ga<sub>2</sub> site.

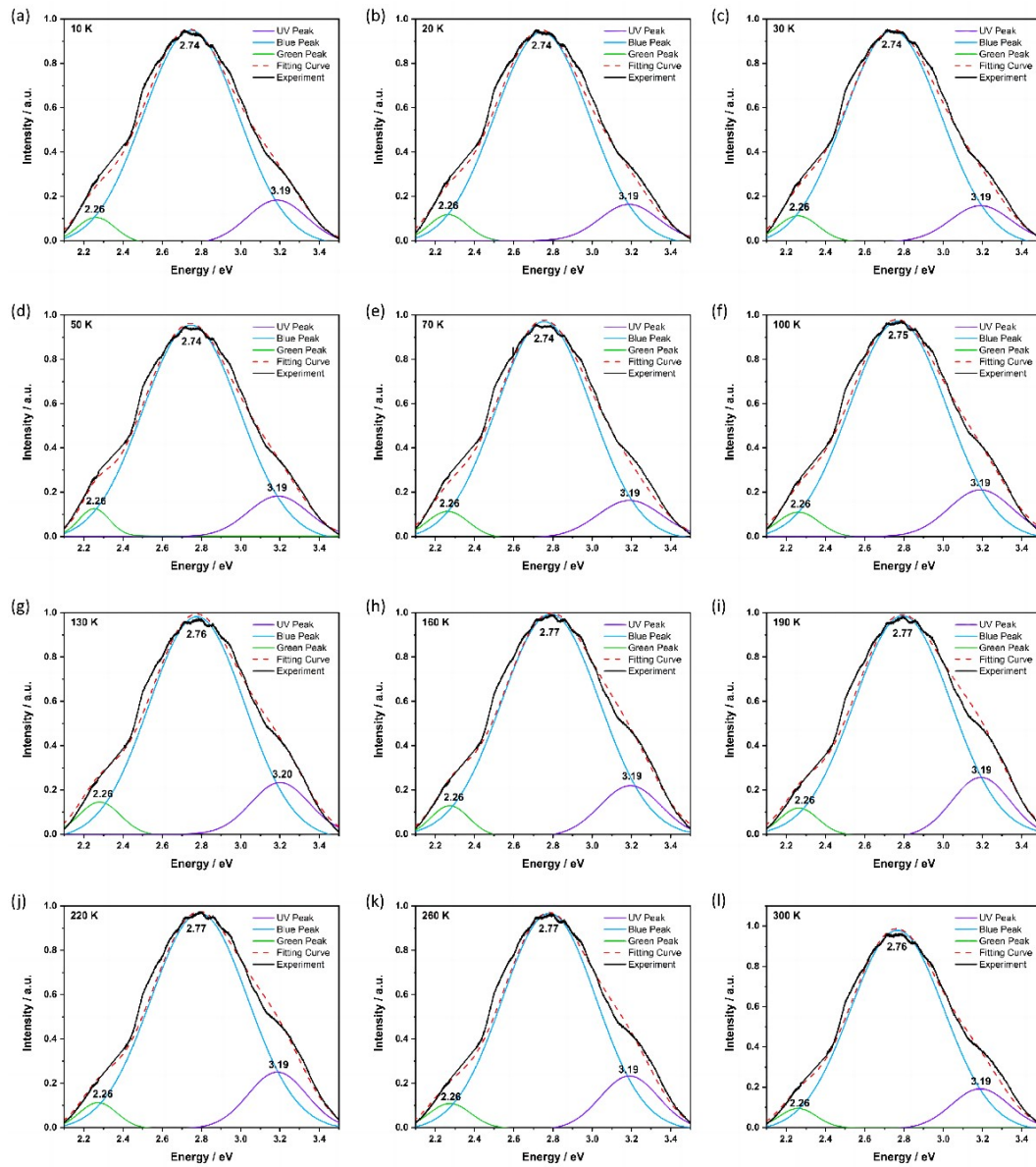


Fig. S5 (a-l) The Gaussian fitting curves of temperature-dependent PL spectra of the  $\beta$ - $\text{Ga}_2\text{O}_3$  microspindles from 10 K to 300 K.



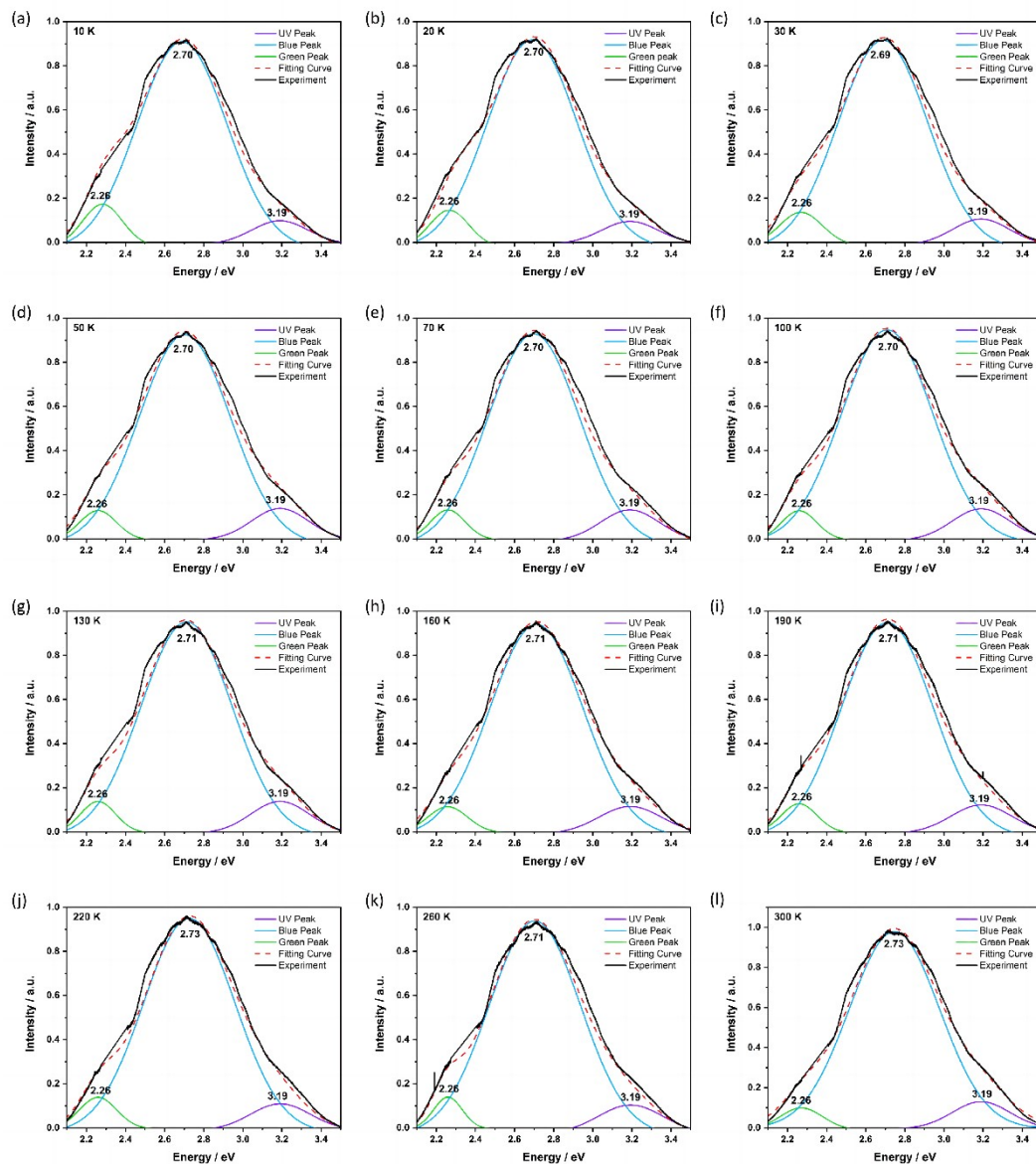


Fig. S6 (a-l) The Gaussian fitting curves of temperature-dependent PL spectra of Zn-doped  $\beta$ - $\text{Ga}_2\text{O}_3$  microspindles from 10 K to 300 K.