

## Supporting Information

### An all-inorganic Li-doped Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> single crystal for dual gamma ray and neutron detection applications

Peng Xiang<sup>1§</sup>, Qinhuai Wei<sup>1\*</sup>, Cheng Wang<sup>2,3§</sup>, Peiqing Cai<sup>4</sup>, Yufeng Tong<sup>1</sup>, Gao Tang<sup>1</sup>,  
Xilei Sun<sup>3\*</sup>, Fan Yang<sup>5</sup>, Hongsheng Shi<sup>6</sup>, Zugang Liu<sup>4</sup> and Laishun Qin<sup>1</sup>

<sup>1</sup> College of Materials and Chemistry, China Jiliang University, Hangzhou 310018

<sup>2</sup> National Engineering Research Center for Rare Earth, GRINM Group Co., Ltd and Grirem Advanced Materials Co., Ltd., Beijing 100088

<sup>3</sup> State Key Laboratory of Particle Detection and Electronics, Institute of High Energy Physics, CAS, Beijing 100049

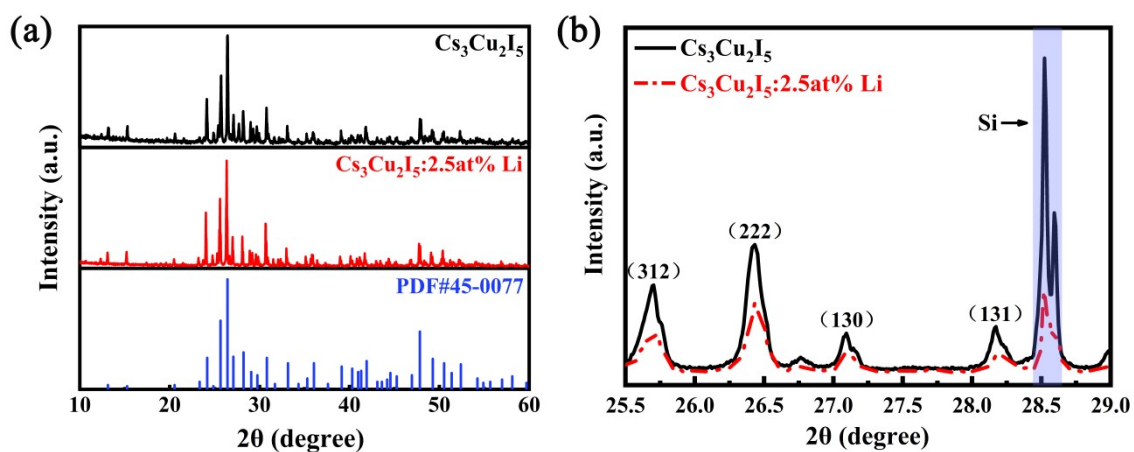
<sup>4</sup> College of Optical and Electronic Technology, China Jiliang University, Hangzhou 310018

<sup>5</sup> The Key Laboratory of Weak Light Nonlinear Photonics, Ministry of Education, School of Physics, Nankai University, Tianjin 300071

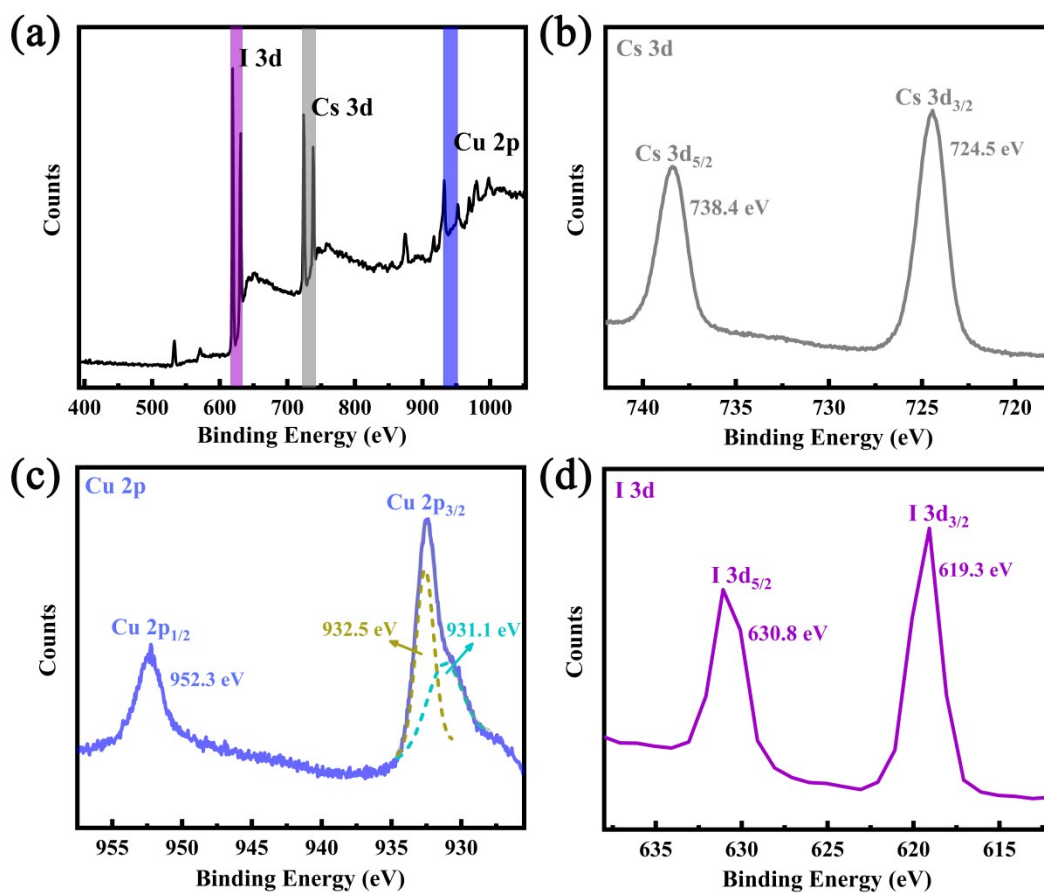
<sup>6</sup> Xinjiang Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Urumqi 830011

§ These authors contributed equally to this work.

\* Corresponding authors (Emails: weiqinhua1985@163.com; sunxl@ihep.ac.cn)



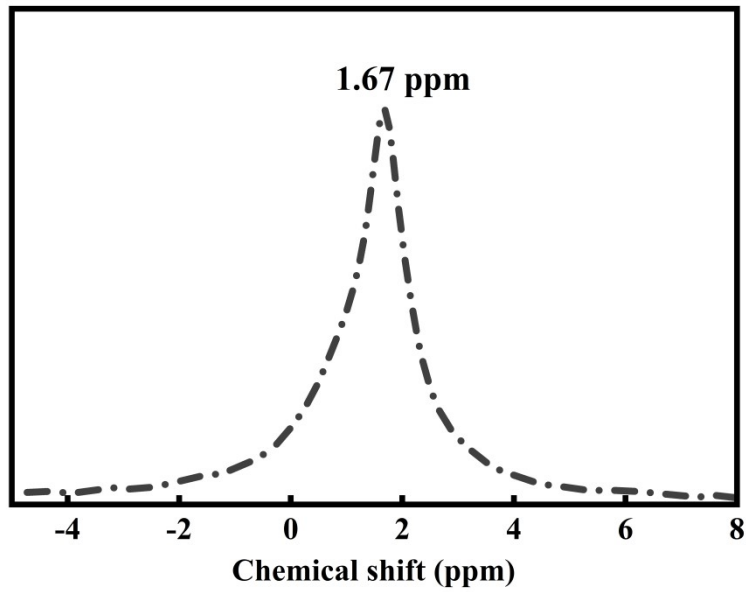
**Figure S1.** (a) Powder XRD patterns of both undoped and  $\text{Li}^+$ -doped  $\text{Cs}_3\text{Cu}_2\text{I}_5$ . (b) Narrow-angle powder X-ray diffraction with high-purity silicon as an internal standard.



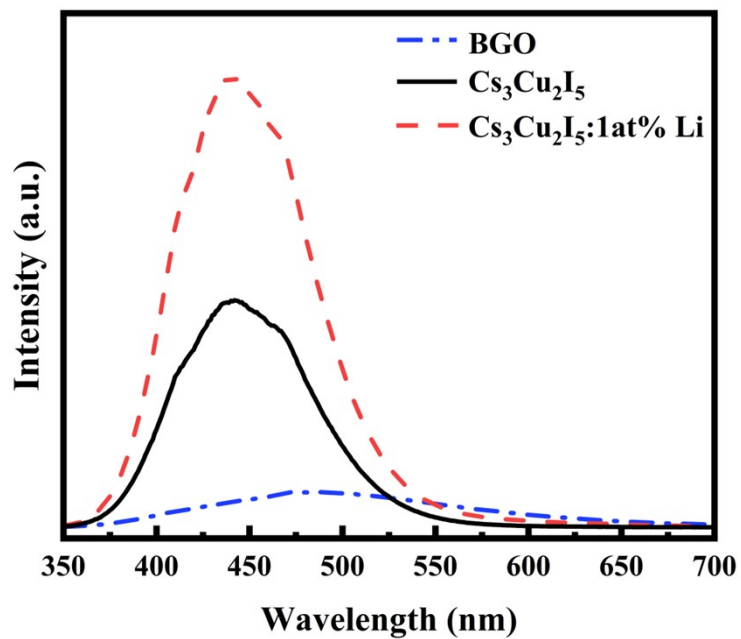
**Figure S2.** (a) XPS survey spectrum of  $\text{Cs}_3\text{Cu}_2\text{I}_5:\text{Li}$ . (b), (c) and (d) High-resolution XPS spectra of Cs 3d, Cu 2p and I 3d, respectively.

**Table S1.** ICP-OES results of  $\text{Cs}_3\text{Cu}_2\text{I}_5:\text{Li}$  with different  $\text{Li}^+$  concentration.

| Calculated concentration (at%) | Measured concentration (at%) |
|--------------------------------|------------------------------|
| 1.0                            | 0.34                         |
| 2.5                            | 0.92                         |



**Figure S3.**  $^7\text{Li}$  NMR spectrum of  $\text{Cs}_3\text{Cu}_2\text{I}_5:\text{Li}$ .



**Figure S4.** X-ray excited luminescence spectra of undoped and  $\text{Li}^+$ -doped  $\text{Cs}_3\text{Cu}_2\text{I}_5$  single crystals and BGO.

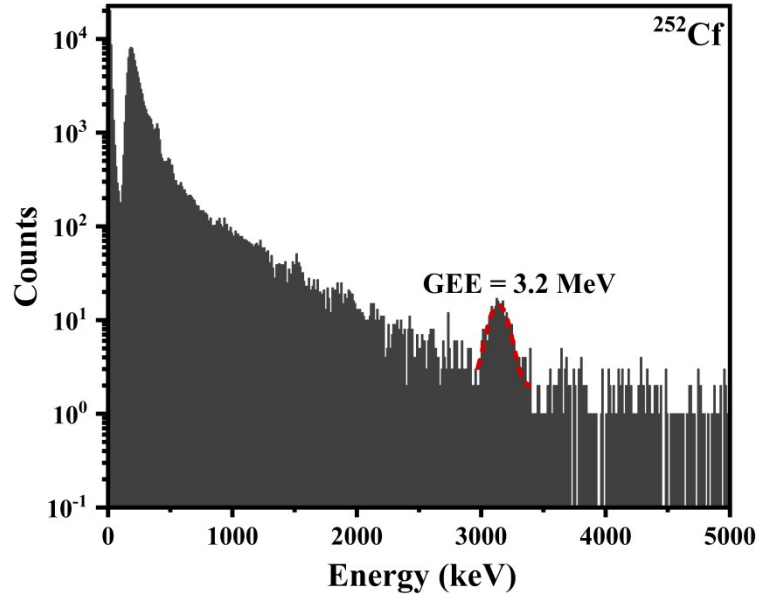


Figure S5. (a) Neutron energy spectra of 2.5at% Li<sup>+</sup>-doped Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> crystal under the excitation of <sup>252</sup>Cf source.

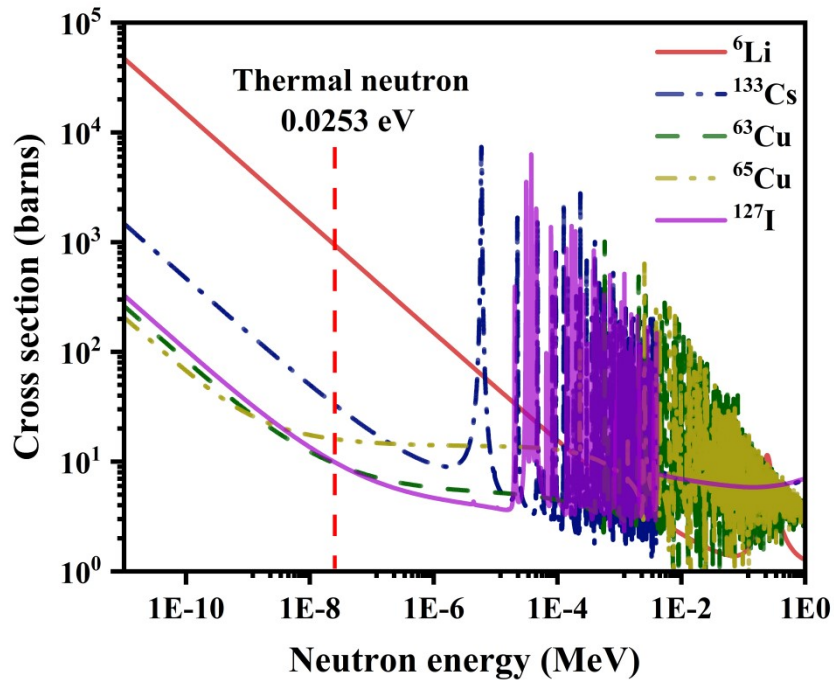


Figure S6. The relationship between neutron energy and reaction cross section of each element in Li<sup>+</sup>-doped Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub>.

Table S2. FOM values of 2.5at% Li<sup>+</sup>-doped Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> single crystal under different prompt integration window combinations.

| Prompt window (ns) | 100  | 200  | 250  | 260  | 275  | 280  | 300  | 400  | 500  |
|--------------------|------|------|------|------|------|------|------|------|------|
| FOM                | 1.66 | 1.91 | 2.01 | 2.09 | 2.19 | 2.25 | 2.10 | 1.95 | 1.57 |