

Supplementary information for

**A new cerium iodate infrared nonlinear optical
material with a large second-harmonic generation
response**

Lei Xiao,^{†,§} Zhenbo Cao,^{‡,*} Jiyong Yao,[†] Zheshuai Lin,[†] and Zhanggui Hu^{†,*}

[†] Center for Crystal Research and Development, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, P.R. China, [‡] Institute of Special Glass Fiber and Optoelectronic Functional Materials, China Building Materials Academy, Beijing 100024, P.R. China, [§] Graduate University of the Chinese Academy of Sciences, Beijing 100049, P.R. China

*To whom correspondence should be addressed. Email: czb824@163.com (Zhenbo Cao) and hu@mail.ipc.ac.cn (Zhanggui Hu)

Figure S1. The superalloy reactor.

Figure S2. Millimetric ($\sim 3 \times 0.3 \times 0.1 \text{ mm}^3$) single crystal of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S3. Experimental (top) and simulated (bottom) X-ray powder diffraction patterns for $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S4. Crystal structure of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S5. UV-Vis-NIR spectra for $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S6. DSC study of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S7. Part of state density of theoretical calculations (PDOS) of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

Figure S8. Local density of states (LDOS) of $\text{Ce}_2\text{I}_6\text{O}_{18}$.



Figure S1. The superalloy reactor.

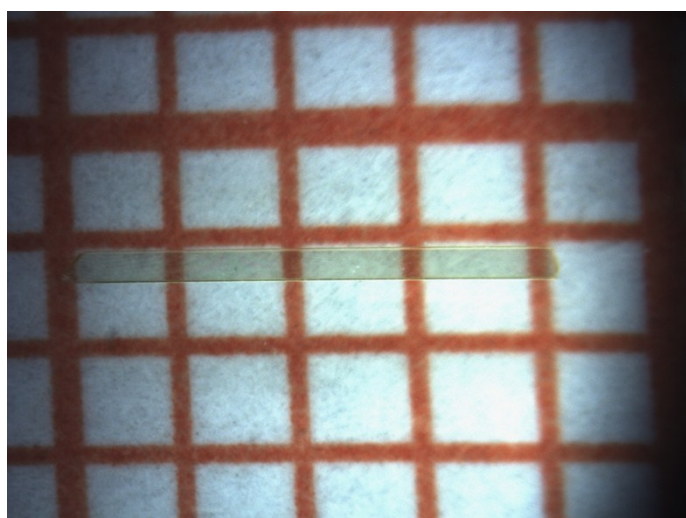


Figure S2. Millimetric single crystal of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

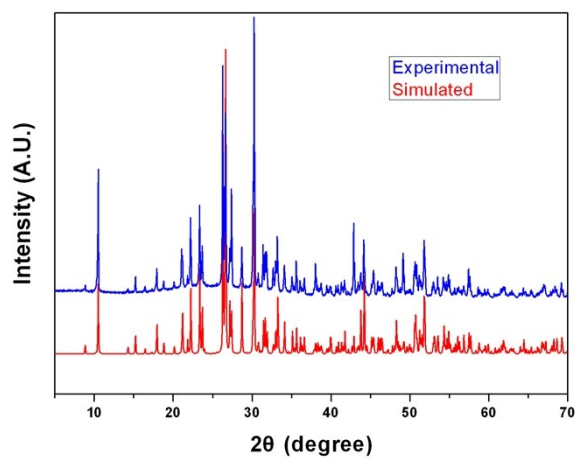


Figure S3. Experimental (top) and simulated (bottom) X-ray powder diffraction patterns for $\text{Ce}_2\text{I}_6\text{O}_{18}$.

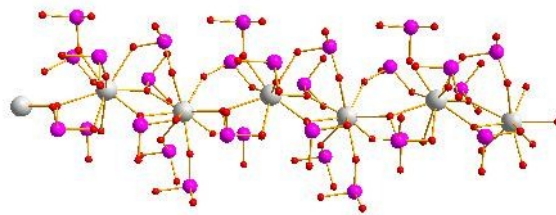
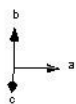


Figure S4-1. Crystal structure of IO_3 and IO_4 polyhedra viewed down the a -axis.

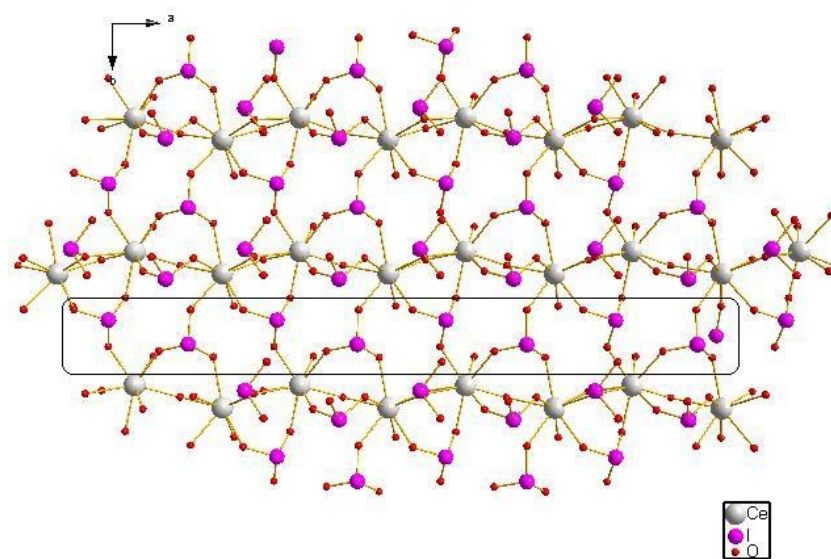


Figure S4-2. The one-dimensional chain continues along the b direction by sharing IO_3 tetrahedral angle.

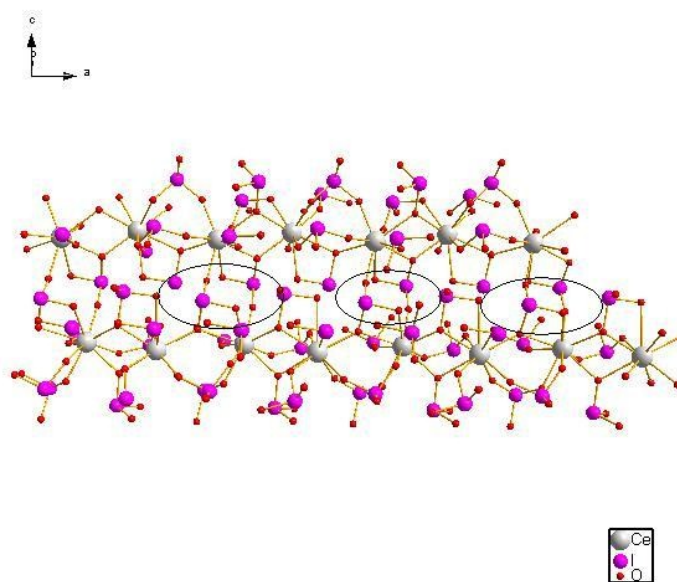


Figure S4-3. Crystal structure of $\text{Ce}_2\text{I}_6\text{O}_{18}$ in the ab plane.

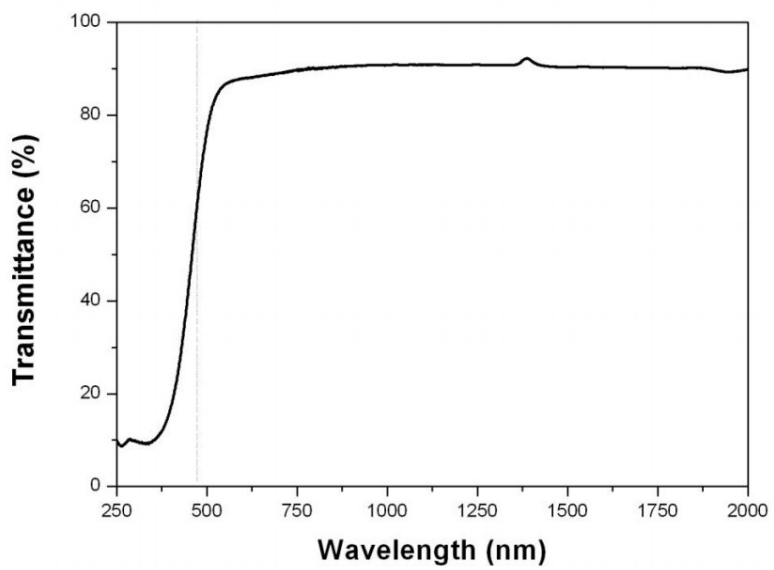


Figure S5. UV-Vis-NIR spectra for Ce₂I₆O₁₈.

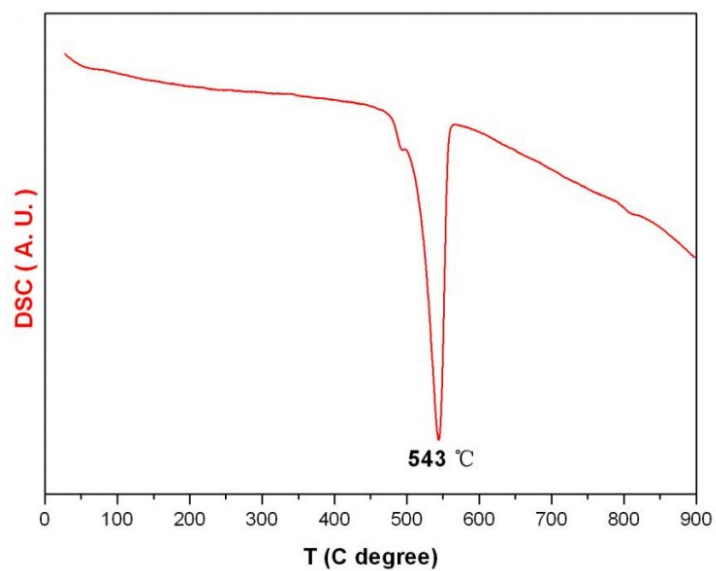


Figure S6. DSC study of Ce₂I₆O₁₈.

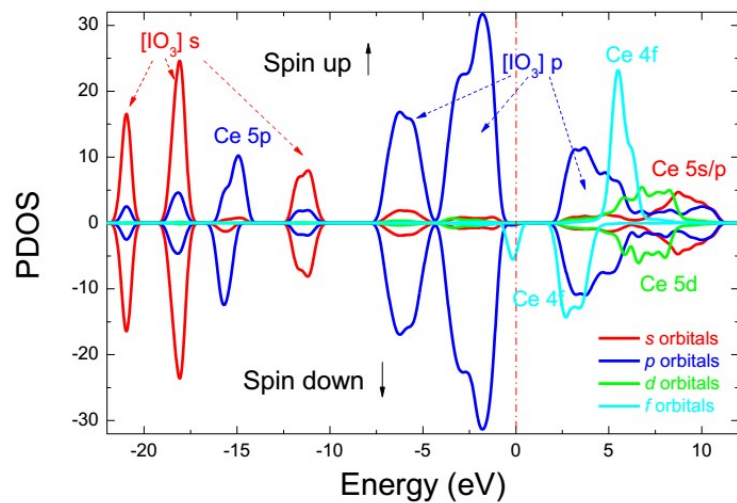


Figure S7. Part of state density of theoretical calculations (PDOS) of $\text{Ce}_2\text{I}_6\text{O}_{18}$.

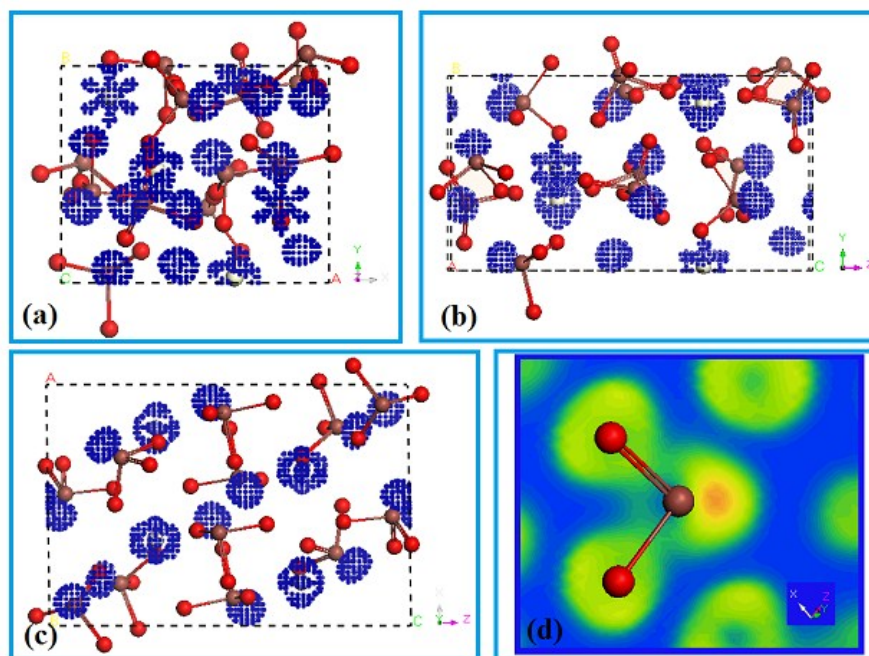


Figure S8. Local density of states (LDOS) of $\text{Ce}_2\text{I}_6\text{O}_{18}$.