Supporting information

Orange Persistent Luminescence and Photo-Darkening Related with Paramagnetic Defects of Non-Doped CaO-Ga2O3-GeO2 Glass

Jumpei Ueda*, Atsunori Hashimoto, Setsuhisa Tanabe

Graduate School of Human and Environmental Studies, Kyoto University, Kyoto 606-8501, Japan

*E-mail: ueda.jumpei.5r@kyoto-u.ac.jp
Figure S1 shows the Tauc plot assuming the direct allowed transition of the CGG glass. From the plot, the band gap was estimated to be 3.17 eV.

Figure S1. Tauc plot of the CGG glass.
Figure S2 shows partial density of states (PDOS) for Ca, Ga, Ge and O atom and total DOS in Ca$_2$Ga$_2$GeO$_7$. The density functional theory (DFT) calculations of the structural and electronic properties of Ca$_2$Ga$_2$GeO$_7$ were performed using the CASTEP module of the Materials Studio 2019 package and the GGA-PBE. The ionic core electrons were replaced by on-the-fly ultrasoft pseudopotentials implemented in the CASTEP. Relativistic effects were taken into account at the level of the Koelling–Harmon approximation of the Dirac equation.

From the PDOS and total DOS results, the conduction band bottom is found to be formed mainly by Ga 4s and Ge 4s.

![Graph showing partial density of states (PDOS) for Ca, Ga, Ge and O atom and total DOS in Ca$_2$Ga$_2$GeO$_7$.](image)

Figure S2. Partial density of states (PDOS) for Ca, Ga, Ge and O atom and total DOS in Ca$_2$Ga$_2$GeO$_7$. 

S3