Supporting information

Design a novel red to near-infrared persistent phosphors of $CaMgGe_2O_6$: Mn^{2+}, Sm^{3+} based on vacuum referred binding energy diagram

Qiangfei Ye, Yuhua Wang*, Haijie Guo, Xufeng Zhou, Peng Feng and Songsong Ding

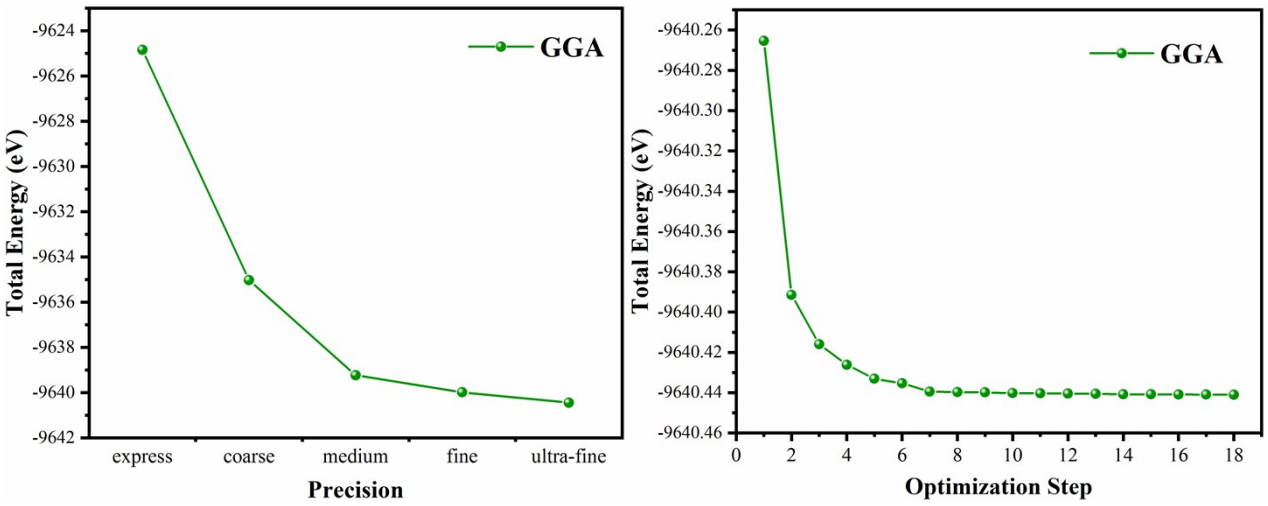

Fig S1. The CASTEP geometric optimization of the $CaMgGe_2O_6$ sample

In order to perform the geometry optimization, we considered different test precision and thresholds in Materials Studio 7.0. The convergence thresholds were (a) Quality: Ultrafine total energy convergence tolerance of less than $5.0*10^{-6}$ eV/atom; (b) maximum force tolerance of less than 0.01 eV/Å; (c) maximum stress tolerance of 0.02GPa;and (d) maximum displacement tolerance of $5.0*10^{-4}$ Å.

When these criteria are satisfied along with successive optimization steps, it is considered that the crystal geometry well converged and the total energy is minimized.

We can see from Fig. S2 that the thermoluminescence peak of the $CaMgGe_2O_6$: Mn^{2+}, Sm^{3+} sample has a distinct peak at 359K and the thermoluminescence curve of $CaMgGe_2O_6$: Mn^{2+}, Tm^{3+} sample does not have this peak, indicating that Sm^{3+} is more suitable as a co-doped rare earth.

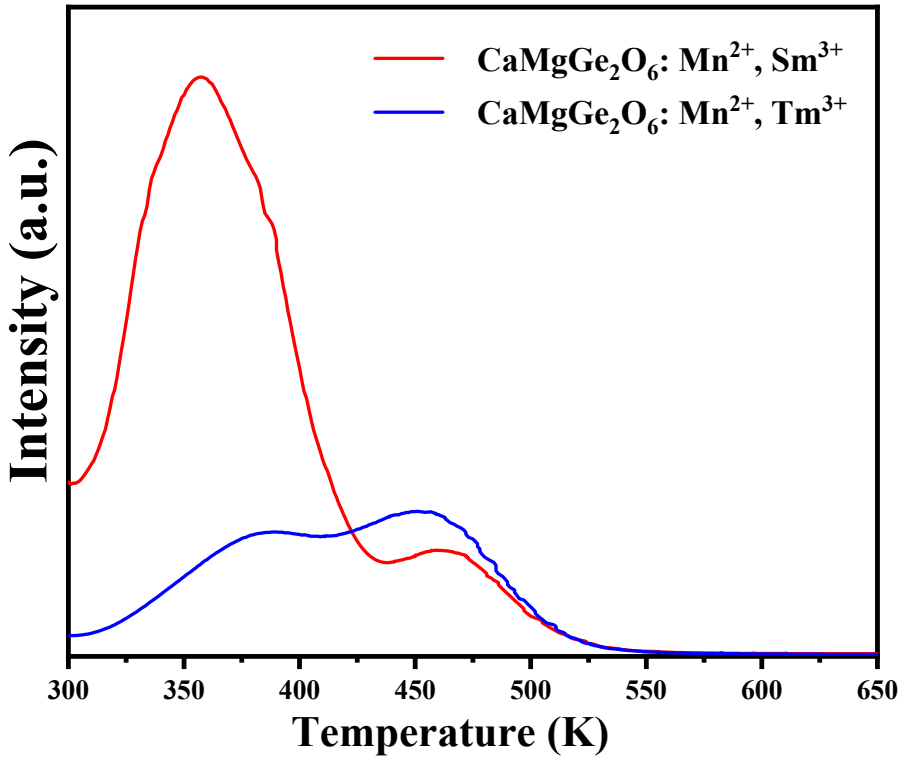

Fig S2. The thermoluminescence curves of the $CaMgGe_2O_6$: Mn^{2+}, Sm^{3+} and $CaMgGe_2O_6$: Mn^{2+}, Tm^{3+} samples