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### Growth, structure and spectroscopic properties of melilite Er: CaLaGa<sub>3</sub>O<sub>7</sub> crystal for use in mid-infrared laser

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#### Abstract

Single crystals of pure and Er<sup>3+</sup> doped CaLaGa<sub>3</sub>O<sub>7</sub> were firstly grown by the Czochralski technology. The structure of CaLaGa<sub>3</sub>O<sub>7</sub> was investigated. The electronic structures of CaLaGa<sub>3</sub>O<sub>7</sub> crystal were performed by using first-principles calculations based on density functional theory (DFT) methods. Its band structure and density of states were presented. The polarized absorption, emission spectra including up-conversion, near-infrared and mid-infrared fluorescence spectra, as well as the fluorescence decay curves of Er: CaLaGa<sub>3</sub>O<sub>7</sub> crystal were measured at room temperature. Detailed spectroscopic analyses of Er: CaLaGa<sub>3</sub>O<sub>7</sub> were carried out. Based on the Judd–Ofelt theory and the polarized absorption spectra, the spontaneous transition probabilities, the fluorescent branching ratios and the radiative lifetimes were calculated. The energy transfer mechanism in Er: CaLaGa<sub>3</sub>O<sub>7</sub> crystal was also studied in this work. It concludes that Er: CaLaGa<sub>3</sub>O<sub>7</sub> crystal can act as a promising candidate for mid-infrared lasers.

**Keywords**: Er<sup>3+</sup>: CaLaGa<sub>3</sub>O<sub>7</sub> crystal, First-principles calculations, Spectroscopic properties, Mid-infrared laser

#### 1. Introduction

In recent years, novel mid-infrared (MIR) solid lasers at the wavelength of  $2.7 \sim 3 \mu m$  have drawn much attention for enormous applications in medicine, detection and remote sensors etc. [1–4]. This is primarily due to the strong absorption by water around this

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