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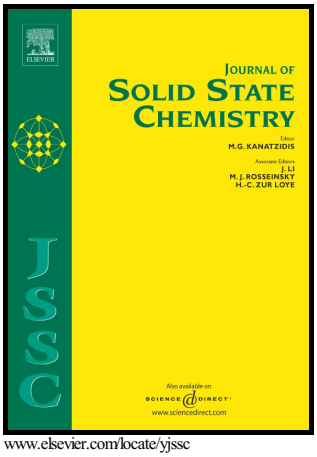

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Theoretical and experimental studies of electronic, optical and luminescent properties for Tb-based garnet materials

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ABSTRACT

Terbium-aluminum ($Tb_3Al_5O_{12}$: TAG) as well as Terbium-scandium-aluminum ($Tb_3Sc_2Al_3O_{12}$: TSAG) garnet materials have attracted tremendous attention around the world owing to their multifunctional applications. However, the electronic structure, optical and luminescent properties for TAG and TSAG are still requiring elucidation. To solve these intriguing problems, firstly, a systematic theoretical calculation based on the density functional theory methods were carried out on them and their electronic structure and optical properties were obtained. The calculated results indicating that both TAG and TSAG belongs to direct band gap materials category with band gap of 4.46 and 4.05 eV, respectively. Secondly, we compared the calculated results with the experimental results (including band gap, refractive index and reflectivity) and found that they were in good coincident. Lastly, we investigated the luminescence properties of TSAG and evaluated its probability for using as visible phosphor and laser matrix. In addition, a Judd-Ofelt theory calculation was performed on TSAG to reveal the radioactive transition of Tb-4*f* configuration and the three Judd–Ofelt intense parameters were obtained to be 4.47, 1.37 and 4.23×10^{-20} cm^2, respectively. All of the obtained results can provide an essential understanding of TAG and TSAG garnet materials and also useful for the further exploration of them.

Keywords: TSAG and TAG; density functional theory; phosphor; visible laser matrix; optical properties; Judd-Ofelt theory

Graphical abstract

The structure and luminescent properties for TSAG crystal.