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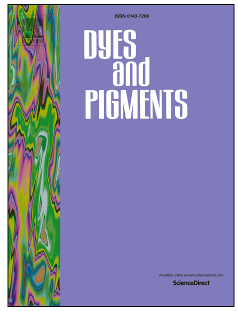

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Electronic structure, photoluminescence and phosphorescence properties in $Sr_2ScGaO_5:Sm^{3+}$

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Abstract

Novel reddish long lasting phosphorescence material $Sr_2ScGaO_5:Sm^{3+}$ was designed and prepared by a solid state reaction. The results of morphology showed that the irregular microparticles were formed by the agglomeration of uniform submicron particles with the size of about 0.5 ~ 1 μm. The electronic structure with an indirect bandgap was evaluated in detail by the density functional theory calculations and the diffuse reflectance spectrum for the first time. By the two different methods, the bandgap energy of Sr_2ScGaO_5 was determined to be about 4.24 and 4.75 eV, respectively. The emission of Sm^{3+} ion at 604 nm is strongest in the photoluminescence process, while in the phosphorescence process the emission at 619 nm is dominant. According to the analysis on the optical properties, the interesting phenomenon about the difference between the photoluminescence and phosphorescence was revealed and explained by the fact that the conduction band played an important role in the phosphorescence process. Additionally, the result showed that the material can be stimulated effectively in very short time and would have great potential in the applications such as AC-light emitting diodes.

Key words: Sr_2ScGaO_5; electronic structure; phosphorescence; conduction band.

1. Introduction

Long lasting phosphorescence (LLP) materials can absorb and store energy under irradiation of high energy electromagnetic waves and then release them slowly in the form of light under thermal stimulation [1,2]. The release can last for several seconds to hours and is of great use in many important fields, e.g. glow-in-the-dark, optical memory, medical diagnostics, photodynamic activation and alternating current driven light emitting diodes (AC-LED), etc. [3-10]. In recent decades, large numbers of LLP materials have been developed and reported by researchers. At present, LLP materials exhibiting blue and green phosphorescence with high brightness are commercially available, while red LLP materials are still in great scarcity and none of them are good enough to be used in practical applications [11,12]. However, in many application fields, red LLP materials are more in demand than the blue or green ones. For example, in the field of AC-LED, LLP materials with short and bright afterglow are usually used to compensate the dimming time in every AC cycle [10]. Meanwhile, there always exists another open issue that LEDs have the lack of red component, resulting in non-standard white light with a high correlated color temperature and a low color rendering index. Herein, red LLP materials would serve a double purpose well. Also, in the biomedical application, it is well known that only red or near-infrared LLP materials can be applicative due to the tissue transparency window [7,13]. Therefore, it is greatly necessary to investigate and develop novel red LLP materials for