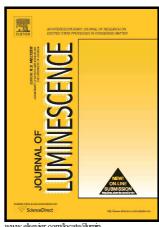
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ACCEPTED MANUSCRIPT

Upconversion Luminescence Properties of Different

Fluoride Matrix Materials NaREF₄ (RE: Gd, Lu, Y)

Doped with Er³⁺/Yb³⁺

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Abstract: The densities of state and optical properties of matrix materials were studied with the help of

first-principles calculations. It is found that the absorption and reflectance of the NaGdF4 system in the infrared

region were comparatively low. Such low values were beneficial to the reduction of the loss of excitation light.

Furthermore, Er³⁺ and Yb³⁺ co-doped NaREF₄ (RE: Gd, Lu, Y) were prepared by a simple hydrothermal method,

which exhibited a regularly shaped hexagonal microrods. Under the excitation of 808 nm, 980 nm, 1064 nm and

1550 nm, three emission peaks were all observed at 521, 540 and 655 nm for these samples, and NaGdF4: Yb/Er

has the highest fluorescence intensity among the three samples. Calculated and experimental results demonstrated

that NaGdF₄ is more suitable than the two other materials as a substrate for UC luminescence.

Keywords: First-principles; Upconversion; NaREF₄; Hydrothermal

1. Introduction

Upconversion (UC) is an anti-Stokes-type emission that involves the sequential absorption of

two or more photons, leading to the emission of light at a wavelength shorter than the excitation

wavelength [1]. Rare earth elements have an unfilled 4f electron layer, shielded by an outer electron

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