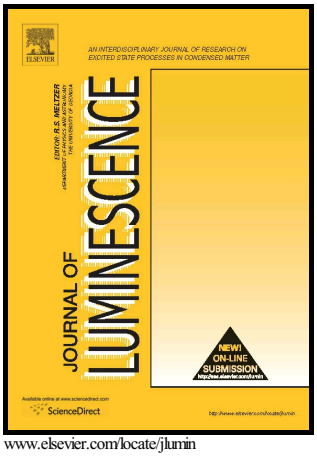

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The First Principles Calculation and Temperature-Sensitive Luminescence Behavior of Optimized Red Phosphor $Mg_2Al_4Si_5O_{18}$: Eu^{3+}

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Abstract

Eu^{3+} doped $Mg_2Al_4Si_5O_{18}$ phosphors were prepared by the solid-state reaction. The first principles calculation, XRD, diffuse reflection spectra, photoluminescence spectra and thermal quenching are carried out to investigate the electron structure, crystal structure, photoluminescence and thermal properties. The calculation results show that $Mg_2Al_4Si_5O_{18}$ possesses the direct band gap of about 5.1 eV. With the introduction of Eu^{3+}, the energy gap becomes obviously smaller due to the discontinuity of exchange-correlation energy. Between HOMOs and LOMOs, a series of f orbitals of Eu^{3+} can be observed, which is the essential condition to realize the efficient 4f-4f transitions of Eu^{3+}. The experimental results indicate that the samples can efficiently absorb the UV-light and emit the red light with the highest peak at 614 nm. With the co-doping of Bi^{3+} as sensitizer, the emission intensity of Eu^{3+} increases by about 49% due to the energy transfer between Bi^{3+} and Eu^{3+}. With the introduction of $Li^+/Na^+/K^+$ as charge compensators, the emission intensities of $Mg_2Al_4Si_5O_{18}$: Eu^{3+} are enhanced by about 22%, 18% and 5%. With the temperature increase, the emission intensity of all samples,