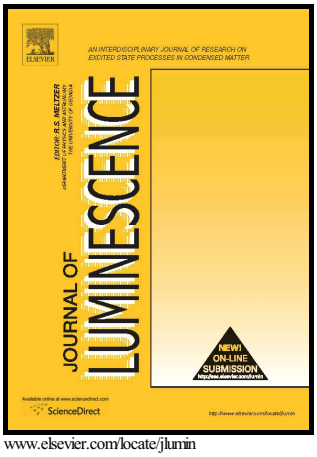

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An integrated first principles and experimental investigation of the relationship between structural rigidity and quantum efficiency in phosphors for solid state lighting

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ABSTRACT

In this paper, we outline an integrated approach for exploring novel near-UV excited phosphors. To test the hypothesis of whether high host structural rigidity results in phosphors with high quantum efficiency (Φ), we calculated the Debye temperatures (Θ) for 27 host materials using density functional theory calculations. We identified Eu^{2+}-activated $Ca_7Mg(SiO_4)_4$ and $CaMg(SiO_3)_2$ as having a relatively high Θ = 601 K and 665 K, respectively, and predicted excitation energies of 3.18 eV (337 nm) and 3.29 eV (377 nm), respectively, both of which are in good agreement with the results of photoluminescence spectroscopy. However, the measured Φ for these two phosphors was < 30%, which indicates that Θ alone is not a sufficient condition for a high Φ. This work demonstrates the potential of combined first-principles calculations and experiments in the discovery and design of novel near-UV excited phosphors.

Keywords: First-principles calculation, density functional theory, near-UV phosphors, Eu^{2+} activation, Debye temperature, quantum efficiency