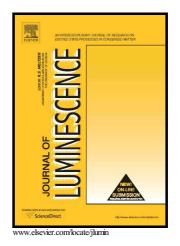
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Luminescence of Mn^{4+} in the orthorhombic perovskite, LaGaO₃

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ABSTRACT

The optical properties of Mn^{4+} ($3d^3$) in the orthorhombic perovskite, LaGaO₃ are investigated. The Mn^{4+} energy levels are calculated using the exchange charge model of crystal-field theory. The calculated Mn^{4+} energy levels are in good agreement with the experimental spectroscopic data. The results of our calculations yield the crystal-field splitting and Racah parameters of Dq = 1926 cm⁻¹, B = 780 cm⁻¹ and C = 2878 cm⁻¹, with C/B = 3.7. The emission spectrum is assigned on the basis of the zero phonon line corresponding to the ${}^{2}E_{g} \rightarrow {}^{4}A_{2g}$ transition and its vibrational sidebands. A comparative study of the variation in the crystal-field splitting and the $Mn^{4+2}E_{g}$ energy level position in materials with the perovskite structure is also presented.

Key words: Mn⁴⁺; LaGaO₃; perovskite; crystal-field splitting; covalence; luminescence

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