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Luminescence of Mn^{4+} in the orthorhombic perovskite, LaGaO_3

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^c Institute of Physics, University of Tartu, Ravila 14C, Tartu 50411, Estonia^d Institute of Physics, Jan Dlugosz University, PL-42200 Czestochowa, Poland**ABSTRACT**

The optical properties of Mn⁴⁺ (3d³) in the orthorhombic perovskite, LaGaO₃ are investigated. The Mn⁴⁺ energy levels are calculated using the exchange charge model of crystal-field theory. The calculated Mn⁴⁺ 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 $Dq = 1926 \text{ cm}^{-1}$, $B = 780 \text{ cm}^{-1}$ and $C = 2878 \text{ cm}^{-1}$, with $C/B = 3.7$. The emission spectrum is assigned on the basis of the zero phonon line corresponding to the ${}^2E_g \rightarrow {}^4A_{2g}$ transition and its vibrational sidebands. A comparative study of the variation in the crystal-field splitting and the Mn⁴⁺ 2E_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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