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Studies of the optical and EPR data and the defect structure for the trigonal Cr^{3+} center in $\text{LaMgAl}_{11}\text{O}_{19}$ crystal

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Abstract

The complete diagonalization (of energy matrix) method based on the two-spin-orbit-parameter model (which takes into account of the contributions from both the spin-orbit parameter of d^n ions in the traditional crystal field theory and that of ligand ions via covalence effect) is adopted to calculate uniformly the optical and EPR data of the trigonal Cr^{3+} center in $\text{LaMgAl}_{11}\text{O}_{19}$ crystal. The calculated results demonstrate that the observed nine optical and EPR data (six optical bands and three spin-Hamiltonian parameters g_{\parallel} , g_{\perp} and D) can be explained reasonably, which proves the effectiveness and practicality of the method in the unified calculations of optical and EPR data for crystals doped with d^3 ions. The defect structure of Cr^{3+} center in $\text{LaMgAl}_{11}\text{O}_{19}$ crystal due to the size mismatch is also estimated.

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