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# Energy Spectra, g Factors and Their Pressure-Induced and/or Thermal Shifts of $SrTiO_3:Cr^{3+}$ and $SrTiO_3:Mn^{4+}$ I: Energy Spectra and g Factors at Normal Pressure

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Abstract: With the strong-field scheme and cubic bases, the complete $d^3$ energy matrix in a tetragonally distorted cubic-field has been constructed. By diagonalizing this matrix, the energy spectra of $SrTiO_3:Cr^{3+}$ and $SrTiO_3:Mn^{4+}$ at normal pressure and various temperatures have been calculated. Correspondingly, the FORTRAN program calculating the g factor of the ground state has been worked out. By using the program and the wavefunction obtained from diagonalizing the complete energy matrix, the g factors of the ground state of $SrTiO_3:Cr^{3+}$ and $SrTiO_3:Mn^{4+}$ at normal pressure and room temperature have been evaluated. The calculated results are in good agreement with the optical-spectral and EPR experimental data. The comparison and analysis of the results of two crystals have been made. It is demonstrated that the covalency of the bonding between $Mn^{4+}$ and ligands ($O^{2-}$) in $SrTiO_3:Mn^{4+}$ is stronger than the one of the bonding between $Cr^{3+}$ and ligands ($O^{2-}$) in $SrTiO_3:Cr^{3+}$. It is shown that the obtained wavefunctions and values of parameters are reasonable.

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