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Anisotropy of the paramagnetic susceptibility in LaTiO3: The electron-distribution picture in the ground state

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Abstract

The energy-level scheme and wave functions of the titanium ions in LaTiO3 are calculated using crystal-field theory and spin-orbit coupling. The theoretically derived temperature dependence and anisotropy of the magnetic susceptibility agree well with experimental data obtained in an untwinned single crystal. The refined fitting procedure reveals an almost isotropic molecular field and a temperature dependence of the van Vleck susceptibility. The charge distribution of the 3d-electron on the Ti positions and the principle values of the quadrupole moments are derived and agree with NMR data and recent measurements of orbital momentum □l□ and crystal-field splitting. The low value of the ordered moment in the antiferromagnetic phase is discussed.

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