ELECTRONIC STRUCTURE AND MAGNETISM OF $LaVO_3$ and $LaMnO_3$

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9.7 cm

$LaVO_3$ and $LaMnO_3$ are a subject of large interest by almost of 30 years due to their anomalous magnetic properties. In this contribution we derive and discuss energy levels of the strongly-correlated d^2 configuration of the V^{3+} ion and of d^4 configuration of the Mn^{3+} ion in the octahedral surroundings in the presence of the spin-orbit coupling and the resulting magnetic properties. We take into account very strong correlations among the d electrons and work with strongly-correlated atomic-like electronic systems, ground term of which is, also in a solid, described by two Hund's rules quantum numbers. In a solid we take into account the influence of crystal-field interactions, predominantly of the cubic (octahedral) symmetry. We describe both paramagnetic state and the magnetically-ordered state getting a value of 1.4 u_B for the V^{3+}-ion magnetic moment in the ordered state at 0 K of $LaVO_3$ ($^3T_{1g}$) and of 3.7 u_B for $LaMnO_3$ (^5E_g). Both values well reproduce the experimental data. A remarkably consistent description of both zero-temperature properties and thermodynamic properties indicates on the high physical adequacy of the applied atomic approach, being somehow a continuation of Van Vleck's studies. The shown ground states have been confirmed recently by other researchers. We point out the necessity to unquench the orbital moment in 3d-ion compounds.

13.4 cm

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