Electronic structure of $LaMnO_3$ and magnetocaloric effects

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For understanding of electronic, magnetic and transport properties of Sr/Ca doped $LaMnO_3$ it is of fundamental importance to know the electronic structure of the maternal stoichiometric compound. Despite of very extensive theoretical studies the consensus about the electronic structure of $LaMnO_3$ is not reached yet. In the current literature there are electronic structures with continuous energy spectrum for *d* electrons as well as with a discrete energy spectrum, with completely different ground state. We advocate for the existence in $LaMnO_3$ the discrete electronic structure related to the Mn^{3+} ion in $LaMnO_3$ with the ^5E_g octahedral subterm as the ground state (Physica B **281-282** (2000) 507; cond-mat/0211595) - such the ground state is, however, questioned, to our big surprise, by the magnetic community, recently by the Scientific Committee of the Strongly-Correlated Electron System Conference SCES-02 [OO015PO]. We hope that the present Conference provides a good scientific forum for the open discussion of the electronic structure of the stoichiometric $LaMnO_3$. We point out that the desired properties of manganites result from strong correlations among *d* electrons, where the relativistic spin-orbit coupling and the local symmetry (Jahn-Teller effect) at the Mn site play fundamentally important role.

The physical superioty of our approach, that we call Quantum Atomistic Solid State Theory (QUASST) lies in the fact that it provides a consistent explanation for the electronic structure of 3*d*-atom-containing compounds (Mott insulators). The crystal-field-based approach completed with spin-orbit interactions accounts both for the ground-state properties and thermodynamics (temperature dependence of the susceptibility, of the ordered magnetic moment, of the heat capacity). Large magnetocaloric effects we take as one of confirmation of the derived by us low-energy electronic structure of the Mn^{3+} in the octahedral symmetry as related to large number of states close to the ground state. The calculated magnetic moment of the Mn atom in $LaMnO_3$ amounts to 3.72 μ_B and is built up from

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the spin and orbital moments of +3.96 μ_B and -0.24 μ_B, respectively. Moreover, the calculated moments order in the a-b plane, i.e. like in the reality.

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