Ground state of the Mn^{3+} ion in $LaMnO_3$ - ^5E_g or $t_{2g}^3e_g^1$?

Z. Ropka[1] *and R. J. Radwanski*[1,2,*]

[1] *Center of Solid State Physics; S^nt Filip 5, 31-150 Krakow, Poland*
[2] *Institute of Physics, Pedagogical University, 30-084 Krakow, Poland*

(presented at XII Krajowa Szkola Nadprzewodnictwa:
"Uklady skorelowanych elektronow wczoraj i dzis",
Ustron 15 IX 2006, Chairman: Prof. dr hab. J. Spalek
Polish version of this abstract was in Acta Physica 3, 35 (2007);
published 30 September 2007; online: www.actaphysica.eu)

Keywords: Strong electron correlation, crystal field, orbital moment, $LaMnO_3$

$LaMnO_3$ is a solid with high application potential in spintronics after a partial substitution of La atoms by Ca or Sr ones. These substitutions lead to ferromagnetic state and, what is more important, to increase of temperature of magnetic ordering close to room temperature what enables practical application. Ground state is/was a subject of long lasting controversy. Results of our calculations, confirming earlier crystal-field theory calculations, for the ^5E_g state as ground state of Mn^{3+} ion in $LaMnO_3$ did not get appreciation in year of 2002, at the SCES-02 Conference. Opponents raise that other researchers gave the ground state as $t_{2g}^3e_g^1$, with the t_{2g} states as the lowest and the e_g state lying higher.

In the present contribution we will explain that the ^5E_g state is one of 80 states of $t_{2g}^3e_g^1$ configuration of the Mn^{3+}. It means that giving by us the ground state as ^5E_g is more specific information than giving a configuration $t_{2g}^3e_g^1$. We will show that formation of the ^5E_g state is a sign of strong electron correlations, including Hunds rules. We will analyze influence of local distorsions, considered often as Jahn-Teller effect nad formation of the magnetically-ordered state connected with breaking of the time reversal symmetrii.

Modern methods enable calculations of electronic structure from first principles. Our calculations from first principles enable consideration of the electronic structure in the energy scale of 1 meV. For these calculations relativistic spin-orbit interaction is fundamentally important.

Our long studies of $3d$ compounds reveal importance of orbital moment and orbital magnetism indicating that it is the highest time to unquech the orbital moment in compounds containing atoms with incomplete $3d$ shell.

* http://www.css-physics.edu.pl; Email: sfradwan@cyf-kr.edu.pl