Comment on "Orbitally degenerate spin-1 model for insulating $V_2O_3$"

R.J. Radwanski

Center for Solid State Physics, St. Filip 5, 31-150 Kraków, Poland,
Institute of Physics, Pedagogical University, 30-084 Kraków, Poland.

Z. Ropka

Center for Solid State Physics, St. Filip 5, 31-150 Kraków, Poland.

e-mail: sfradwan@cyf-kr.edu.pl

We criticize the model proposed by Mila et al. (Phys.Rev.Lett. 85 (2000) 1714) for the description of the $V^{3+}$ ion in $V_2O_3$ by pointing out that it is completely artificial because the condition about the degenerate (doublet) orbital ground state required for the authors’ model cannot be realized in the reality. We claim that the $V^{3+}$ ion should be considered as described by the quantum numbers $S=1$ and $L=3$ and with taking into account the orbital moment and the intra-atomic spin-orbit coupling.

In a recent Letter [1] Mila et al. have proposed a new "orbitally degenerate spin-1 model for the insulating $V_2O_3$". By this Comment we criticize [2] this model pointing out that the model proposed by authors for the description of the $V^{3+}$ ion in $V_2O_3$ is completely artificial because i) the condition about the degenerate (doublet) orbital ground state required for the authors’ model cannot be realized in the reality. Moreover, we criticize ii) the description of the $V^{3+}$ ion in $V_2O_3$ by an "orbitally degenerate spin-1 model" (i.e. with $S=1$ and $L=1/2$) as we iii) claim that the $V^{3+}$ ion in $V_2O_3$ should be described by the quantum numbers $S=1$ and $L=3$ [3,4].

The critiques i) and ii) are associated with the Jahn-Teller theorem that states that each system tends to, if possible, to the singlet ground state. Thus, the orbital ground state, demanded by the authors’ model, will be not realized in the reality.
The claim iii) follows from the two Hund’s rules (two rules, i.e. 1° the maximal S and 2° the maximal L for two d electrons) [5]. These two Hund’s rules yield S=1 and L=3. The 21-fold degeneracy will be removed by crystal-field and spin-orbit interactions [3,4], and finally by spin-dependent interactions yielding a singlet ground state of the V$^{3+}$ ion in the atomic scale. Despite of the singlet ground state state magnetism can develop by moment-induced mechanism like in many praseodymium compounds. Our understanding of 3d-ion compounds is close to an original idea of Van Vleck from 1932 [6], that electronic and magnetic properties are largely determined by the atomic-like electronic structure.

In favour of the authors’ model we would like to point out that their model with S=1 and L=1/2 is already closer to the reality than a model of Castellani et al. [7], a S=1/2 orbitally degenerate model, and a S=1 model without an orbital degeneracy [8]. These different models, currently discussed, clearly show that a description of V$_2$O$_3$, as well as many other 3d-ion compounds, is far from being established calling for the normal open scientific discussion.

In a conclusion, the model proposed by authors is much artificial because the condition about the degenerate (doublet) orbital ground state required for the authors’ model cannot be realized in the reality. We claim that the V$^{3+}$ ion in V$_2$O$_3$ should be considered as described by the quantum numbers S=1 and L=3. We are convinced that taking into account the orbital moment and the intra-atomic spin-orbit coupling is indispensable for the physically adequate description of electronic and magnetic properties of V$_2$O$_3$.

E-mail for correspondence: sfradwan@cyf-kr.edu.pl

[1] F.Mila, R.Shiina, F.-C.Zhang, A.Joshi, M.Ma, V.Anisimov and T.M.Rice, Phys.Rev.Lett. 85, 1714 (2000).

[2] We are not in favour of writing of the Comment, in which as the editorial obligation one has to criticize or correct somebody’s paper - thus please treat the Comment as an extended normal
scientific discussion. We are forced to write the Comment due to a hardly understandable and unacceptable politics of the Editors of Phys.Rev.Lett., that finds some papers, on the electronic structure and the magnetism of 3d-ion compounds pointing out the importance of the spin-orbit coupling and the orbital moment, as inappropriate for the publication in Phys.Rev.Lett.. This controversy about the role of the spin-orbit coupling and the discrete states in description of electronic and magnetic properties of compounds containing 3d ions is a subject of an scientific bet for 1 million USA dollars to Editors of Phys.Rev.Lett. (with 1:4000 subsequent inputs, taking into account the 40 involved referees and 100 times, at least, greater their scientific experience), namely the Editor-in-Chief Dr M.Blume, Dr W.E. Brown, Dr. Z. Fisk and Dr. M. Sandweiss.

[3] R.J.Radwanski and Z.Ropka, Relativistic effects in the electronic structure for the 3d paramagnetic ions, http://xxx.lanl.gov/abs/cond-mat/9907140.

[4] R.J.Radwanski and Z.Ropka, Quantum numbers of the V^{3+} ion in V_2O_3, submitted to Phys.Rev.Lett.; http://xxx.lanl.gov/abs/cond-mat/0010218.

[5] C.Kittel, in: Introduction to Solid State Physics (John Willey, 1976) ch. 14.

[6] J. H. Van Vleck, The theory of electric and magnetic susceptibilities, Oxford Univ. Press, 1932.

[7] C.Castellani, C.R.Natoli and J.Ranninger, Phys.Rev. B 18, 4945 (1978); 18, 4967 (1978); 18, 5001 (1978).

[8] S.Yu.Ezhov, V.I.Anisimov, D.I.Khomskii and G.A.Sawatzky, Phys.Rev.Lett. 83, 4136 (1999).