Comment

Comment on Phys. Rev. B "Orbitally driven spin pairing in the three-dimensional nonmagnetic Mott insulator $BaVS_3$: Evidence from single-crystal studies" - wrong description of the V^{4+} ion

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In a recent Letter [1] Mihaly *et al.* have discussed properties of $BaVS_3$ recalling the crystal-field splitting of the vanadium *d* levels associated with the V^{4+} ion ($3d^1$ configuration) shown in Fig. 4a. By this Comment we would like to point out [2] that the analysis of the crystal field splitting recalled by authors for the description of the V^{4+} ion in the octahedral crystal field with distortions is wrong. We should say that we are in favour of the CEF theory but it should be correctly considered. By this Comment we would like to point out that there is the spin-orbit coupling that, though weak in 3*d* ions, always exists. It drastically changes the electronic structure and the magnetism of the V^{4+} ion. The calculated effect of distortions on the electronic structure

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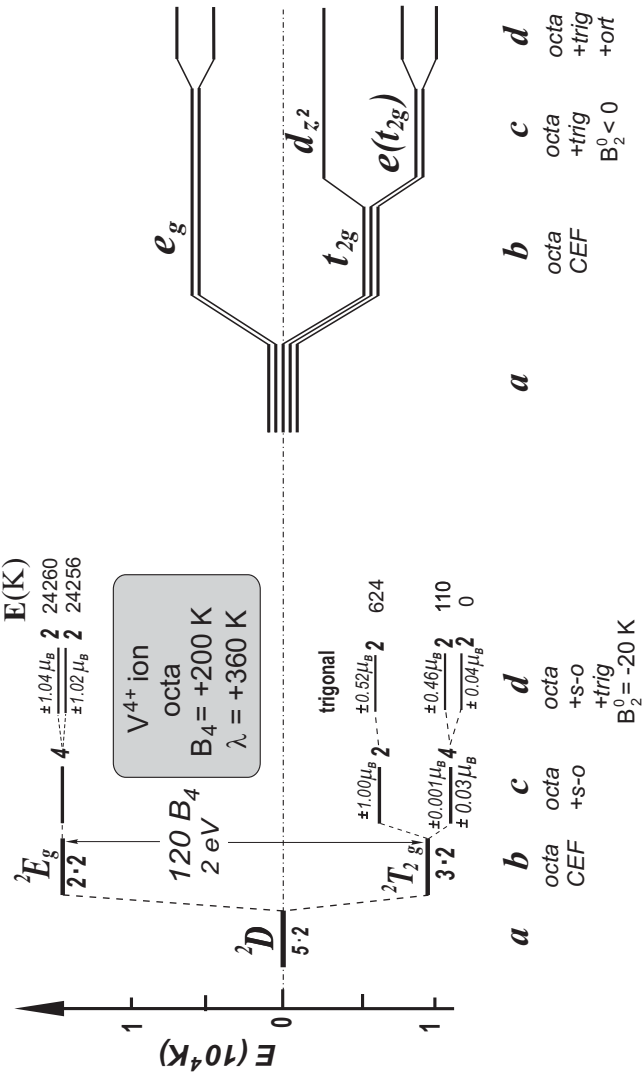

FIG. 1: Crystal -field splitting of the vanadium 3*d* levels due to the symmetry reduction from the octahedral symmetry with the intraatomic spin-orbit coupling (left side: a, b, c taken after our Refs 3, 5) and without the spin-orbit coupling (right side, after the commented Ref. 1). There is a drastic change of the electronic structure by taking into account the intra-atomic spin-orbit coupling what is the main point of our understanding of 3*d* compounds.

in the presence of the spin-orbit coupling is shown on the left side in Fig. 1 [3–5]. One can see that the electronic structure with taking into account the spin-orbit coupling differs significantly from the very simplified electronic structure presented in the commented paper on Fig. 4a. One of the consequences of the spin-orbit coupling is that the spin and the orbital degrees of freedom are correlated. From the values of the magnetic moments shown in Fig. 1a one can see that there is the very large orbital moment present. Thus, the V^{4+} ion cannot be considered as the S=1/2 system.

In conclusion, for consideration of the crystal-field electronic structure of the V^{4+} ion the intra-atomic spin-orbit coupling has to be taken into account. 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 $BaVS_3$ (as well as other $3d$-ion containing compounds). Calculations without the spin-orbit coupling suffer invalidated simplification.

[1] G. Mihaly, I. Kezsmarkt, F. Zamborsky, M. Miljak, K. Penc, P. Fazekas, H. Berger, and L. Forro, Phys. Rev. B **61**, R7831 (2000); arXiv:cond-mat/9911122 (1999).

[2] We are not in favour of writing of Comment, in which as the editorial obligation one has to criticize or correct somebody's paper - thus please treat Comment as an extended normal scientific discussion. We are forced to write Comment due to a hardly understandable and unacceptible politics of the Editors of Phys. Rev., 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. The paper of Ref. 1 clearly shows that taking into account the spin-orbit coupling is not the rule in Phys. Rev.

[3] R. J. Radwanski and Z. Ropka, [Acta Physica **21-22**, 1 (2008)], arXiv:cond-mat/9907140 (1999), *Relativistic effects in the electronic structure for the 3d paramagnetic ions.*

[4] a very simplified analysis of the spin-orbit coupling with the quartet-doublet sequence (in fact, the orbital doublet-singlet sequence) one can find already on p. 417 in A. Abragam and B. Bleaney, in: *Electron Paramagnetic Resonance of Transition Ions* (Clarendon Press, Oxford) 1970.

[5] Z. Ropka, R. Michalski, and R. J. Radwanski, [Acta Physica **14-15**, 29 (2008)], arXiv:cond-mat/9907141 (1999), *Anomalous temperature dependences of the susceptibility for the one-3d-electron cation.*