Comment

Comment on Phys. Rev. B "Electronic structure, phase stability, and magnetic properties of $La_{1-x}Sr_xCoO_3$ from first-principles full-potential calculations" - the neglect of the orbital moment

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In Ref. [1] Ravindran *et al.* have presented generalized-gradient-corrected, relativistic first-principles full-potential density functional calculations for $LaCoO_3$.

By this Comment [2] we would like to point out that there is a text-book knowledge [3] that the Co^{3+} ion should be considered as the system with S=2 and L=2, but not as the system with S=2 or S=0 only. According to us the orbital magnetism has to be taken into account for the understanding of properties of $LaCoO_3$.

Authors of Ref. 1 write that "In the cubic perovskites, the octahedral ligand field produced by the O atoms surrounding each Co atom split the tenfold degenerate d levels of Co ..." (p. 16426, left column). It is not true as the lowest term of the Co^{3+} ion in the octahedral field is 25-fold degenerated [4–7], see also [2] and [3]. The statement of Ref. 1 is valid only for the single d electron, but not for 6 d electrons existing in the Co^{3+} ion.

We fully agree with the authors of Ref. 1 that "the present (i. e. of Ref. [1]) theory is unable to predict the semiconducting state of $LaCoO_3$" (p. 16426, right column), i.e. the insulating state at 0 K. Moreover, we can add that also thermodynamics cannot be calculated within the approach of Ref. [1].

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In conclusion, despite of the very complex name of the approach, the approach of Ref. [1] suffers substantial limitations related to the neglection of the orbital magnetism [8]. This deficiency causes that the results are incompatible to the reality. It means that we still need to look for the understanding of the old problem related to $LaCoO_3$. Here we can only mention our atomic-like approach, that give surprisingly good results for $LaCoO_3$ [5–7]. Our approach yields the discrete energy spectrum for the d states in $LaCoO_3$ in contrary to the continuum energy spectrum of Ref. [1] (see Fig. 3), but further discussion goes beyond the present Comment.

[1] P. Ravindran, P. A. Korzhavyi, H. Fjellvag, and A. Kjekshus, Phys. Rev. B **60**, 16423 (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] A. B. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions* (Clarendon Oxford) 1970, ch. 7; B. N. Figgis, *Introduction to Ligand Fields* (Interscience, New York, 1966) ch. 7.

[4] P. D. Adams and P. Boucher, editors of Phys. Rev. B, during the long referee process of the paper: Influence of the spin-orbit coupling on the cubic crystal-field states of the d^6 system (BNR670), submitted 22.01.1998, strongly state that the 25-fold degeneracy is quite obvious. The commented paper, Ref. 1, shows that it is not so.

[5] R. J. Radwanski and Z. Ropka, Solid State Commun. **112**, 621 (1999) [for final our description of $LaCoO_3$ see Phys. Rev. B **67**, 172401 (2003)].

[6] 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.*

[7] Z. Ropka and R. J. Radwanski, [Acta Physica **25**, 21 (2008)], arXiv:cond-mat/0005505 (2000), *The existence of the fine electronic structure in $LaCoO_3$.*

[8] A. M. Begley, editor of Phys. Rev. B, maintains the statement of a Phys. Rev. B referee that, as $LaCoO_3$ is nonmagnetic, there is no orbital magnetism. This statement is, according to us, incorrect. The orbital magnetism is related to $L \neq 0$.