Why a paper to Phys. Rev. Lett.: "Relativistic effects in the electronic structure for the 3d paramagnetic ions" has been written and WHY WE DO CHALLENGE Phys. Rev. Lett. and Phys. Rev. B? – steps of a scientific discrimination in Phys. Rev. Lett. and Phys. Rev. B

The paper "Relativistic effects in the electronic structure for the $3d$ paramagnetic ions" (LE6945) is a rather simple paper. However, for its today judging it is worth to know why it was written. It has been submitted to Phys. Rev. Lett. 30 May 1997 (sent date by post 19.05.1997) in situation when:

1. the referee of Phys. Rev. B referring our paper "The orbital-doublet E_g state the ground state of the Mn^{3+} ion in $LaMnO_3$" BZR586 in his report of January 8, 1997 wrote that "The orbital doublet state (E_g) is unaffected by the spin-orbit coupling." [the original report is in Acta Physica **9-10** (2007) 24]. On this basis our paper has been rejected because we have got that the ^5E_g state for the Mn^{3+} ion is split by the spin-orbit coupling as is seen in Fig. 1 of our paper. The referee wrote that our calculation is wrong. Later, March 25, 1997, in his 3^{rd} report the referee has admitted that our calculations are correct writing "I am full of apologies to the author." [the original 3^{rd} report is in Acta Physica **9-10** (2007) 31]. In meantime, despite of our explanation of January 15, 1997 (see Acta Physica **9-10** (2007) 26) he wrote the 2^{nd} report, February 12, 1997, still claiming the our computer program is incorrect (see Acta Physica **9-10** (2007) 27]. Taking into account that Phys. Rev. has the best referees and being sure of our calculations we have submitted 21 January, 1997 to Phys. Rev. Lett. next our paper "Influence of spin-orbit interactions on the cubic crystal-field states of the d^4 system" which has been registered as LA6567 [Acta Physica **9-10** (2007) 46]. This paper was written just after getting the 1^{st} negative report of January 8, 1997.

2. In May 1997 Editor of Phys. Rev. Lett. has accepted a referee report (C) to the above mentioned paper LA6567 with a reproach "The author (i.e. me) may learn about the spin-orbit calculations by searching with names like Solovyev" [see the following page 12]. In such the circumstances I have found that Solovyev in just published paper [Phys. Rev. B **53** (1996) 7158] does not take into account the spin-orbit coupling at all. The neglect of the spin-orbit coupling is clearly admitted

on p. 7164, left column, 16 lines bottom, "We leave the effects of the spin-orbit coupling for future investigations". This paper of Solovyev *et al.* was important because its aim was to explain magnetic properties and the electronic structure of $LaMO_3$ (M=Ti-Cu) perovskites from first principles. One of the consequence of leaving off the s-o coupling is that Solovyev *et al.* can calculate the spin moment only (Table III) whereas we have claimed the importance of the orbital moment. At present the orbital magnetism is generally accepted confirming that I was right though my papers have not been published. In a situation of continuous rejection of my papers in Phys. Rev. Lett. and Phys. Rev. B, finding them "not to be suitable and not of wide interest" in June 24, 1997 I have submitted a Comment to Solovyev's paper which has been registered BFK631 [Acta Physica **18** (2008) 23, my submission letter on p. 27].

Thus, one can see that the simple paper grew up to a scientifically-important paper. The referee wrote erroneous report, the Editor rejected the paper, and later the Editor did not like to admit the error. We remind that all started with our paper: "The E_g ground state of the Mn^{3+} ion in $LaMnO_3$" in which we calculated the E_g doublet as the ground state in $LaMnO_3$ instead of always drawn electronic structure with the lowest triplet t_{2g} and excited e_g doublet (see also Acta Physica **9-10** (2007) 39). Having belief that the Phys. Rev. Lett. and Phys. Rev. B, being very prestigous scientific journals, have the best referees in the world we were entitled to point out the importance of the spin-orbit coupling and the orbital magnetism in description of $3d$-ion containing compounds. The applicability of our CEF approach to NiO and calculations of the orbital moment has been submitted to Phys. Rev. Lett. in 1999 (LF7313: Orbital moment in NiO) - its rejection has led to the discrimination decision udertaken by the Editor-in-Chief dr M. Blume March 7, 2000 [the original decision on page 34]. **At present everybody knows that the crystal-field, spin-orbit coupling and strong correlations are fundamentally important for description of magnetic, electronic and optic properties of 3d-ion containing compounds.**
We think that we have a quite significant contribution to this understanding - a hundred of referees have learned our approach named the Quantum Atomistic Solid State theory (QUASST) with the discrete atomic-like electronic structure. Despite of discrimination we described at the atomic scale properties of NiO, CoO, FeO, $LaCoO_3$, $Nd_2Fe_{14}B$, $ErNi_5$, Ho_2Co_{17}, UGa_2, UPd_2Al_3, $YbRh_2Si_2$, and many others.

September 25, 2008

R. J. Radwanski

PHYSICAL REVIEW
PHYSICAL REVIEW LETTERS

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14 May 1997

Re: Influence of spin-orbit interactions on the cubic crystal-field states of the d^4 system

By: R.J. Radwański LA6567

Dear Dr. Radwański:

The above manuscript has been reviewed by our referee(s).

On the basis of the resulting report(s), we conclude that the paper is unsuitable for publication in Physical Review Letters. We enclose comments from the criticism that led to this editorial decision. In accordance with our standard practice (see enclosed memo), this concludes our review of your manuscript.

Yours sincerely,

Gene L. Wells
Editor
Physical Review Letters

Referee C

Manuscript Number: LA6567

Author: R.J. Radwanski

Title: Influence of spin-orbit interactions on.....

Referee Report

The author's statement ' Nowadays performed band-structure calculations generally ignores spin-orbit interactions ' is incorrect. The author may learn about these calculations by searching with names like Solovyev (e.g. Phys. Rev. B55 (1997) 8060 and references therein). It is true, however, that a band calculation, even if it includes spin-orbit coupling, does not deal with the ionic state in the way this author does, who considers a single-ion Hamiltonian, his eq. (2). The result is perhaps interesting (in-spite of the peculiar ref.7), but is of little relevance for the manganites where, surely, hybridization effects are important which are not part of the phenomenological Hamiltonian, eq. (2). Thus one is left to judge the isolated results that appear in the figures and here I must agree with the previous referees: This is not enough to warrant publication in Phys. Rev. Letters or in Phys. Rev.

Submission to Phys. Rev. Lett.: LE6925 "Relativistic effects in the electronic structure for the 3d paramagnetic ions"

Krakow, 19 May 1997

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Phys.Review Lett.,
Editor 1 Research Road,
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Dr G. Wells

The submittal to Phys. Rev. Lett.

Dear Sir,

Please find enclosed the manuscript, plus 2 copies, of my paper entitled:
"Relativistic effects in the electronic structure for the 3d paramagnetic ions" that I submit for publication in Phys. Review Lett.. Also floppy: radwanre.wp5 in Word Perfect 5.1.

Paper accounts 6 pages with 22 references, 2 figures and 1 table in total length less than 450 PR lines.

The Phys. Rev.Letter Journal has been chosen due to continuously going discussion in Phys. Rev. Lett. about the electronic structure of 3d paramagnetic ions. Many of them, if not all, constituent widely-known Mott insulators, a class of compounds of important theoretical interest.

The Letter presents new interesting results. **For the first time the effect of spin-orbit coupling has been correctly calculated for the 3d^n systems.** Most of presently-published papers do not discuss

the spin-orbit coupling at all. The spin-orbit coupling makes that d electrons cannot longer be treated as nearly-free electrons as is assumed in standard band-structure calculations. It is concluded in this Letter that the discussed now the relativistic spin-orbit coupling is indispensable for the proper evaluation of the electronic structure of $3d$ paramagnetic ions.

The presented results will have enormous impact on our understanding of properties of $3d$-ion compounds both the diluted systems like semimagnetic semiconductors, the dense $3d$ compounds like FeO, NiO, $LaCoO_3$ or $LaMnO_3$ as well as other complex $3d$-ion containg systems (NENP, NENC and so on). Results will be of large interest to physicists and chemists working on $3d$ paramagnetic-ion compounds and alloys.

I would appreciate the fast referee process and the acceptance of this letter for publication in Phys. Rev. Letters. **As this Letter presents new theoretical results that reveal the large shortage of the nowadays understanding, please take personal responsibility for the referee process. I would remind a Karl Popper thesis about the revolutionary way of the developing Science.**

Please, keep me informed about the referee procedure. **Please insist the referee for the clear scientific report.**

Sincerely Yours,
R. J. Radwanski

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Krakow, 4 September 1997

The Editor of
Phys. Review Letters

LE6925

Dear Editor,

In the answer to a letter of your Assistant of 8.08.1997 concerning my paper: **Relativistic effects in the electronic structure for the 3*d* paramagnetic ions" (LE6925)** please find included:
1) my appeal to The Editor-in-Chief of the APS
2) with information for the Chairman of the American Physical Society.
3) My answer to the referee report A.

My claims and arguments you can find in these letters.

In this situation please transfer my appeal to the Editor-in-Chief and send the copy to the Chairman of the American Physical Society.

Please, ask the referee for the detailed information where results similar to mine have been published. Please inform me what is the answer of the referee.

I repeat, **I have chosen Phys. Rev. Letters expecting the best referees and the best, honest scientific treatment.** I still expect your cooperation for progress in Physics. Please, realize that I am spending enormous time, life energy and my private money for this scientific work and the heavy correspondence. Instead of working on Physics I am writing these nonsens appeals and answers to undefined unscientific referee reports.

As you know I have sent to you a number of papers - it shows the real prediction power, a good sign of any valuable theory. Please take care seriously for the real scientific arguments. Your treatment of my Comment LGK652 is unacceptible.

I am preparing appeals on your other negative decisions. I am ready for the open real scientific discussion. Please, insist on the referees for

good clear scientific reports. I will still send new papers for publishing - I consider PRL to have the best referees. I suppose you agree with it.

I cannot accept often made arguments in other my papers of "unsufficient importance and not broad interest". Such not-to-discussion arguments have been given in Poland by the communistic regime. It is surely not scientific arguments. Do not you have better referees?

At the end, let me say that the treatment of my papers in Phys. Rev. Letters goes to the scientific scandal. It becomes already a beautyful example for the Karl Popper's theory. It is a reason for informing the Chairman of the American Physical Society - I hope that there is a number of philosophers of science ready to study it.

In such circumstances I call for fast publication of my paper. Otherwise, I expect clear scientific arguments.

Sincerely Yours,
R. J. Radwanski

Author answer to the referee report A

Krakow, 4 September 1997

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LE6925: Author answer to the referee report A concerning my paper:
Relativistic effects in the electronic structure for the 3d paramagnetic ions" (LE6925)

Dear Referee,
Sorry, but you are completely mistaken.

I repeat - my paper presents for the first time exact results of the influence of spin-orbit coupling on crystal-field states. Please, give the detailed reference.

But point by point. Two first sentences are simply descriptive. In the 2^{nd} sentence it is not clear if the referee, repeating part of my conclusions, agrees or disagrees with this my conclusion. I think that for any physicists it is obvious that the existence of localized states with so dramatically different magnetic characteristics, as shown in Fig. 1, will affect the low-temperature properties. The calculations of specific systems, as the referee suggested in the end of his report, have been performed already - due to the shortage problem they constituates separate papers. For example, I have prepared already d^4 related with $LaMnO_3$ (LA6567), d^6 system applicable to $LaCoO_3$ (LE6485); Comments: $LaTiO_3$- BFK631; $FeBr_2$ - BHK634; $LaCoO_3$ - BHK633). Please be advised that discussion of all properties of one compound takes more than one paper - there is hundrends of papers in literature devoted to $LaCoO_3$, for instance. In the present paper results for the Fe^{2+} ion in MgO and NiO have been obtained in good agreement with experiment.

The first two sentences of the second akapit reveals the shortage of the text-book knowledge about the crystal field and spin-orbit interactions. **This diagonalization has never been done -if you disagree, please give the reference to a book or journal.** 40 years ago this

kind of calculations have been done by the perturbation method, that are only very approximate. Results can be found in a Bible-book of Abragam and Bleaney (1970), mentioned in my paper as ref. 17, in Fig. 7.19 and 7.20. My calculations have revealed new features with respect to 1) the existence of extra splittings, 2) the evaluation of magnetic characteristics. Please put also the attention to values of magnetic moments of ground states.

Prof. John Goodenough, one of the most prominent experts in this field, has recently admitted to me that he was one of people who has always believed that the ^5E_g state for the d^4 system never splits. On similar argument one of my papers has been originally rejected in Phys. Rev. B - after a 3-letters discussion the referee has admitted that I am right about the splitting of the ^5E_g state. We agreed that it results from the second-order effect of the spin-orbit coupling not performed by the perturbation method.

Moreover, found by me very small moments for the d^1 system will help to understand behaviour of $LiV2O_4$, exotic properties of which have been just published in PRL (78, 3729).

In such situation saying by the referee that "paper does not present any new physical information" indicates on his enormous shortage of the 3*d*-magnetism subject.

Dear referee, did you notice that studies, as mine, of many-electron crystal-field states have been almost stopped about 40 years ago when the 3*d* physics had been directed into one-electron crystal-field states and one-particle band-structure theories.

In such circumstances I call to you - please write where figures similar to mine have been published.
I expect you to behave as the real honest scientistist.
I expect clear scientific arguments.

Sincerely Yours,
R. J. Radwanski