2^{nd} APPEAL TO CHAIRMAN of DAE
J. Sandweiss

Krakow, 17 September 1999

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Prof. J. Sandweiss
Editor and Chairman of DAE
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LE 6925: Relativistic effects in the electronic structure of 3d-ion by me and Z.Ropka.

Dear Editor and Chairman of DAE,
Thank you very much for your very kind letter of 15.07.1999 being the answer to my letter of 18.02.1999. I appreciate very much your statement that you can be convinced by the scientific arguments. It should be obvious in the scientific journal but it is not often the case up to now. The Editor too often rejects the paper as not being suitable that is not at all the scientific argument.

Sorry for the delay but I have been for Conference in Japan (Strongly-Correlated Electron Systems in Nagano) and Budapest (Neutrons).
In your nice letter in fact you put two scientific points:
1. in the acapit 3 (I do think ....) However, that such effects (i.e. the relativistic effects are important in atomic physics) are present is not, at this time surprising. Nor do the effects overturn in, any basic way, our understanding of systems you have studied.
Although the first sentence could be true in atomic physics this is not the case in solid-state physics dealing with systems containing enormous number of $3d$ ions, each of them representing many-body problem. In fact, in solid-state physics, according to me, the main scientific point is how far the atomic physics is applicable to the solid state physics. Presently in fashion view is that atoms forming a solid loose largely their atomic properties and form a black box. Examples

of such treatment you can find in papers published in PRL and cited in my paper: Ref. 1 (PRL **75** (1995) 1126); Ref. 9 (PRL **75** (1995) 3910) where instead of atomic-like states of 3d electrons the bands are considered. Note that these bands are hundred times wider than the derived by me the fine electronic structure. Thus, the discussed by me effects are hundred times more subtle than discussed at present in the solid-state physics.

Although the s-o coupling is obviously known in atomic physics it is neglected in description of $3d$-ion compounds as this is weak interaction for $3d$-ions. I gave a number of examples in previous answers to the referees you can look to the just published paper in PRL 83 (1999) 1387 from 16.08.1999 (I found it today i.e. 17.09.1999) for the approach to Vanadium oxides. In these compounds vanadium is as V^{4+} ion i.e. as one electron system. They describe it as collection of the S=1/2 spin (just effect of the neglect of the spin-orbit coupling). The problem is the origin of anomalous temperature dependence of the susceptibility with a maximum about 50 -300 K and a dramatic lowering at low temperatures. It completely violates the Curie law. Authors of PRL **83** (1999) 1387 get this behavior by manipulating the directions of spin due to different values of exchange interaction parameters. According to me this behavior is due to single-ion effects and you can find its origin already in my figure of the paper LE6925. You can see that for the d1 system the ground state has very small magnetic moment whereas the excited state has moment close to 1. As a consequence the temperature dependence will show anomalous temperature behavior with a non-magnetic (weakly-magnetic) low-temperature ground state and a maximum. This has been calculated by us in the Letter submitted in June [1999] to PRL (LF7379) [Acta Physica **14-15** (2008) 1]. The curve 4 of Fig. 4 of our paper is quite similar to that what authors of paper PRL **83** (99) 1387 have got by manipulation of the direction of spins at different sites by means of different exchange parameters. It means that authors of just published paper in PRL do not know this atomic physics because going to very complex explanation should check the simpler i.e. atomic physics explanation. Soon we will write the Comments on paper PRL **83** (1999) 1387.
Thus:
i) I (with my coworkers) am not claiming to invent the spin-orbit coupling but
ii) I claim that the spin-orbit coupling is essentially important for description of electronic and magnetic properties understanding of compounds containing 3d elements,

iii) It means that I think that taking the spin-orbit into account can overturn our understanding of many 3*d*-ion systems, ...

In conclusion, the inclusion of the spin-orbit coupling, known from the atomic physics, to solid-state physics can overturn largely our understanding of many systems.

2. the spin-orbit coupling for transuranic systems.
I have analyzed more than 50 rare-earth systems within the single-ion approach, starting from my work for the University of Amsterdam, revealing the atomic-like electronic structure (crystal-field levels) with energy details below 1 meV ($ErNi_5$ - Physica B **177** (1992) 291; $NdNi_5$- J. Phys.: Cond. Mat. **6** (1994) L15; J. Magn. Magn. Mat. **157/158** (1996) 407). This analysis has been very successful. It works also for heavy-fermion superconductor $Nd_{2-y}Ce_yCuO_4$ Solid St. Commun. **99** (1996) 981.
Moreover, this atomic-like picture I have applied to actinides like URu_2Si_2 (J. Magn. Magn. Mater. **103** (1992) L1; UGa_2 J. Alloys and Comp. **219** (1995) 260; J. Magn. Magn. Mater. **140-144** (1995) 1373; $NpGa_2$ J. Phys.: Cond. Mater. **8** (1996) 10467 and very consistent description has been obtained. Here also is worth to mention very successful analysis of UPd_2Al_3 in Physics of Transition Metals, (World Scientific 1992) eds. Oppeneer and Kubler, p. 38.

In conclusion, the spin-orbit coupling has been found already to be important for actinides.

In final conclusion, the very similar approach we have applied in LE6925 to 3*d* ion compounds but the s-o coupling is thousands times smaller for the 3d ions. **Despite of this weakness we conclude that the atomic spin-orbit coupling has to be taken into account for description of 3*d*-ion systems.**

I hope that you are satisfied with our answer. Please give the positive opinion about our Letter and recommend it for publication. It could be with a note about the referee objections.
In the final conclusion, **I ask for publication of our Letter. It enables the open scientific discussion on important physics of 3*d* magnetism.**
We ask you for the scientific cooperation,

Sincerely Yours,
Ryszard Radwanski and Z. Ropka

PHYSICAL REVIEW LETTERS

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18 November 1999

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31-150 Krakow, POLAND

Re: Relativistic effects in the electronic structure...

By: R.J. Radwanski LE6925

Dear Dr. Radwanski:

I am writing in response to your e-mail of 9-November-99 concerning the appeal of your manuscript "Relativistic Effects in the Electronic . . ." LE 6925, submitted to PRL.

Unfortunately, I have not changed my view about the appropriateness of the manuscript for PRL. As I mentioned in my earlier letter, I do believe that you would be much better served by writing a longer, more complete article which could put forward your results and their consequences in a coherent and manifest fashion.

Sincerely,

Jack Sandweiss
Editor and Chairman of the
Divisional Associate Editors
Physical Review Letters

JS:pm

Appeal
1 million USD scientific bet to Dr J. Sandweiss

From: sfradwan@cyf-kr.edu.pl
To: prl@aps.org
Subject: appeal -bet to Dr Sandweiss, LE6925 Radwanski
Date sent: Mon, 29 Nov 1999 08:21:57 +0100

Krakow, 27 November 1999

From: Dr R.J. Radwanski
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with the information to Editor-in-Chief Dr M. Blume

LE 6925: "Relativistic effects in the electronic structure of 3d-ion"
by R. J. Radwanski and Z. Ropka.

Dear Editor and Chairman of DAE, Dr Sandweiss,
Thank you very much for your letter of 18.11.1999 (obtained by the post today) being the answer to my appeal of 9.11.1999.

I appreciate your not changing view about the appropriateness of my manuscript LE6925 for PRL. I am even in favour of it provided you undertake the full responsibility for your decision and undertake the scientific bet proposed by me.

In case when you and your "established experts in the relevant areas of solid state physics" reject my paper due to the different scientific opinions please take the full responsibility for it.

In this rejection situation I think that the normal scientific honesty requires from you to undertake this bet for 1 million USA dollars. I

increase my input for 500, please establish the bet. You still have rights to increase/decrease your evaluation according to your estimation of your experts. In fact, as you are convinced about my wrong approach you simply easily win. Do not hesitate.

Without this responsibility Phys. Rev. Lett. can freely manipulate Science.

Your sugestion that a longer, more complete article will be better served in Phys. Rev. Lett. does not have any guarantee. With a longer paper I can less know what is wrong in my paper. A statement on the first or may be on the second page. After the 2.5 year discussion I do not know what is wrong in my manuscript LE6925.

I hope that You undertake this scientific bet. In fact, the scientific honesty requires it from you. If you are sure of your knowledge and of your experts you do not loose anything

Looking hearing you in two weeks time (say to 12.12.1999).

Sincerely Yours,
R. J. Radwanski
Z. Ropka

PS. The best greetings for the Thanksgiving Day.