Spin-orbit singlet magnetism - Induced atomic U- and Ru-moment in URu_2Si_2 and in Sr_2RuO_4

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Despite the fact that spin-orbit (s-o) interactions are well know in the atomic physics its importance in the solid-state physics was only recognized about 15 years ago with studies of $5d/4d$ oxides like Sr_2IrO_4 or Sr_2RuO_4 [1,2]. Earlier a scientific papers pointing out the fundamental importance of the s-o interactions also in more-discussed $3d$ oxides have been rejected [3,4,5,6,7] even in the most prestigious journal as PRL or PRB with arguments that they are weak interactions, not of importance compared to U and J_H parameters of the energy size of 5 and 0.5 eV, respectively. Also, that there is no needs for such interactions for explanation of known, at that time, phenomena. A "revolution" about the importance of the s-o interactions seems to start with two Phys.Rev.Lett.'s papers of Jackeli and Khaliullin in 2009 [1,2]. In the first one they interpreted INS excitations in Sr_2IrO_4 as due to s-o interactions in the Ir^{4+}-ion in the $5d^5$ configuration [1]. In the second paper they managed to convince the PRL Editor that weak s-o interactions in the $V^{4+}(3d^1)$-ion produce the nonmagnetic state of the whole Sr_2VO_4 oxide [2] in contrary to my earlier submissions from 1997-2010. This nonmagnetic state is clearly shown in Fig. 1 of Ref. [4] from 1999 with detailed examples of the V^{4+} ions in $BaVS_3$ [6,7] and in Sr_2VO_4.

In this contribution I will discuss $3d/4d/5d$ compounds/oxides underlying i) formation of the charge ionic state with the well-defined integer valency, like U^{4+} and Ru^{4+} ions, ii) the discrete quasi-atomic crystal-field+s-o spin-orbital low-energy electronic structure and iii) the preservation of this low-energy (below 1 meV) quasi-atomic $3d/4d/5d$ electronic structure also in solid crystals. As the s-o effects I will discuss the formation of the singlet nonmagnetic ground state of the $U^{4+}(5f^2)$ and $Ru^{4+}(4d^4)$ ions and their preservation in URu_2Si_2 [3] and in Sr_2RuO_4. In the presented approach, which one could call as Quantum Atomistic Solid-State Theory (QUASST), the orbital moment, as the s-o effect, will be discussed in NiO (Ni^{2+}) [5] and in $FeBr_2$ (Fe^{2+}) [8].

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