Valence Fluctuations in Actinides

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The long-standing issue of non-magnetic δ-Pu, which could not be captured by conventional Denstity Functional Theory, triggered lot of interest in fundamentals of electronic structure of actinide systems. At present, the non-magnetic state can be obtained already by various types of calculations, although this does not help to distinguish, which types processes are dominant when forming or suppressing magnetic moments in Pu based systems and in general in light actinides. Recent DMFT calculations [1] deduce the Kondo effect responsible for the lack of magnetism in δ-Pu. On the other hand, static LDA+U calculations [2,3] also lead to a non-magnetic state if the 5*f* occupancy exceeds approximately 5.3.

This situation requires to refer carefully to various regimes know from anomalous rare earths (Ce,Yb,Sm,Eu,Tm), which exist on the path between the localized, atomic, 4*f* states on one side and band states on the other side. Here, besides the Kondo regime, acting close to integral 4*f* occupancy (i.e. weak 4*f* instability), a regime of valence fluctuations occurs. In this case, the average 4*f* occupancy is significantly different from integer, but the fluctuations $4f^{n}$ -> $4f^{n-1}$ + 1 cond. el. are still relatively slow, with the characteristic timescale interfering with the scale of thermal fluctuations. The charge fluctuations are the reason for the destruction of magnetic moments without invoking any spin-compensation mechanisms.

It is very difficult, in case of Pu systems, to obtain a direct insight in the dynamics of charge fluctuations e.g. by neutron scattering. But the valence fluctuators are characterized by very specific bulk properties and photoelectron spectra. Here we will discuss analogies between properties of Pu compounds and rare-earth valence fluctuators from the point of view of spectroscopies and occurrence of other specific markers as a negative value of elastic coefficient c_{12}.

References

1. Shim J.H., Haule K., Kotliar G., *Nature* **446**, 513 (2007).
2. Shick A.B., Drchal V., Havela L., *Europhys. Lett.* **69**, 588 (2005).
3. Shick A., Kolorenc J., Havela L., Drchal V., Gouder T., *EPL* **77**, 17003 (2007).

Spontaneous and Field-Induced Magnetic Transitions in $RBaCo_2O_{5.5}$

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A detailed study of magnetic properties of cobaltites $YBaCo_2O_{5+x}$ has been performed in high (up to 35 T) magnetic fields and under hydrostatic pressure up to 0.8 GPa. The oxygen