Electronic structure and magnetism in UGa_2 - DFT+DMFT approach

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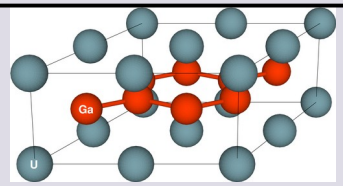
Banhi Chatterjee, Jindřich Kolorenč

Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

We investigate the effects of dynamical correlations between the 5f electrons on the magnetic moments of the uranium atom in the intermetallic compound UGa_2 using DFT+DMFT. We analyze how well this method describes the experimental XAS, valence-band PES and Sommerfeld coefficient. We compare all our results with the static mean-field approximation LSDA/LSDA+U.

- Ferromagnetic ordering below T_c=125 K.
- Magnetic moment of 3 μ_B on the U atom along (100).
- Large spin orbit coupling, crystal field splitting, Coulomb interaction between 5f electrons influence moments in a non-trivial manner.
- U 5f electrons: Itinerant? Localized? Debated….



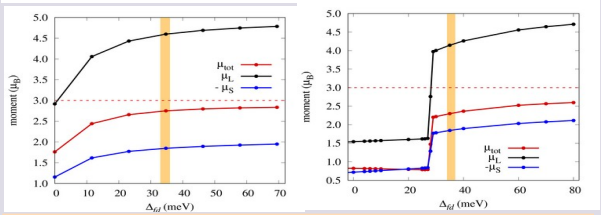
UGa_2: AlB_2-type hexagonal structure

LSDA: Local Spin Density Approximation

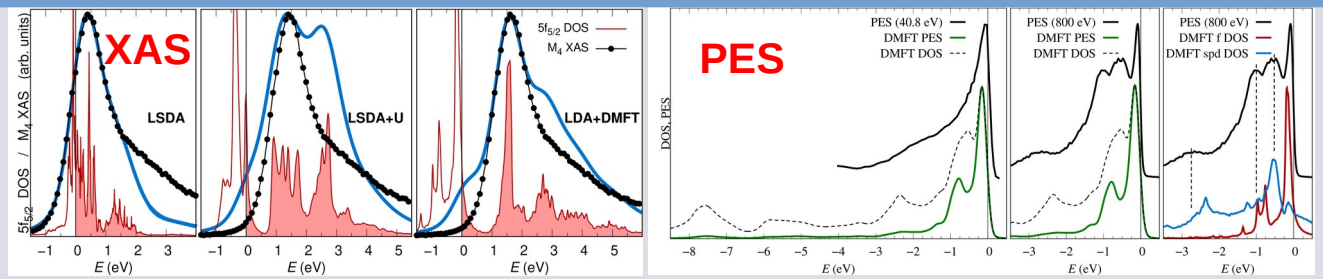
- Severely underestimates the magnetic moments.
- Fails to reproduce experimental spectra (XAS, PES).
- Overestimates Sommerfeld coefficient.
- **Will inclusion of correlations improve the picture?**

Electronic correlations are treated by combining the density functional theory with the dynamical mean-field theory: LSDA+DMFT.

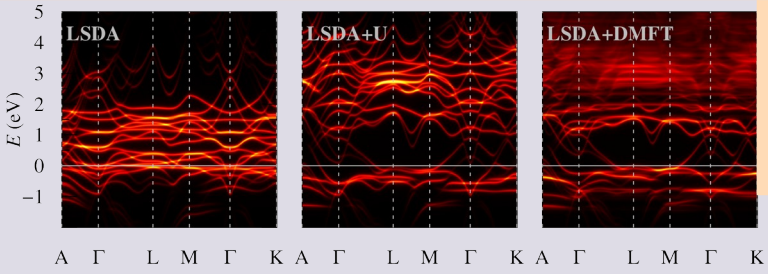
method	μ_S μ_B	μ_L μ_B	μ_{tot} μ_B	n_f	γ mJ/mol K^2
LSDA	-1.82	2.64	0.54	2.72	26.7
LSDA+U(FLL)	-1.64	4.43	2.54	2.78	8.4
LDA+DMFT	-1.85	4.60	2.75	2.76	8.2
LSDA+DMFT	-1.66	4.15	2.3	2.82	7.2
Expt			3.07		11.0



L(S)DA+DMFT can reproduce the experimental magnetic moments with a judicious choice of spin polarized double counting simulating the 5f-6d exchange interactions [1,2].



L(S)DA+DMFT reproduces the experimental spectroscopic features (both in the XAS and PES) better than LSDA+U. Certain features could be identified as finger-prints of atomic multiplets [1-5].



Momentum resolved 5f spectral density with electronic correlations described by an increased level of sophistication (left to right).

LSDA+U spectra close to LSDA+DMFT. **Our calculations point towards a close-to-localized picture of the 5f states in UGa_2 [1-3].**

1) **B. Chatterjee, J. Kolorenč, arXiv: 2102.08224 (2021)**
2) **B. Chatterjee, J. Kolorenč,** *MRS Adv*. **5,** 2639(2020)
3)A.V. Kolomiets, M. Paukov, J. Valenta, **B. Chatterjee**, A.V. Andreev, K. Kvashnina, F. Wilhelm, A. Rogalev, D. Drozdenko, P. Minarik, **J. Kolorenč**, M. Richter, L. Havela (submitted to Phys. Rev B, 2021)
4)S. Fujimori *et. al*, Phys. Rev. B **99**, 035109 (2019)
5) T. Gouder *et. al, J. Alloys. Comp.* ***314,7*** *(2001)*

Correspondence: **banhi29@fzu.cz**

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