Electronic structure of the U_5Ge_4 compound

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The U_5Ge_4 compound crystallizes in the hexagonal Ti_5Ga_4 type structure having $P6_3/mcm$ space group [1]. The unit cell has a complex structure and contains 18 atoms: the uranium atoms occupy two inequivalent sites, 4d and 6g, and germanium also two sites: 6g and 2b. Following the Hill diagram [2], the magnetic properties of the uranium compounds depend on the interuranium distances, which in the case of U_5Ge_4 are the following: U(4d)-U(4d)≈2.93 Å, U(4d)-U(6g)≈3.48 Å, and U(6g)-U(6g)≈3.83 Å, below and above the Hill limit ~3.4 Å. Magnetic measurements [1] indicate nearly temperature independent paramagnetic behaviour down to 2 K. The band structure *ab-initio* calculations [3], presented below for the paramagnetic state, show the influence of hybridization on degree of localization of the 5f electrons: the peaks for U(4d) are more broadened than for U(6g) atoms. The preliminary results of spin polarized calculations indicate that the magnetic moments can be formed on uranium atoms, and their values depend on the local environments.

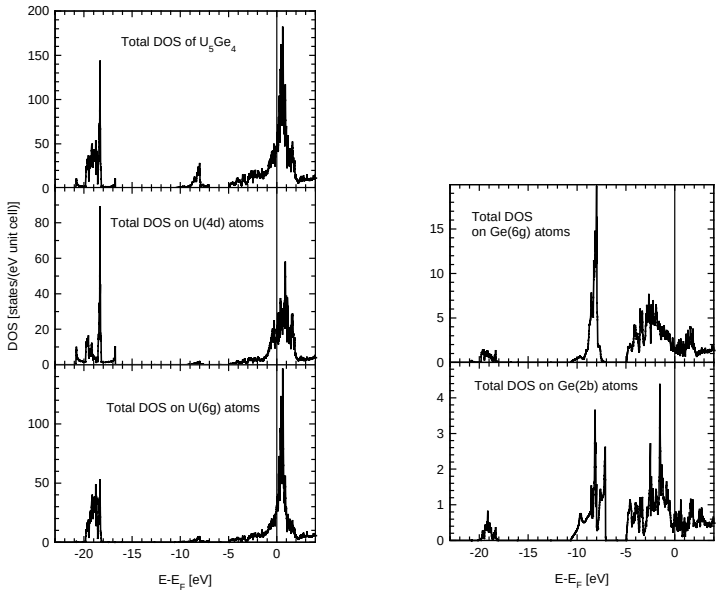

Fig.1. Densities of electronic states for paramagnetic U_5Ge_4 compound.

[1] P. Boulet, M. Potel, J.C. Levet, H. Noël, J. Alloys Compd. **262-263** (1997) 229.
[2] H.H. Hill: in „*Plutonium and Other Actinides 1970*", W.N. Miner (ed.), Metal. Soc. AIME, New York 1971, vol. 1, p. 2.
[3] O.K. Andersen, O. Jepsen, M. Šob, w *Electronic Structure and Its Applications* M.S. Yussouff (ed.), Springer, Berlin 1987, p. 2.

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