ELECTRONIC STRUCTURE OF THE U_5Ge_4 COMPOUND

A. Szajek[a], M. Werwiński[a], W.L. Malinowski[a], P. Leśniak[a], M. Richter[b]
[a]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
[b]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

9.7 cm

The U_5Ge_4 compound crystallizes in the hexagonal Ti_5Ga_4 type structure having space group $P6_3/mcm$ [1]. The unit cell has a complex structure containing 18 atoms: the uranium atoms occupy two inequivalent sites, 4d and 6g, and germanium ones 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: $U(4d) - U(4d) \approx 2.93$ Å, $U(4d) - U(6g) \approx 3.48$ Å, and $U(6g) - U(6g) \approx 3.83$ Å, below and above the Hill limit ~ 3.4 Å. Magnetic measurements [1] indicate nearly temperature independent paramagnetic behaviour down to 2 K. Previously reported band structure $ab - initio$ calculations [3] showed that the magnetic moments can be formed on uranium atoms, and their values are dependent on the local environments. In this paper we present results of calculations obtained based on fully relativistic FPLO code [4]. The values of magnetic moments on uranium atoms are equal to 0.08 and 0.05 μ_B/atom for U(4d) and U(6g) atoms, respectively.

[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] A. Szajek, Materials Science-Poland 25 (2007) 515.
[4] FPLO-5.10-20 improved version of FPLO code by K. Kopernik and H. Eschrig, Phys. Rev. B 59 (1999) 1743; http:// www.fplo.de

13.4 cm

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Corresponding author :
W.L. Malinowski

Address for correspondence :
Institute of Molecular Physics, Polish Academy of Sciences
ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

Email address :
wlm@ifmpan.poznan.pl