ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF THERMAL METAMAGNET UPdGe

M. Samsel-Czekała, R. Troć and V.H. Tran
Institute of Low Temperature and Structure Research, Polish Academy of Sciences,
P.O. Box 1410, 50-950 Wrocław 2, Poland

9.7 cm

We present results of relativistic spin- (LSDA) and orbital- (OP) polarized band structure calculations for orthorhombic UPdGe performed by the FPLO code [1]. Previous bulk experiments showed that this compound exhibits two phase transitions, at $T_C = 30$ K to ferromagnetic (FM) and at $T_N = 50$ K to amplitude-modulated antiferromagnetic states. Interestingly, a giant transverse magnetoresistivity value of -73% was found exactly at T_C and at $B = 8$ T for a polycrystalline sample [2]. Our calculated magnetic moment in the FM ground state (LSDA+OP) is in good agreement with the experimental one, concerning both its value of 1.5 B.M./U at. and orientation in a simple collinear magnetic structure along the b axis [3]. The calculated density of states (DOS), in this FM state, resembles that in halfmetals while non-magnetic (LDA) DOS is semimetallic-like. The computed Fermi surface (FS) in the FM state is typically metallic, containing four electron and hole FS sheets, whereas the non-magnetic FS is semimetallic-like (with reduced FS sheets). This is in accord with our transport measurements indicating a Kondo-like behavior of UPdGe at temperatures $T > T_N$.
References: [1] K. Koepernik, H. Eschrig, PRB **59**, 1743 (1999); [2] R. Troć, J. Alloys Compd. **442**, 34 (2007); [3] S. El-Khatib et al. J. Appl. Phys. **93**, 8352 (2003).

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Corresponding author :
M. Samsel-Czekała

Address for correspondence :
Institute of Low Temperature and Structure Research, Polish Academy of Sciences,
P.O.Box 1410, 50-950 Wrocław 2, Poland

Email address :
m.samsel@int.pan.wroc.pl