Electronic band structure, XPS and bulk physical properties of UCoGe

M. Samsel-Czekala\textsuperscript{a,b}, R. Troc\textsuperscript{b}, E. Talik\textsuperscript{c}, S. Elgazzar\textsuperscript{d} and P. M. Oppeneer\textsuperscript{d}

\textsuperscript{a}Leibniz Institute for Solid State and Materials Research, IFW Dresden, P.O.Box. 270116, D-01171 Dresden, Germany
\textsuperscript{b}Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box. 1410, 50-950 Wroclaw 2, Poland
\textsuperscript{c}Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland
\textsuperscript{d}Department of Physics, Box 530, Uppsala University, S-751 21, Uppsala, Sweden

The electronic structure as well as bulk physical properties of orthorhombic TiNiSi-type UCoGe have been investigated. The results of band structure calculations, employing the modern full-potential local-orbital (FPLO) code \cite{1}, are compared with experimental data of x-ray photoelectron spectroscopy (XPS), transport and magnetic properties, obtained for single crystalline samples. Based on measurements on polycrystalline samples, Huy et al. \cite{2} have interpreted the ground state of this compound as weak itinerant ferromagnetism ($T_C = 3$ K) coexisting with superconductivity ($T_{SC} = 0.8$ K). In contrast, our sample does not confirm their findings but turns out to be paramagnetic and non-superconducting down to the lowest values of temperature. A ferromagnetic phase is, however, close in energy to the non-magnetic phase according to our spin- and orbital-polarized calculations. Good agreement between results of non-magnetic calculations and XPS experimental data is achieved mainly for the U 5f electrons but not as much for the Co contributions. This indicates that the real electronic structure could be different from the predicted one.

\cite{1} FPLO 3 and 5 [improved version of the original FPLO code by K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999)]; www.FPLO.de;
N.T. Huy et. al, Phys. Rev. Lett. 99, 067006 (2007);

\textbf{Subject category :}
3. Magnetic Structure and Dynamics

\textbf{Presentation mode :}
oral

\textbf{Corresponding author :}
M. Samsel-Czekala

\textbf{Address for correspondence :}
Leibniz Institute for Solid State and Materials Research, IFW Dresden, P.O.Box. 270116, D-01171 Dresden, Germany

\textbf{Email address :}
m.samsel@int.pan.wroc.pl