

Electronic properties of ThCu_5Sn and ThCu_5In compounds

M. Werwiński and A. Szajek

*Institute of Molecular Physics, Polish Academy of Sciences
M. Smoluchowskiego 17, 60-179 Poznań, Poland*

Recently uranium compounds have attracted interest because of many interesting properties such as the Pauli paramagnetism, spin fluctuations, heavy fermions, magnetic ordering, or superconductivity. Wide range of properties in these compounds is caused by the uranium $5f$ electrons, which show an intermediate character between the localized $4f$ electron system and itinerant character of $3d$ electrons. The role of $5f$ electrons is important in actinides and the question is if they are localized or itinerant or perhaps the two situations coexist giving rise to a new character of the electronic structure, referred to as the duality of the behaviour of $5f$ electrons. It is very useful to compare properties of isostructural systems with and without $5f$ electrons treating the systems with thorium as reference ones. Results of investigations of the electronic structure of UCu_5M ($\text{M} = \text{In}, \text{Sn}$) compounds were recently published in Refs. 1, 2.

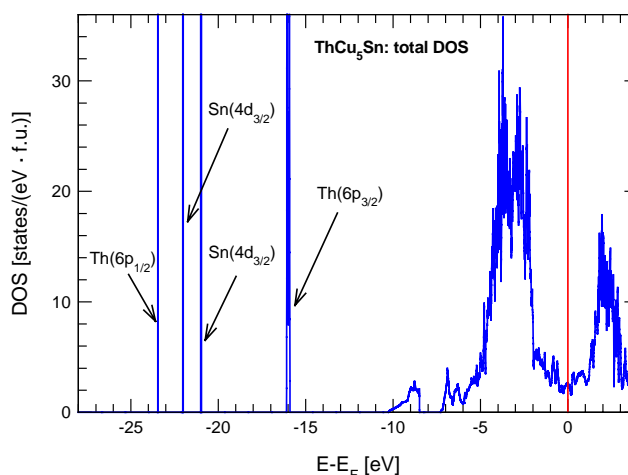


Fig. 1. Total density of electronic states for ThCu_5Sn .

X-ray phase analyses of annealed and as-cast alloys of ThCu_5In and ThCu_5Sn alloys indicated that they are isostructural and that their structure is similar to that of the $\text{UCu}_5\text{In(Sn)}$ compound (CeCu_5Au -type structure, space group $Pnma$) [3, 4]. The aim of this paper is to calculate band structure of the $\text{ThCu}_5\text{In(Sn)}$ compounds based on fully relativistic FPLO® code [6, 7]. As an example, the results for ThCu_5Sn are presented in Fig. 1.

- [1] G. Chełkowska, J.A. Morkowski, A. Szajek, R. Troć, J. Phys.: Condens. Matter **14** (2002) 3199
- [2] G. Chełkowska, J.A. Morkowski, A. Szajek, R. Troć, Phil. Mag. B **82** (2002) 1893
- [3] V. Zaremba, V. Hlukhyy, J. Stepień-Damm, R. Troć, J. Alloys Compd. **321** (2001) 97
- [4] V. Zaremba, J. Stepień-Damm, R. Troć, D. Kaczorowski, J. Alloys Compd. **280** (1998) 196
- [5] K. Koepnick and H. Eschrig, Phys. Rev. B **59** (1999) 1743
- [6] I. Opahle, K. Koepnick, and H. Eschrig, Phys. Rev. B **60** (1999) 14035

Name of the presenting author (poster session II): Mirosław Werwiński
e-mail address: wemir@ifmpan.poznan.pl
<http://www.ifmpan.poznan.pl>