

Photoemission spectra of some uranium compounds

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Uranium intermetallic compounds, especially those containing a transition metal T and a p -metal M , form an interesting class of materials. In recent two decades they attracted particular interest because of their frequent anomalous behavior at low temperatures, mainly caused by the simultaneous occurrence of the magnetically ordered state together with heavy fermion and sometimes even with superconducting states.

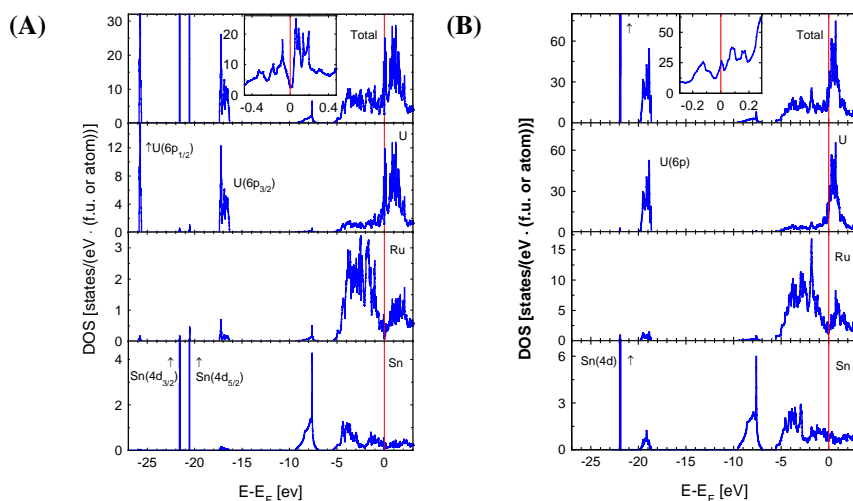


Fig.1. DOS plots for $\text{U}_2\text{Ru}_2\text{Sn}$ (total and local) obtained by FPLO (A) and TB LMTO ASA (B) methods.

The aim of the present work is to extend our knowledge on the electronic structure of some actinide compounds ($\text{U}_2\text{Ru}_2\text{Sn}$ and UCu_5M , $\text{M}=\text{Al}, \text{In}, \text{Sn}$) by theoretical (*ab-initio* calculations) and experimental investigations (X-ray photoemission). Earlier calculations [1, 2] were based on nonrelativistic TB LMTO ASA [3] method. In the present approach we use fully relativistic FPLO® code [4, 5]. The computational results will be compared with experimental XPS measurements. As an example, the results for $\text{U}_2\text{Ru}_2\text{Sn}$ are presented.

- [1] G. Chełkowska, J.A. Morkowski, A. Szajek, R. Troć, Phys. Rev. B **64** (2001) 075119;
J. Phys.: Condens. Matter **14** (2002) 3199; Phil. Mag. B **82** (2002) 1893
- [2] G. Chełkowska, et al., European J. Phys. B **35** (2003) 349
- [3] O. Andersen, Phys. Rev. B **12** (1975) 3060
- [4] K. Koepernik and H. Eschrig, Phys. Rev. B **59** (1999) 1743
- [5] I. Opahle, K. Koepernik, and H. Eschrig, Phys. Rev. B **60** (1999) 14035

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