Electronic band-structure and X-ray photoemission studies of ternaries APdGe (A= Th,U) in the paramagnetic state

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Previous investigations showed that UPdGe, crystallizing in the orthorhombic TiNiSi-type (*Pnma*), reveals not only an interesting complex magnetic behavior but also extremely specific electrical properties [1]. This compound undergoes at 28 and 50 K two magnetic transitions into ferro- and antiferromagnetic state, respectively. At low temperatures a simple ferromagnetic canted alignment of the magnetic moments within the orthorhombic *a*-*c* plane was first proposed [2] but recently it has been suggested by magnetic-space group analysis and neutron-diffraction studies [1,3] to form the collinear ordering of uranium moments along the orthorhombic *b* axis. It should be mentioned that in the ferromagnetic state at temperatures 20-30 K a conical structure with the net magnetic moment along the *c* axis was reported in Ref. [4]. This finding turns out to be in good agreement with the last study of thermopower and magnetoresistivity. In turn, between 28 and 50 K there was proposed a sinusoidally modulated antiferromagnetic structure in Ref. [2]. As regards electrical properties, the most interesting feature is that UPdGe exhibits a giant value (73 %) of the magnetoresistivity at the transition temperature from ferro- to antiferromagnetic state [1].

This presentation is considered to be the first step in understanding the magnetic and electrical properties based on the electronic structure studies of UPdGe and its non-5f-electron counterpart ThPdGe in the paramagnetic state. With this motivation fully relativistic (4-component) band-structure computations were performed, using the full-potential local-orbital (FPLO) minimum-basis code [5], treating *f* electrons as itinerant. The obtained theoretical band energies and electron densities of states (DOS) were compared with experimental X-ray photoemission spectra (XPS). However, some disagreement was achieved probably due to mostly localized character of *f*-electron states observed in the XPS spectra. This requires further investigations.

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