9.7 cm

ELECTRONIC STRUCTURE OF THE URANIUM MONOSTANNIDE USn

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The uranium monostannide USn crystallizes in the orthorhombic $ThIn$-type structure with the space group $Pbcm$ [1]. Uranium and tin atoms each occupy three crystallographic positions. The uranium atoms located in (4c) sites form metallic chains running along c axis, with a $U-U$ interatomic distance of 3.10 Å. USn orders ferromagnetically below $T_C = 55K$, with an ordered moment of $1.20\mu_B/U$ measured on a polycrystallized sample. Because of short distance $U(4c)-U(4c)$ and expected hybridization with the conduction-band electron states it would be interesting to know if this uranium sublattice is also ordered magnetically. $Ab-initio$ calculations would clarify this situation. In this work, spin-polarized band structure calculations results will be presented based on the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation ($TB\ LMTO\ ASA$). The calculations showed that all three types of uranium atoms are magnetically ordered and their moments depend on local environments.

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[1] P. Boulet and H. Noël, *Solid State Commun.* **107** (1998) 135

13.4 cm

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