Electronic structure of Th_7Ru_3

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Physical properties of non-centrosymmetric Th_7T_3 (T= Co, Fe, Rh, Os, Ir, Ru), were studied by Matthias et al. [1]. The authors showed that expect for Th_7Ru_3, the remaining compounds have superconducting transition at approximately 1.5 - 2 K. Owing to the aspect of non-centrosymmetric superconductivity, there is a need to perform an investigation of electronic band structures. Such studies have recently been presented by us for Th_7Co_3 [2] and Th_7Fe_3 [3]. In this contribution, we report the results of scalar and fully relativistic calculations for Th_7Ru_3, using the full potential linearized-muffin-thin-orbital method. The obtained data reveal that effect of asymmetric spin-orbit coupling with splitting energy of 10 - 40 meV is much weaker, and simultaneously the van Hove singularity-like peak locates at -2.1 eV with respect to the Fermi level, is much deeper as compared to those of Fe-, Co-based superconductors. The findings can explain the existing difference between the studied Th_7T_3.

References:

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