Electronic band structure of Ru_3Sn_7

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The first-principle band structure calculation of Ru_3Sn_7 was carried out using the full-potential linearized muffin tin orbital (FP-LMTO) method. The self-consistent (SC) charge density convergence was achieved using the local density approximation (LDA) for the exchange correlation potential. It was shown that the essential valence band contribution is due to the 4d electrons of Ru, while the contribution from the 5p-Sn orbitals is relatively small. Furthermore, the 4d-Ru and 5p-Sn orbitals located near the Fermi level have the non-hybridized characters, thus contributing independently to the total density of states. A high concordance was observed between the results and those obtained from the full-potential local orbital (FPLO) method. The purpose of the present work is to study in detail the electronic band structure of Ru_3Sn_7 as a reference compound, in comparison with that of the superconducting Mo_3Sb_7.

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