Electronic structure of novel superconductor AuSb₆Te

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Binary compounds AuₓSb₁₋ₓ are known to take cubic π-phase and show superconductivity[1], while the ternary compound Au₀.125Sb₀.75Te₀.125 (or AuSb₆Te) was known as a semiconductor. Recently we have found that AuSb₆Te becomes superconducting below Tₜ~6.7K[2], contrary to the previous report.

We have investigated the electronic structure of this newly found superconductor AuSb₆Te from first principles. The density of states curve has a sharp peak just at the Fermi level. Complex feature of the Fermi surfaces shows the possibility of the multi-gap superconductivity in this system. The obtained number of Au valence electrons is ~8.7, which means Au almost takes 2+ valence on average. We discuss the possibility that this Au²⁺ ion works as an attractive center by the valence-skipping mechanism.