

ELECTRONICS STRUCTURE AND TRANSPORT PROPERTIES

$\text{Mo}_3\text{Sb}_{7-x}\text{Te}_x$

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Mo_3Sb_7 is a very interesting compound, since the competition of superconductivity with spin fluctuations was recently experimentally observed [1]. Moreover, the Fermi level in this compound is located very close to the energy gap, on a very steep slope of electronics density of states function. This opens the possibility of interesting thermoelectric properties, especially for the electron-doped system. In this work we present the electronic structure calculations results, obtained with the Korringa-Kohn-Rostoker method applying the coherent potential approximation (KKR-CPA) to study the disordered alloy structure of Mo_3Sb_7 doped with Te. The site-preference, evolution of the Fermi surface and densities of states upon doping are shown. The kinetic and transport properties are also discussed, basing on the electronic band calculations with complex energy. Theoretical results are compared with our experimental results [2], as well as with those recently published [3].

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[1] C. Candolfi, B. Lenoir, A. Dauscher, C. Bellouard, J. Hejtmanek, E. Santava, and J. Tobola, *Phys. Rev. Lett.* **99**, 037006 (2007).

[2] C. Candolfi, B. Lenoir, A. Dauscher, J. Tobola, S. J. Clarke, *to be published*

[3] F. Gascoin, J. Rasmussen and G.J. Snyder, *J. All. Comp.* **427**, 324(2007)

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