Electronic structure of Fe_2VGa

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The physics of *d*-electron intermetallic compounds with electronic gaps or pseudogaps at the Fermi level continues to attract attention. This gap (pseudogap) in materials containing localized magnetic orbitals may be due to hybridization or Kondo-type singlet formalism (*e.g.* [1]). Recently, the Heusler-type Fe_2VAl [2] and Fe_2TiSn [3] compounds were discussed as the *d*-Kondo-insulators of the FeSi-type [4] due to their unusual electric transport and thermodynamic properties. Namely, the electrical resistivity of the both compounds exhibits semiconducting behavior and the low-T specific-heat data revealed an unusual upturn in C/T, commonly observed in most heavy fermion systems. From the band-structure calculations and infrared studies, however, Fe_2VAl [5] and Fe_2TiSn [6] are semimetals with a pseudogap at the Fermi level. In our recent work [7] we discussed the low-T properties of these Fe-compounds on the base of Kimball-Falicov model [8], which well describes the temperature characteristics attributed to the narrow *d*-antisite band, strongly correlated and located at the Fermi level. Now, we present the band-structure calculations for Fe_2VGa, which also has a pseudogap at the Fermi level and is nonmagnetic. An atomic disorder leads to a weakly magnetic behaviors, and the antisite Fe-defects also locate the *d*-states at the Fermi level, which form a narrow and strongly correlated *d*-band.

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