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EINLADUNG zum IFP-SEMINAR

The electronic pseudo band gap states of the full Heusler compound Fe_2VAl

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Host: Ernst Bauer

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Ort: Institut für Festkörperphysik, TU Wien
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Abstract:

For Fe_2VAl the temperature dependent Seebeck coefficient $S(T)$ and electrical resistivity $\rho(T)$ were calculated by means of density functional theory (DFT) based approaches and compared to measurements. The DFT calculations were extended in terms of a DFT/LDA+U approach with U-J values attributed to Fe-d like states. For simulating the general features of the measured data, a large range of U-J values was scanned through with U-J = 2.145 eV as a recommended value. For this value a very small negative indirect gap of $E(X)-E(\Gamma)$ = -0.0093 eV occurs which is significantly reduced as compared to the DFT-GGA value of -0.158 eV. Charge transfer was derived by Bader's approach resulting in a significant transfer of 0.75 electronic charges to each Fe atom from Al (1.03) and V (0.48). The pseudo-gap states around the Fermi energy were analyzed in detail in terms of density of states, band structures and charge density contours. These states almost exclusively govern $S(T)$ and $\rho(T)$. They have large dispersions and are centered at Γ and X. They consist of tails of localized V and Fe-states, dangling to the Al-site. The dispersion of the band along the k-space direction X-Γ was modelled in terms of a tight-binding ansatz, resulting in k dependent matrix elements. From our study based on the findings for $S(T)$ and ρ(T) it appears that Fe_2VAl has a very small negative and possibly zero indirect gap in the electronic structure.