

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Effect of electron correlation on thermoelectric properties of the full-Heusler compound Fe_2VAI ¹ DAT DO, MAL-SOON LEE, S.D. MAHANTI, Department of Physics and Astronomy, Michigan State University — Heusler-type alloys have been studied extensively since they were first discovered by Heusler in 1903. Among those Fe_2VAI became interesting when Nishino *et. al.*[1] suggested that it might be a heavy fermion system. LDA/GGA calculations have shown that Fe_2VAI is a pseudo-gap system with sharp edges in the density of state near the Fermi level. This feature makes it a promising thermoelectric material. Since then electronic properties of nominally pure and doped Fe_2VAI have been studied extensively. However the exact nature of the ground state of this system is still not well understood. Since it contains d-electrons one expects electron correlation effects to be important. We have carried out band structure calculations using GGA+U method with several values of the on-site Coulomb interaction parameter U. Using the obtained band structure, transport coefficients were calculated within Boltzmann approach. Electronic structure and thermoelectric properties were studied for different values of U and compared to available experiments.

[1] Y. Nishino *et. al.*, *Phys. Rev. Lett.* **79** (10), 1909 (1997).

¹This work was supported by the US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center.

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Date submitted: 22 Dec 2010

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