CORRELATIONS EFFECTS ON THE ENERGY BAND GAP IN HEUSLER ALLOY Ru_2CrGe

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ABSTRACT. Magnetic and electronic proprieties of the ternary alloys Ru_2CrGe have been studied using DFT calculation in conjunction with full potential Linear Muffin-Tin Orbital FP-LMTO method. The conventional density functional theory DFT fails for materials with strongly correlated electrons, therefore, the LDA+U method [1] was used to study the effect of on-site correlation at the transition metal sites on the magnetic and electronic properties of the Ru_2CrGe compound. It was shown that our obtained equilibrium lattice parameter is in good agreement with the experimental results.

KEYWORDS: *FP-LMTO, Heusler, LDA+U*