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Study of the Structural, Electronic, Thermodynamic and Magnetic Properties of AgCr2Ga Heusler Alloys by First Principals Approachs

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The purpose of this study is to exploit structural, electronic, magnetic and thermodynamic properties of the full Heusler Ag2CrGa compound using the method of calculation of linear Muffin-tin-orbital potential (FP-LMTO) in the L21 phase with the local approximations density (LDA), local spin density and the local spin (LSDA)density coupled(LSDA-couple). The calculation made on the structural properties such as modulus, pressure derivatives and electronic properties have enabled us to deduce the nature of this alloy which proved a metal. While the calculated magnetic properties has enabled us to evaluate the magnetic moment of the test compound Ag2CrGa and the magnetic moments of each constituent element of the latter. The calculated thermodynamic properties are apparent change in modulus, heat capacity and the Debye temperature [from 0 to 1600 °C].