# Investigation of Structural Stability and Mechanical properties for full Heusler alloy: Co2FeGa

Labidi Salima*[1]

[1]LNCTS Laboratory, Department of Physics, Faculty of Sciences, BadjiMokhtar University (UBMA) – LNCTS Laboratory, Department of Physics, Faculty of Sciences, BadjiMokhtar University, Algeria

**Abstract**

By using the full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT). The physical properties such: structural and mechanical properties for the full Heusler alloy Co2FeGa are investigated and discussed. The exchange-correlation potential was treated using two of approximations where the WC-GGA is used to calculate the stable state of the material for both Fm -3m and F43-m space groups from the FM, NM, and the AFM states by calculating all of their structural parameters from the lattice parameter a (Å) to the enthalpy Hf and to calculate also the elastic constants. The three-dimensional plots of different mechanical moduli exhibit that the bulk modulus is isotropic, whereas Young's modulus, Poisson's ratio and shear modulus of Co2FeGa compound are highly anisotropic. The effects of temperature and pressure on the heat capacity, thermal expansion coefficient and Debye temperature are also studied.

*Speaker