

Project Proposal

Investigation of Electronic structure And Magnetic properties of Heusler Alloys using VASP

In my post graduation we had successfully used Heusler alloys $YFeCrZ$ ($Z=Al,Sn,Sb$) to study the ground state, electronic and mechanical properties of heusler alloys. The main purpose is to study the magnetic properties of heusler alloys, because of their unique and interesting properties. Heusler alloys were investigated by using first principle calculation. All our total energy calculations are performed based on density functional theory as implemented in Vienna Ab- initio Simulation package (VASP). The result shows that $YFeCrZ$ alloys exhibit a half metallic character.

Heusler alloys used for a spintronic devices these alloys shows high curie temperature. In future spin based device such as amplifiers it can be used and electron spin is used in quantum computer. In medical field it is used to detect cancer. Current research is Energy harvesting along with thermoelectric materials has been investigated. These alloys used for several application such as Magnetoresistance, Magnetocaloric etc.

References

- Heusler Fr. Verh. Deutsch. Phys. Ges 5(1903) 219.
- G. Kresse, J. Hafner, Phys. Rev. B 47(1993) 558
- M.N. Rasool, A. Javed, M.A. Khan, A. Hussian, J. Magan Mater. 476(2019)398.