Theoretical Investigations of Structural, Electronic, Thermoelectric, and Magnetic Properties of Heusler Alloys

UNIVERSITY OF ARKANSAS
Graduate School & International Education
Microelectronics-Photonics

Student: Shuruq Alsayegh Degree: M.S., May 2022
Major Professor: Dr. Bothina Hamad-Manasreh

Modeling & Simulation

Background/Relevance

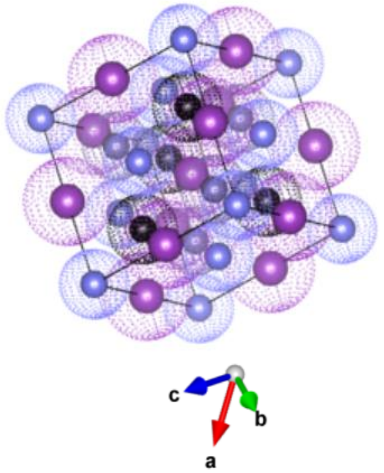
- Heusler compounds have received a great deal of interest since their discovery. These compounds became an important research field due to their novel properties such as high Curie temperature and high spin polarization that can be utilized in different applications.

Innovation

- Discovering new Heusler Alloys to use in different spintronic applications.
- Improving the performance of spintronic devices is essential for the development of modern technology

Approach

- Model new quaternary Heusler alloys.
- Analyze structural, electronic, magnetic, thermodynamic and thermoelectric properties.
- Boltzmann theory was employed to study the thermoelectric properties, which includes electrical conductivity, electronic thermal conductivity and Seebeck coefficient.



Key Results

- using Wien2k and VASP code, the equilibrium lattice parameters of CoHfFeZ, Z=Ge,Al,Si,In are determined.
- The formation and total energies are calculated for antistites defects in the CoHfFeZ alloys.
- New quaternary Heusler alloys show half-metallic behavior, high magnetizations, high thermoelectric power factors, and low lattice thermal conductivity.

Conclusions

- These compounds could be spin gapless semiconductors where, in addition to the gap in one spin channel, there is a zero-band gap in the other spin channel across the Fermi level (Ef). The half metallicity and the spin gapless properties made Heusler compounds good candidates for spintronic devices.

Future Work

- Calculating electronic, thermodynamic, and thermoelectric properties for different Heusler alloys in their bulk and low dimensional structures.