Theoretical Investigations of the electronic, magnetic, and thermoelectric properties of Quaternary Heusler Alloys

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Background/Relevance

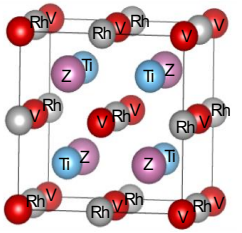
- Thermoelectric (TE) materials are solid state devices that could be designed using two dissimilar materials such as n-type and p-type semiconductors. They are designed to convert thermal energy from a temperature gradient into electrical energy and visa versa.
- Quaternary Heusler alloys have received a great deal of attention due to their novel electronic structure, magnetic, and thermoelectric materials nature.

Innovation

- Using Quaternary Heusler Alloys in thermoelectric and spintronic applications.

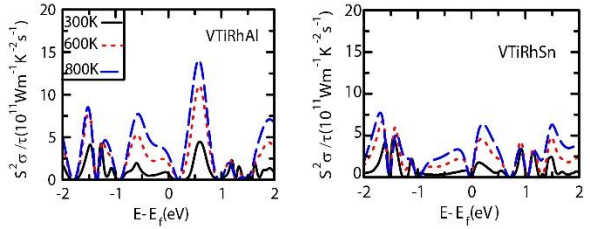
Approach

- Calculations using density functional theory (DFT) were performed to investigate the structural, dynamical, electronic, magnetic, and thermoelectric properties of VTiRhZ (Z = Al, Ga, In, Si, Ge, Sn) alloys.
- The semi-classical Boltzmann transport theory is used to calculate the thermoelectric properties that include seebeck coefficient, electrical conductivity, and electronic thermal conductivity of the materials.



Key Results

- Electronic, magnetic and thermoelectric properties of VTiRhZ (Z = Al, Ga, In, Si, Ge, Sn) alloys are investigated.
- The total magnetic moment of VTiRhZ (Z=Al,Ga,In) was found to be 3μB, and for VTiRhZ (Z=Si, Ge, Sn) exhibit integer values of 2μB.
- The value of the power factor per relaxation time ranges between $7.2 \times 10^{11}\ Wm^{-1}\ K^{-2}\ s^{-1}$ and $14 \times 10^{11}\ Wm^{-1}\ K^{-2}\ s^{-1}$.



Conclusions

- The band gap obtained using GGA-PBE approximation is slightly smaller than that obtained by GGA-mBJ. The calculations using GGA-mBJ functional are considered to give more reliable predictions for the band structure.
- Quaternary Heusler Alloys can find significant applications as thermoelectric and spintronic materials.

Future Work

- Calculating lattice thermal conductivity.
- Calculating figure of merit.