Electronic, Magnetic and Thermoelectric Properties of Perovskite: $BaTbO_3$

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Outline

Introduction:Thermoelectric (TE) Effect

- The Seebeck effect (process that converts temperature gradient directly in to electricity).
- Peltier effect (process that converts electrical energy in to temperature gradient).

- TE performance of a material measured by the figure of merit (ZT)

$$ZT = \frac{\alpha^2 \sigma T}{\kappa_e + \kappa_l}$$

- $\alpha = \frac{8\pi^2 k_B^2}{3eh^2} m^* T \left(\frac{\pi}{3n}\right)^{\frac{2}{3}}$

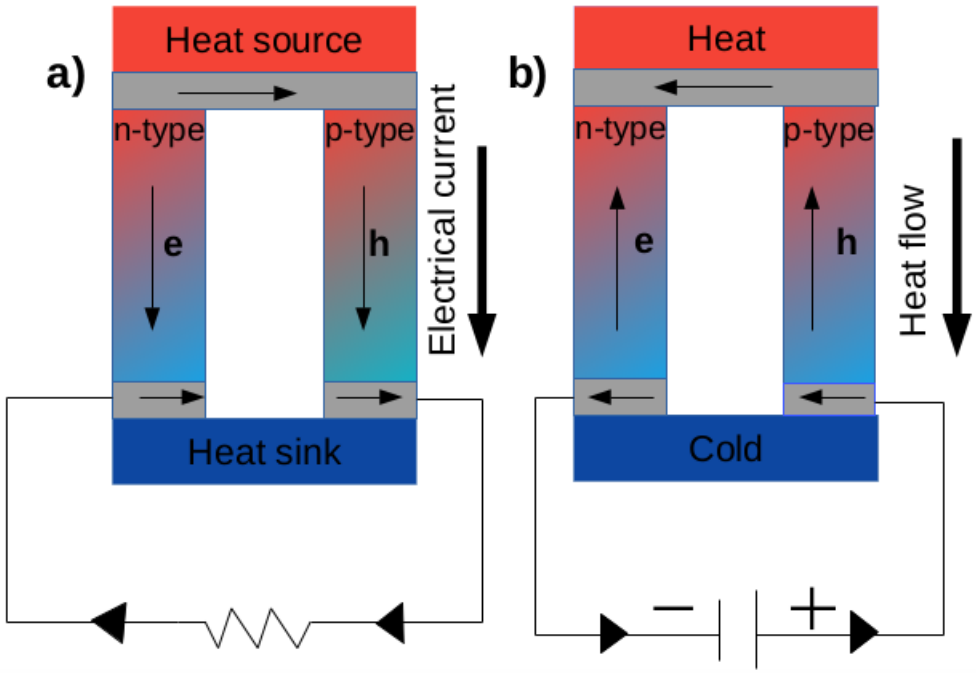


Fig. 3: Schematic representation of a) Power generation and b) Cooling.

Introduction: Requisites for Better TE Materials

- Insulator
- Semiconductor
- Metal

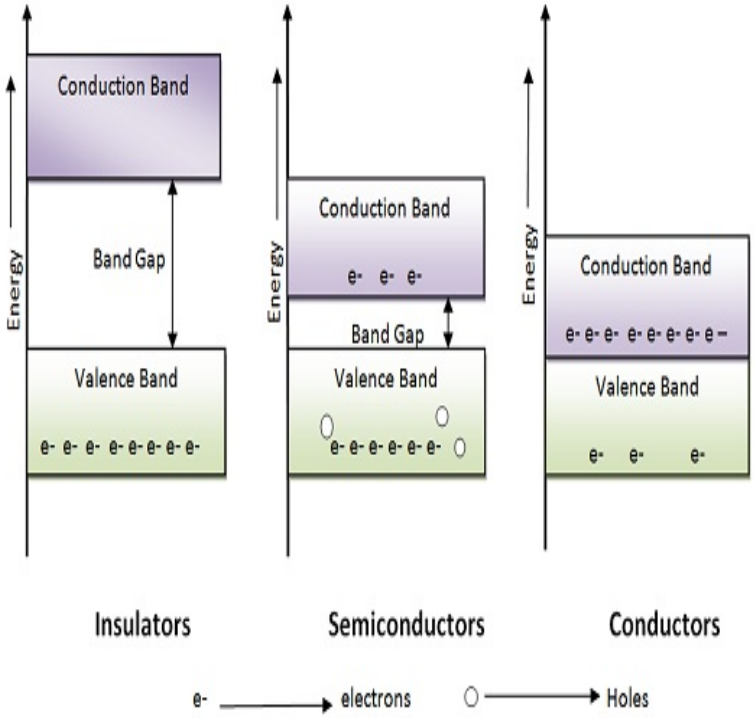


Fig.1: Classification of the materials on the basis of energy gap

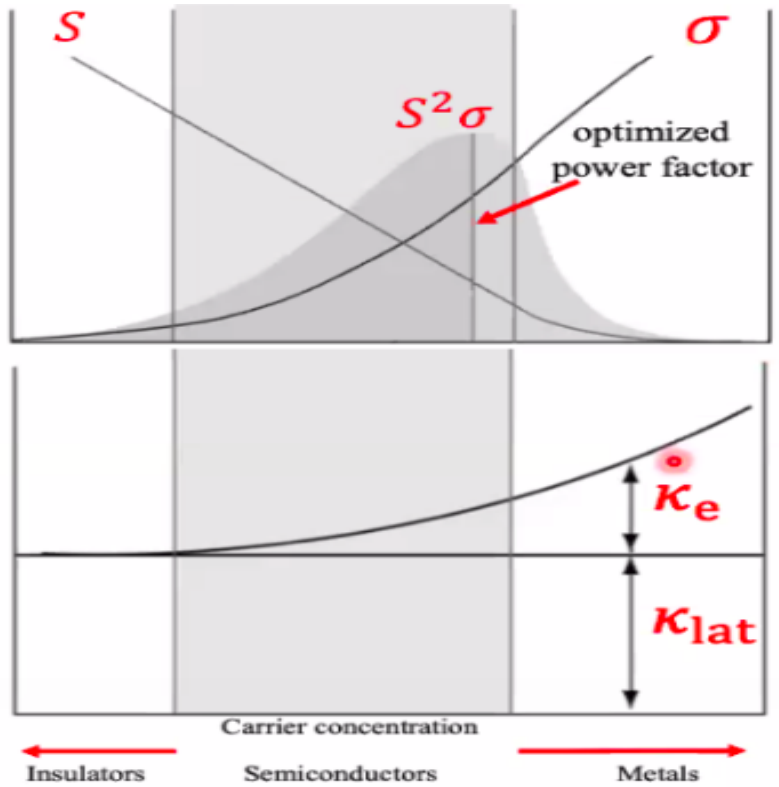


Fig.2: Schematic dependence of the electrical conductivity, Seebec coefficient, power factor, and thermal conductivity on the carrier concentration (Snyder *et al. Nature 7, 105-114, (2008)).*

Introduction:Perovskite

- TE materials have applications: cooler, power generation, temperature sensor etc.
- Silicon-Germanium, chalcogenides, Heusler alloys, Clathrates used for fabricating TE devices.
- Perovskite have various interesting properties such as:
  - Ferromagnetic
  - Half-metallic
  - Semiconductor
  - Topological insulator
  - Thermoelectric
- Oxides Perovskite:
  - Structural stability
  - Low cost
  - Naturally abundance
  - Non-toxic

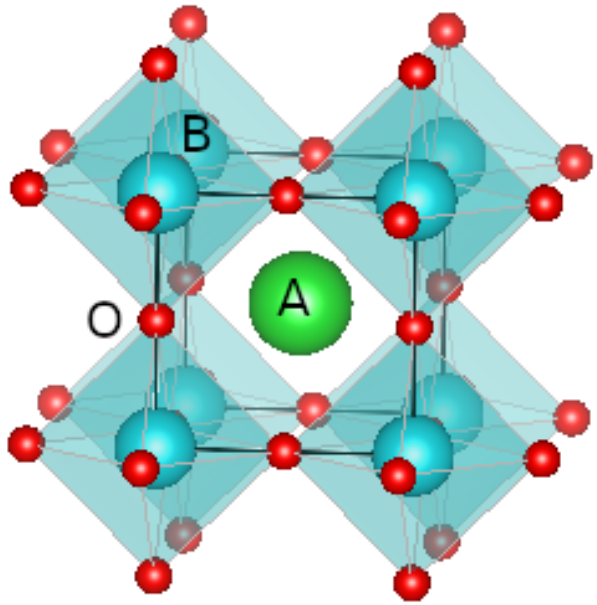
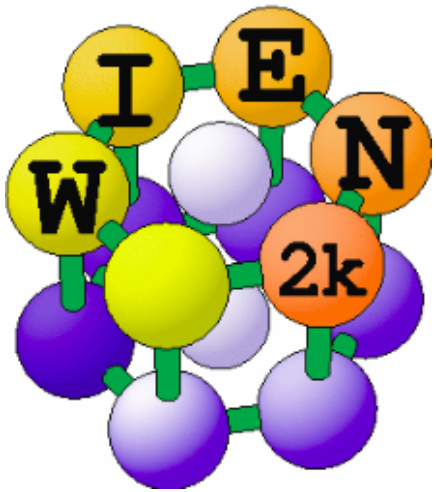


Fig.4: Ideal Cubic perovskite crystal structure of ABO_3.

Computational Details

- Density functional theory (DFT) is used to study the electronic, magnetic and transport properties based on the full-potential linearized augmented plane wave + local orbital (FP-LAPW+lo) using generalized gradient approximation (GGA) as exchange correlation functional.



- WIEN2K code used for the electronic/magnetic properties calculation.

- BoltzTraP code to study the transport properties based on constant relaxation time approximation (CRTA) and the rigid band approximation (RBA).

Crystal Structure and Optimization

Space group $Pm\bar{3}m$ (223)

- $a = 4.36$ Å, $\alpha = 90^\circ$

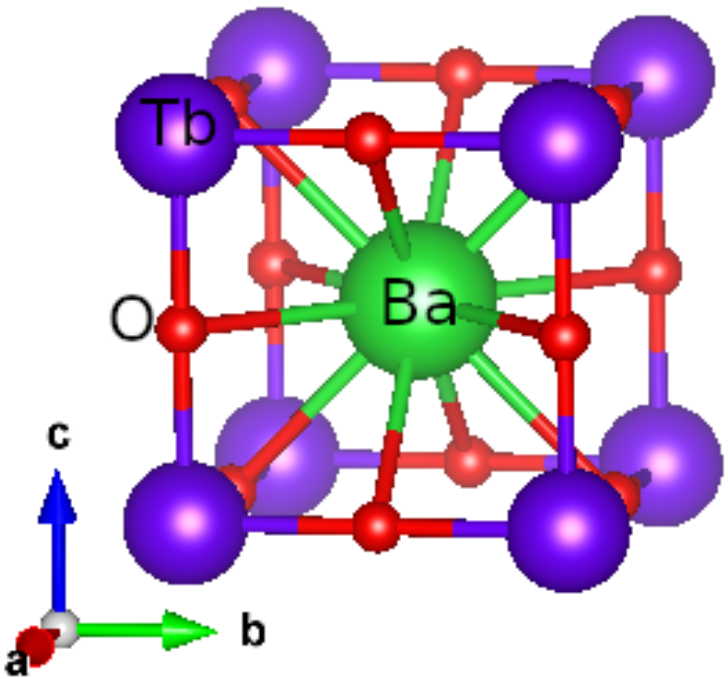


Fig.5: Optimized crystal structure of $BaTbO_3$.

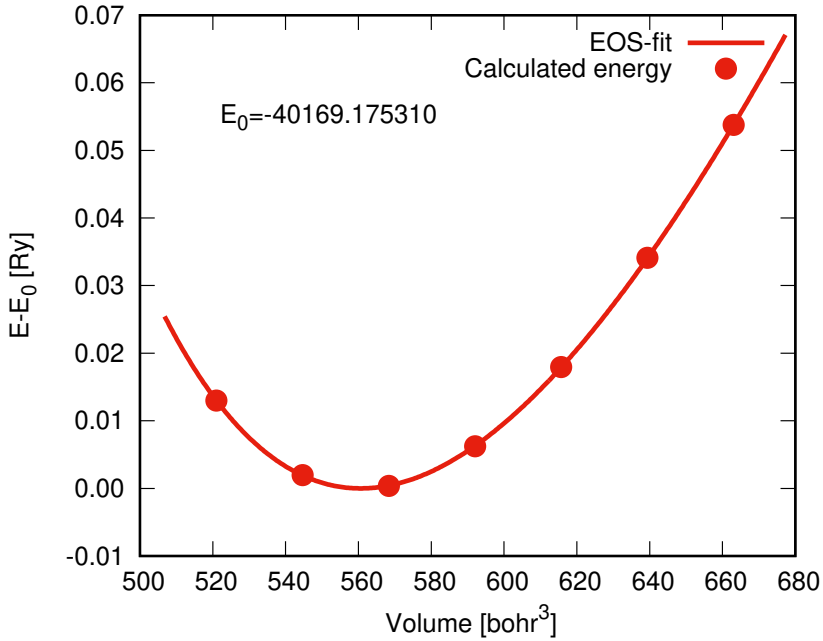


Fig.6: Structure optimization.

- The calculated value of the energy with respect to the volume, fitted using the Murnaghan equation of state.

Results and Discussion

- Ground state – antiferromagnetic, and direction of easy axis is found along [010] direction.

Table3: Total magnetic moment, spin and orbital magnetic moment of antiferromagnetic $BaTbO_3$

	Magnetic moment (μ_B)		
	m_s		m_l
	GGA	GGA+SOC	
Total	0.0	0.0	
Tb1	6.25	6.18	0.32
Tb2	-6.25	-6.18	-0.32

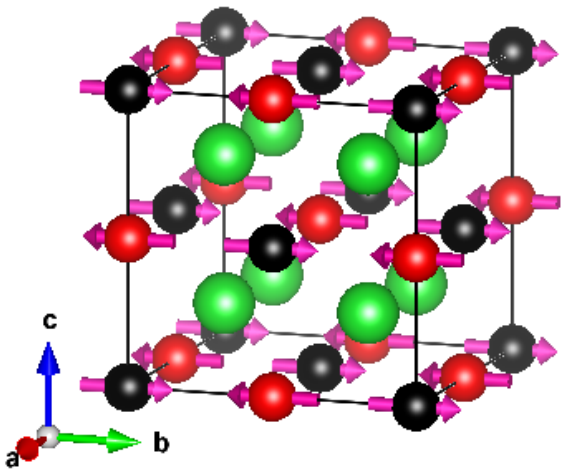


Fig.8: Crystal structure of antiferromagnetic $BaTbO_3$ with direction of easy axis along [010]. The sphere in black, red, and green color represents Tb1, Tb2, and Ba atoms, respectively.

Results and Discussion

Density of States

- Conduction region is mainly contributed by Tb$-4f$ orbital.
- Valence region is contributed by O-2p orbital near Fermi level.

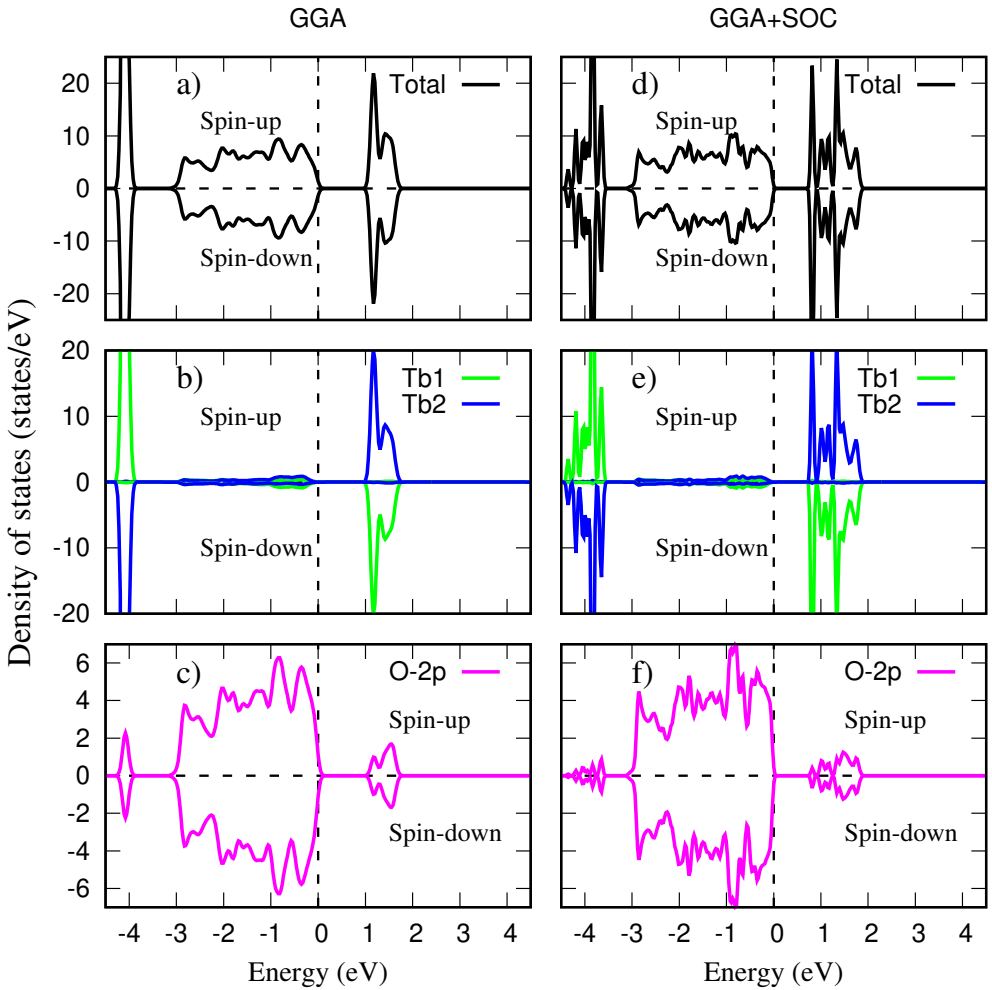
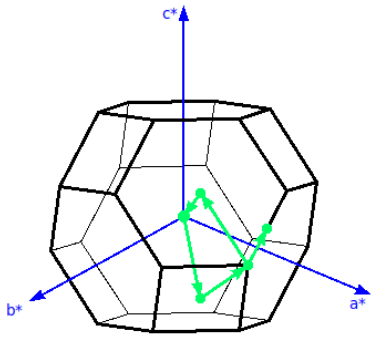


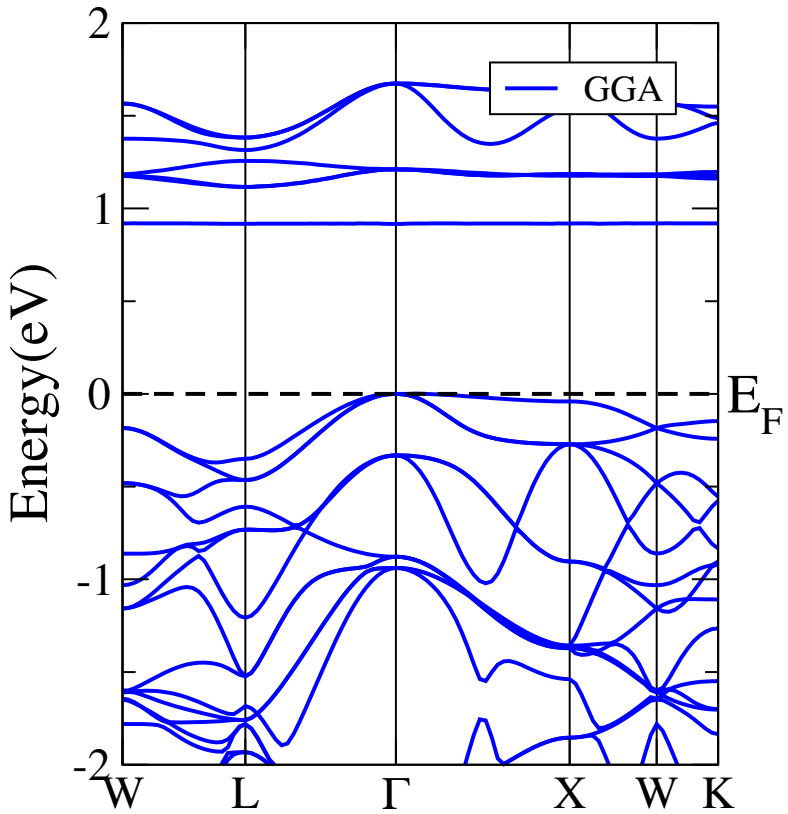
Fig.7: Density of states.

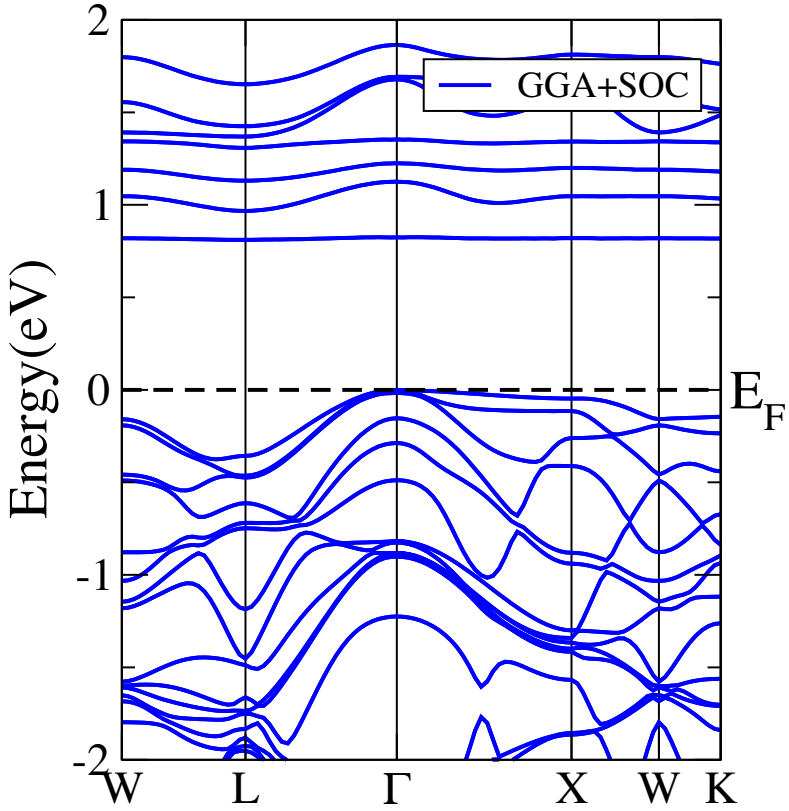
Results and Discussion

Band Structure

- 0.81 eV band gap







Results and Discussion

Transport Properties

- The Seebeck coefficient decreases with the temperature.
- σ increased with the temperature signifies semiconducting in nature.

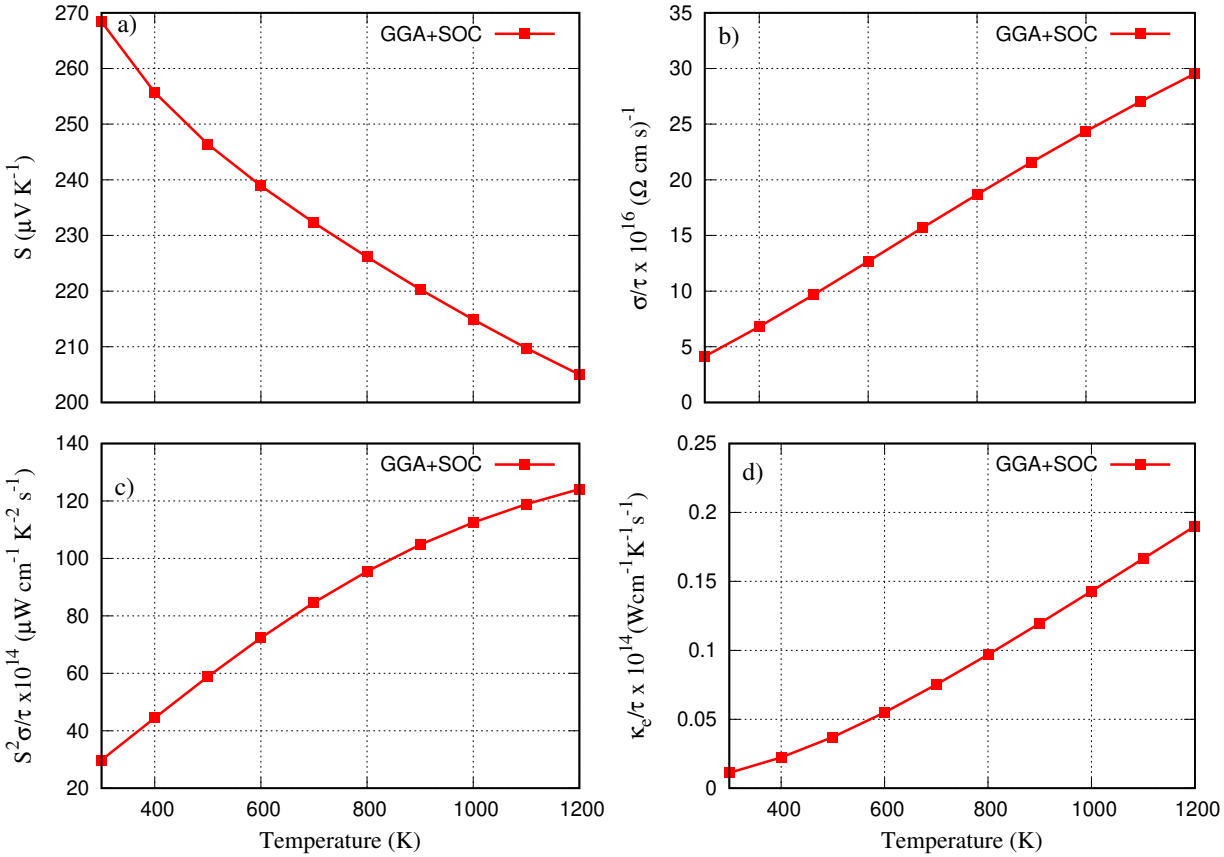


Fig.9: Variation of a) Seebeck Coefficient (α) b) Electrical Conductivity (σ/τ) c) Power Factor ($\alpha^2\sigma/\tau$) and d) Electrical Thermal Conductivity (κ_e/τ).

Results and Discussion

Transport Properties

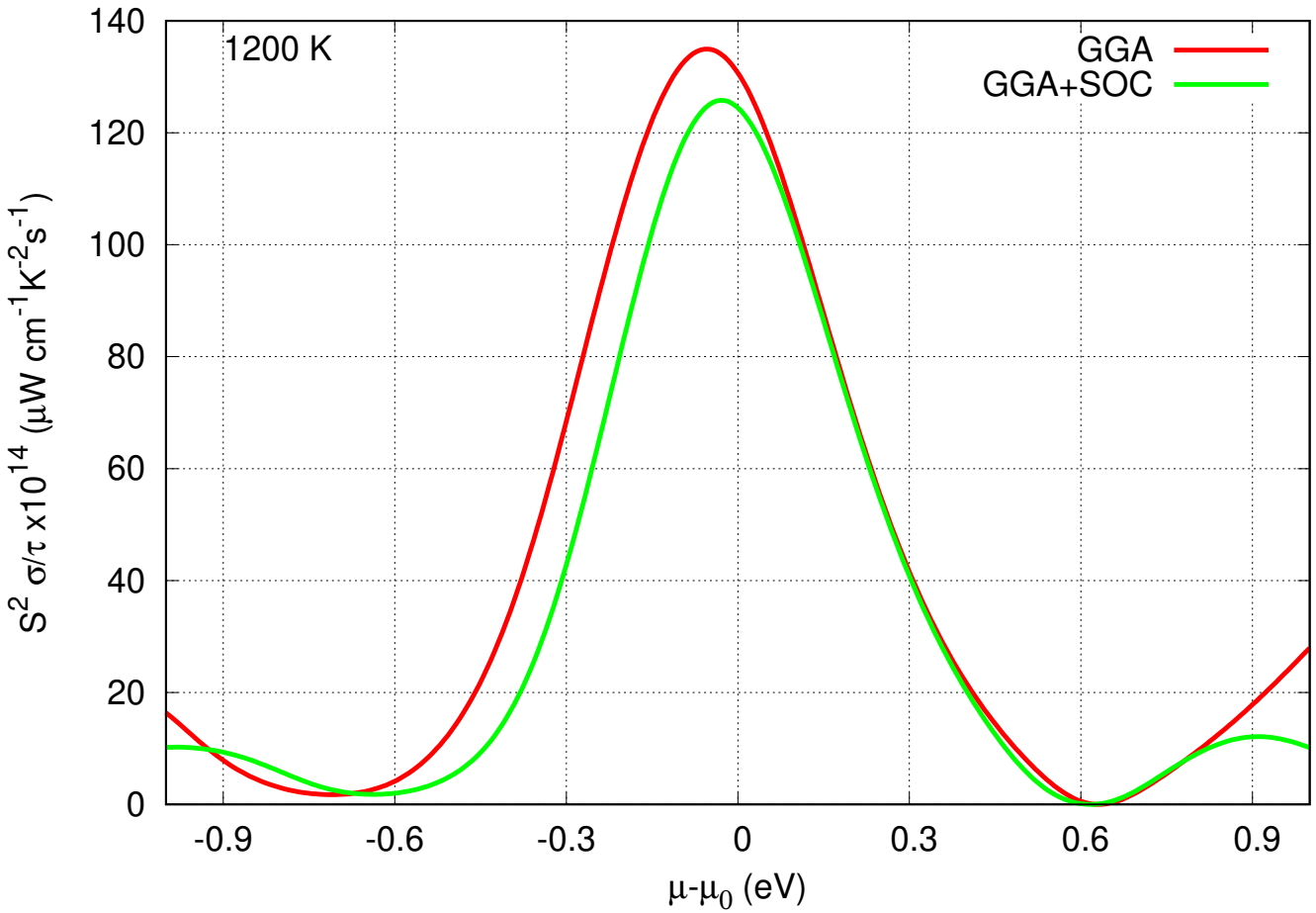


Fig.10: Variation of the power factor with the chemical potential.

Results and Discussion

Transport Properties

- Positive value of α is due to p-type charge carrier.
- High value of the ZT is obtained due to the flat nature of degenerate states in valence region near E_F.

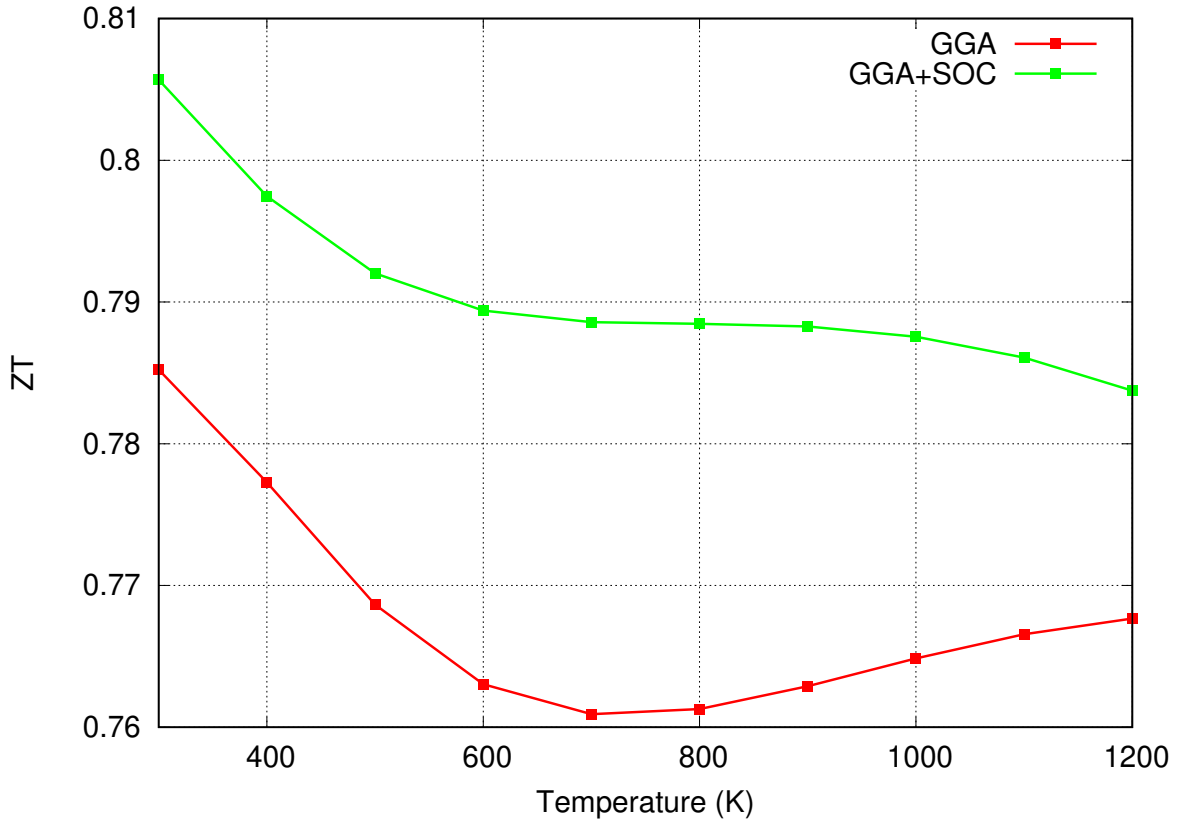


Fig.11: Variation of the figure of merit (ZT) with the temperature (K).

Conclusions

- We investigate the electronic, magnetic and thermoelectric properties using density functional theory.
- The ground-state found as antiferromagnetic with the energy gap of 0.81 eV.
- Large value of the Seebeck coefficient $\sim 205\ \mu VK^{-1}$ observed even at 1200 K signifies suitable for a high temperate TE devices.
- Based on the CRTA, obtained value of the power factor $\sim 124\ \mu W\ cm^{-1}\ K^{-2}$ at 1200 K indicates suitability for potential TE devices.
- We only consider the electronic part of the thermal conductivity, lattice part is dominant over the high temperature region, which affect the final value of the ZT.

Acknowledgments

- Central Department of Physics, Tribhuvan University, Nepal
- Condensed Matter Physics Research Center (CMPRC) Butwal, Nepal

THANK YOU !!!