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Enhancing the Conversion Efficiency of a Chalcogenide-Based Thermoelectric Module via Biaxial Strain

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INTRODUCTION & AIM

Climate change is one of the greatest challenges facing our planet today. It is mainly caused by human activities, which increase the concentration of greenhouse gases in the atmosphere. In response to this global issue, thermoelectric technology offers a promising solution for sustainable energy generation. Thermoelectric materials can directly convert heat into electricity through the Seebeck effect, without any moving parts or harmful emissions. Therefore, thermoelectricity represents an innovative and environmentally friendly approach to combating climate change. Improving the performance of these materials mainly focuses on increasing their figure of merit (ZT), which involves the application of several advanced material design techniques such as **nanostructuring, doping**, **composite materials** and **low-dimensional structures**

Deformation, also known as **strain engineering**, is an effective method to improve the performance of thermoelectric materials.

In this work, we try to enhance the Conversion Efficiency of a **CuGaTe2-Based** Thermoelectric Module via Biaxial Strain

METHOD

This study is an ab initio investigation performed using the **WIEN2k** code, which is based on density functional theory (**DFT**) and employs the full-potential linearized augmented plane wave (**FP-LAPW**) method. The structural and electronic properties were calculated using WIEN2k, while the thermoelectric properties were evaluated using the **BoltzTraP** code. The parameters required for the calculation of the lattice thermal conductivity (κ_l) were obtained using the **Gibbs2** code.

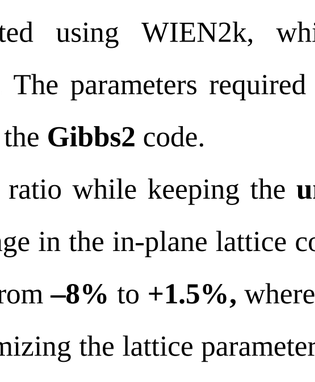
The biaxial strain in the **ab-plane** was simulated by varying the **c/a** ratio while keeping the **unit cell volume constant**. The strain is expressed in terms of the relative change in the in-plane lattice constant, as $\boldsymbol{\varepsilon = {\Delta a}/{a_0} = {a}/{a_0} - 1}$. The applied biaxial strain values range from **–8%** to **+1.5%,** where tensile strain corresponds to **ε > 0** and compressive strain to **ε < 0**. After optimizing the lattice parameters a and c, the atomic positions were also fully relaxed.

the dispersion energy was calculated using the **GGA-WC** and **TB-mBJ** approximations, including the **spin–orbit coupling (SO)** effect.

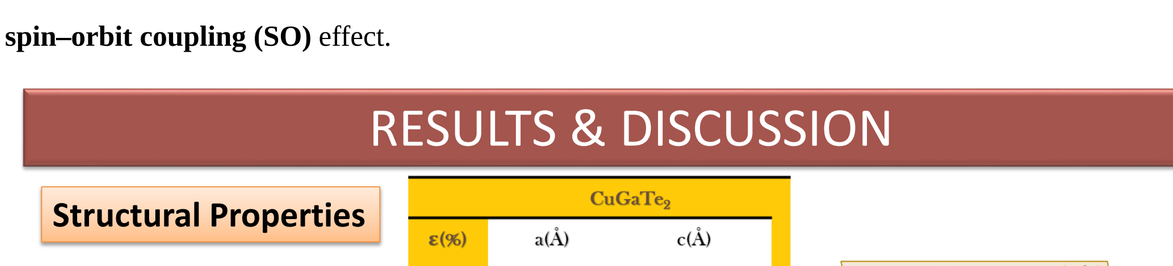
RESULTS & DISCUSSION

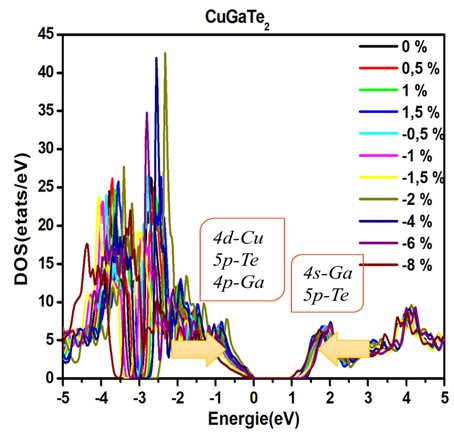
Structural Properties

CuGaTe$_2$		
ε(%)	a(Å)	c(Å)
+1.5	5.908	11.828
+1	5.8791	11.727
+0.5	5.850	11.680
0	5.82	11.64
-0.5	5.791	11.579
-1	5.762	11.486
-1.5	5.733	11.423
-2	5.704	11 ?371
-4	5.588	11.126
-6	5.471	10.888
-8	5.355	10.656



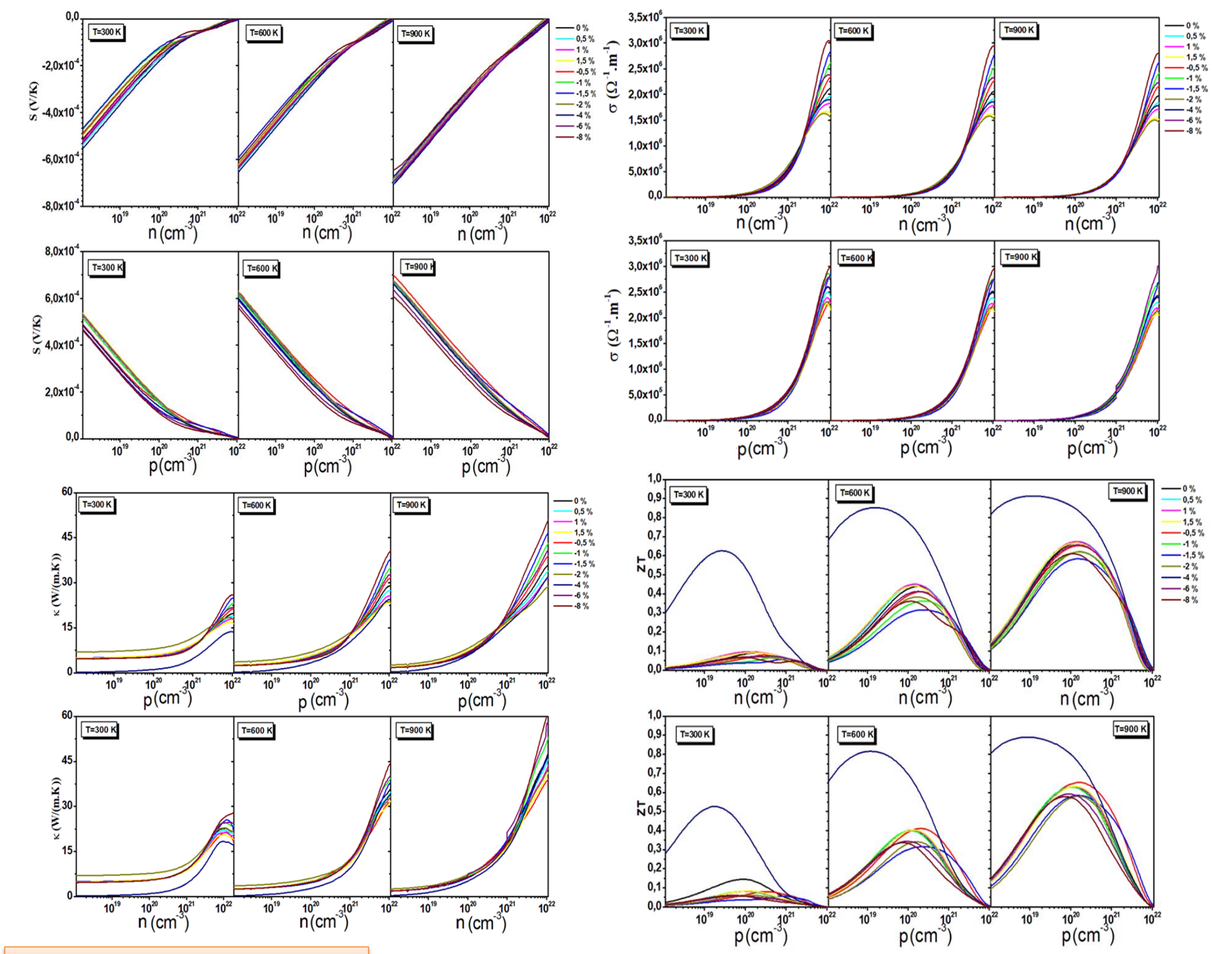
Electronic properties



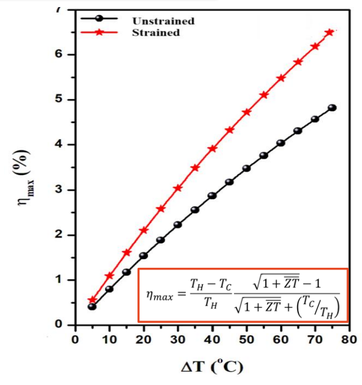


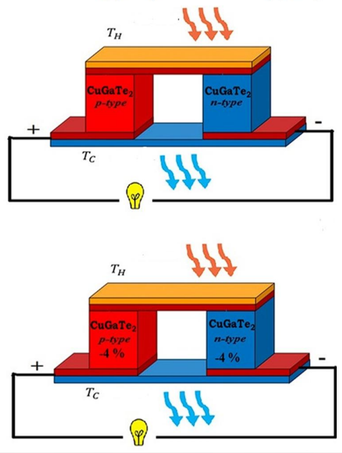
Eg(eV)			
	CuGaTe2		
ε(%)	GGA-WC	TB-mBJ	TB-mBJ+SOC
1.5	0.674	1.346	1.126
1	0.764	1.370	1.170
0.5	0.807	1.367	1.176
0	0.856	1.363	1.183
-0.5	0.887	1.355	1.172
-1	0.881	1.340	1.158
-1.5	0.866	1.326	1.142
-2	0.849	1.313	1.126
-4	0.856	1.360	1.124
-6	0.825	1.293	1.093
-8	0.690	1.170	0.963

Thermoelectric coefficients



Conversion efficiency





CONCLUSION

- ✓ Applying strain can modify the energy band gap near the Fermi level, enhancing the Seebeck effect.
- ✓ Deformation can scatter phonons, reducing the lattice thermal conductivity and thus improving the overall figure of merit (ZT).
- ✓ Compressive strain leads to improved efficiency, with ZT rising from 0.63 to about 0.9, showing clear performance enhancement.
- ✓ $CuGaTe_2$ demonstrates strong potential as a high-performance and environmentally friendly thermoelectric material, contributing to future sustainable energy technologies.

FUTURE WORK / REFERENCES

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