Thermoelectric Properties Of Chalcogenide Perovskites

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Background

- Thermoelectric materials are useful in addressing energy crisis and also serve as an alternative source of energy for future technological applications.
- Chalcogenide perovskites typically contain the Group-IIA elements such as Ba, Ca and Sr, the Group-IVB elements such as Hf, Zr, and Ti, S or Se atoms.
- Orthorhombic Barium Zirconium Sulfide ($BaZrS_3$) is a promising thermoelectric with a band gap close to the optimum value for single junction photovoltaics (1.35 eV)
- There are no detailed reports on the thermoelectric and optical properties of $BaZrS_3$. To bridge this gap a study on the accurate details of the thermoelectric properties has been conducted.

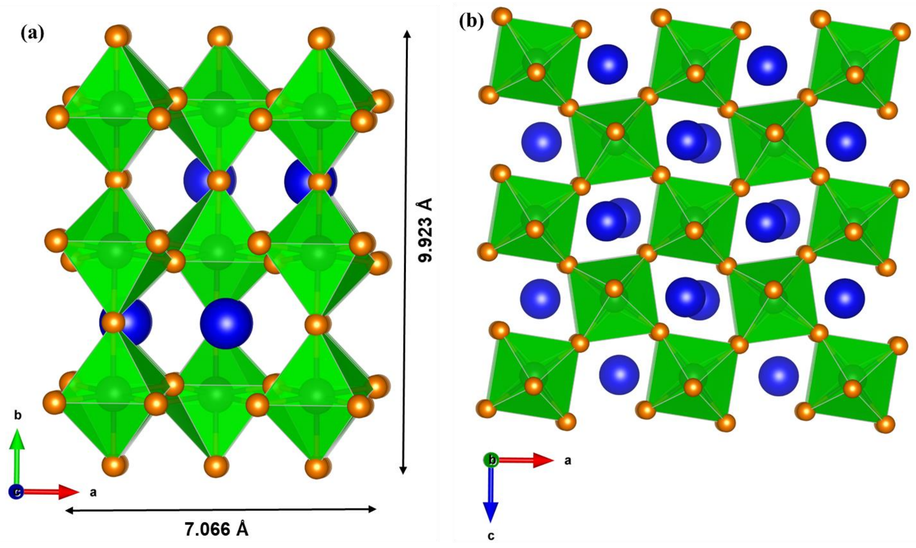
Motivation

- The commonly available thermoelectrics like $CuInSe_2$ and CdTe contain toxic metals and the need for other thermoelectrics containing earth abundant and less toxic elements arises.
- Finding materials with good thermoelectric figure of merit ZT (1 or above) requires exploration of chalcogenide perovskites as they possess good optical properties

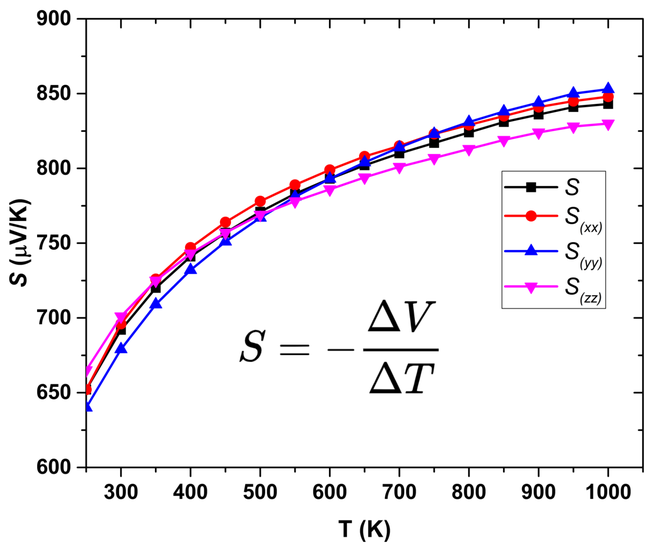
Conclusion

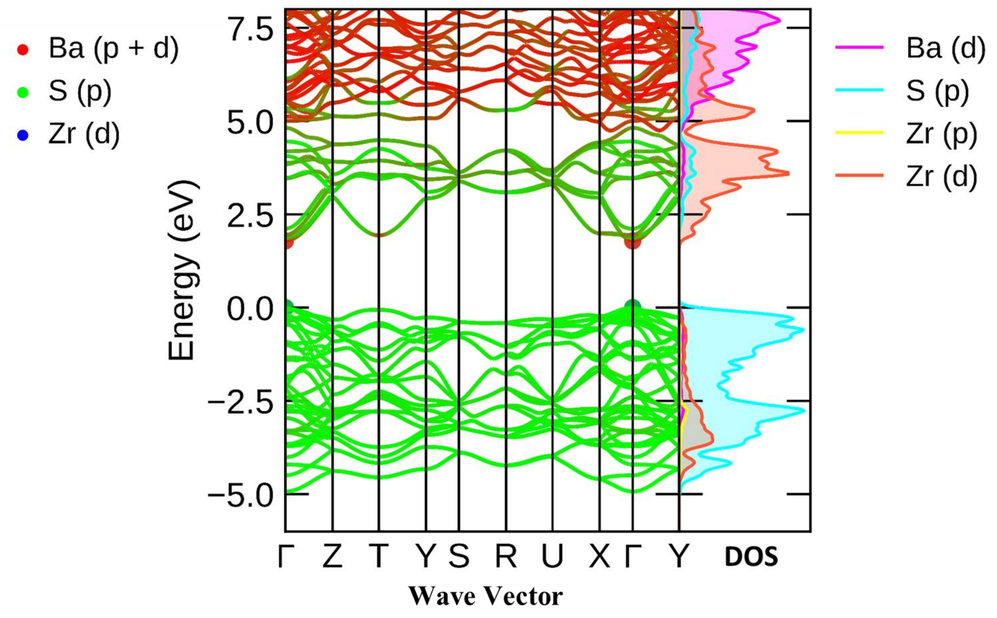
- We observe that $BaZrS_3$ possesses high Seebeck coefficients from 300 K to 900 K with the highest values along the a and b crystal lattices.
- $BaZrS_3$ exhibits low electrical conductivity and negligible electronic thermal conductivity within the same chemical potential range.
- The highest *ZT* value of 1.00 is obtained at 800 K for *n*-type doping at a carrier concentration of 10^{22} cm^{-3}.
- If operated at this given parameter, $BaZrS_3$ is an excellent thermoelectric with very promising prospects as a possible photovoltaic material.

Results and Discussion

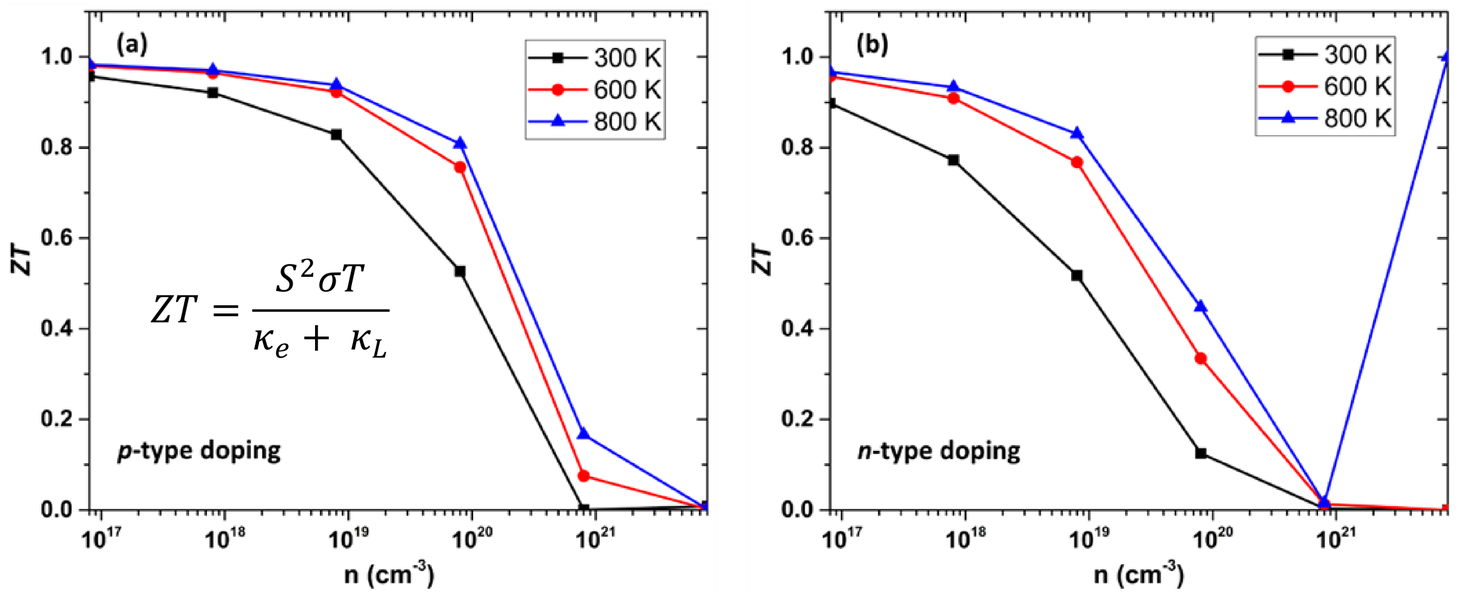


- Density Functional Theory calculations are used to optimize the $BaZrS_3$ to optimize the structures.
- Visualization of the BaZrS3 unit cell (left image) is produced with VESTA
- Side view(a) and top view (b) of the distorted perovskite structure of BaZrS3. Blue and brown spheres represent Ba and S atoms respectively while Zr atoms are inside the polyhedrals





- DFT calculations of the relaxed $BaZrS_3$ structure reveal a band gap of 1.79eV
- $BaZrS_3$ achieves a high optical absorption of 3 x 10^5 cm^{-1} at 3 eV of photon energy.
- There is a large contribution to the Seebeck coefficient (S) from the *a* and *b* lattices of $BaZrS_3$ at all temperatures.



- $BaZrS_3$ perovskites can achieve high thermoelectric figure of merit (*ZT*) values of 0.92-0.98 for both *p*-type and n-type doping at carrier concentrations of 10^{17} and 10^{18} cm^{-3} at 300-800 K.
- At lower carrier concentrations, *p*-type doped $BaZrS_3$ shows better performance in terms of the thermoelectric figure of merit while better thermoelectric figure of merit performance is achieved for *n*-type doping at higher carrier concentrations.

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