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Thermoelectric Properties of Manganese and Lead Telluride from First Principle

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Abstract: In this paper, we have employed the first principle calculation together with the Boltzmann transport theory to study the thermoelectric behavior of Manganese and Lead telluride between the temperature range of 100K to 1200K using the density functional theory and boltztrap as implemented on quantum espresso. Our results reveal that, even though tellurides are good TE materials but some are better than the others when compared. The thermal conductivity of the two materials is almost the same even though MnTe have higher thermal conductivity, other calculated parameters like the Seebeck coefficient, electrical conductivity and power factor reveals clearly that MnTe perform better as TE material when compared PbTe.

Keywords: *Thermoelectric; Telluride; BoltzTraP; Density Functional Theory; Seebeck coefficient*

1. Introduction

In the quest for sustainable energy solutions, thermoelectric materials emerge as pivotal contenders, harnessing waste heat and converting it into useful electrical power (Witting *et al*. (2019).

For instance, in a thermoelectric effect, heat is converted to electricity through the Seebeck effect. When there is a temperature gradient across a thermoelectric material, charge carriers (electron and holes) diffuse from the hot side to the cold side thereby creating an electric potential difference (Adachi *et al.* (2013). Conversely, in a thermoelectric cooler or heat pump, electricity is used to create temperature difference across thermoelectric material. This is achieved through the Peltier effect. When current flows through the material, one side absorb heat while the other side releases it creating a cooling effect or the heating effect depending on the direction of the current (Drebushchak (2008).

Among the many materials that find applications in TE, telluride compounds exhibit good thermoelectric properties, holding promise for efficient energy conversion (Guptar *et al. (*2020). It is important to highlight some breakthroughs attained so far in sustainable energy via TE materials, for instance (Dughaish (2002) in his work discussed that lead telluride PbTe can be used to convert waste heat to electricity in a power generator. It is also worth mentioning that even MnTe has a good thermoelectric property according to the work of (Hooshmand Zaferani, *et al.* (2021). MnTe show

excellent thermoelectric characteristic due to the presence of paramagnon drag above the Neel temperature. Traditional chalcogenides like Bismuth telluride and lead telluride are generally known to have good figure of merit as an indication of their thermoelectric performance (Sharma *et al* (2021). In this work we seek to explore specifically by comparing MnTe and PbTe the distinction in thermoelectric performance of these two chalcogenides to gain an insight as to which one of them will be more preferred in terms of practical applicability. To achieve these, we have employed the first principles methodologies using the density functional theory as implemented on quantum espresso (Miyata *et al. (*2018). Through this exploration, we endeavor to shed light on the potential applications and avenues for optimization of these materials in the pursuit of sustainable energy technologies according to (Junior *et al.* (2018).

2. Computational Method

The structural, electronic, and thermal transport properties of MnTe and PbTe were investigated using Density Functional Theory (DFT) as implemented in the quantum espresso code (Giannozzi, *et al*. (2020). The Perdew-Burke-Ernzerhof (PBE) parameterization using generalized gradient approximation was used to handle the exchange–correlation functionals (Tran. *et al. (*2020). The cut-off energy, lattice parameter and kpoints were converged and the best values were chosen. A dense K-mesh of 15x15x15 which uses over 400 k points in the irreducible brillouin zone (IBZ). The transport properties were obtained using Bolztrap code (Madsen *et al. (*2006), which solved the semi classical Boltzmann transport equation while having a constant value of relaxation time. This code was used to determine factors like power factor, Seebeck coefficient, electrical conductivity and thermal conductivity.

3. Results and Discussion

3.1 Seebeck Coefficient

This is an important parameter in determining the transport property of a material, it is the voltage induced in a material as a result of a temperature difference across it. When a Seebeck coefficient of a material is positive, it signifies that the material is p-type semiconductor but in our case, we observed that at higher temperature the materials become n-type. From our results, the PbTe material have lower Seebeck coefficient as compared to MnTe with a peak value of 4.31μV/K at 296K while the MnTe has a higher value of 28.3μV/K at 200K (figure 1). This implies that MnTe will accommodate more potential difference across in a ranges of temperature difference. We also noticed that higher temperature of 700K and above the two materials becomes n-type 100% and maintain the same value of Seebeck coefficient which decreases monotonically to 1100K

3.2 Thermal Conductivity

Thermal conductivity is the parameter that measures the ability of a material to transport heat along its length. In our case we calculated the thermal conductivity of MnTe and PbTe with respect to elctron relaxation time as in figure 2. In our result, we noticed that at lower temperature ranges of 200K to 400K, the two materials have their thermal conductivity correlating but at higher temperature of 600K and above MnTe exhibit higher conductivity. For instance, at a temperature of 1100K, the thermal conductivity of MnTe and PbTe are 9.12x10^{15} and 8.22 x10^{15} W/mK respectively. By this, the results suggest that lower voltage will be induced to MnTe because of its high thermal conductivity while PbTe will attract high voltage induced to it by virtue of its thermal conductivity value.

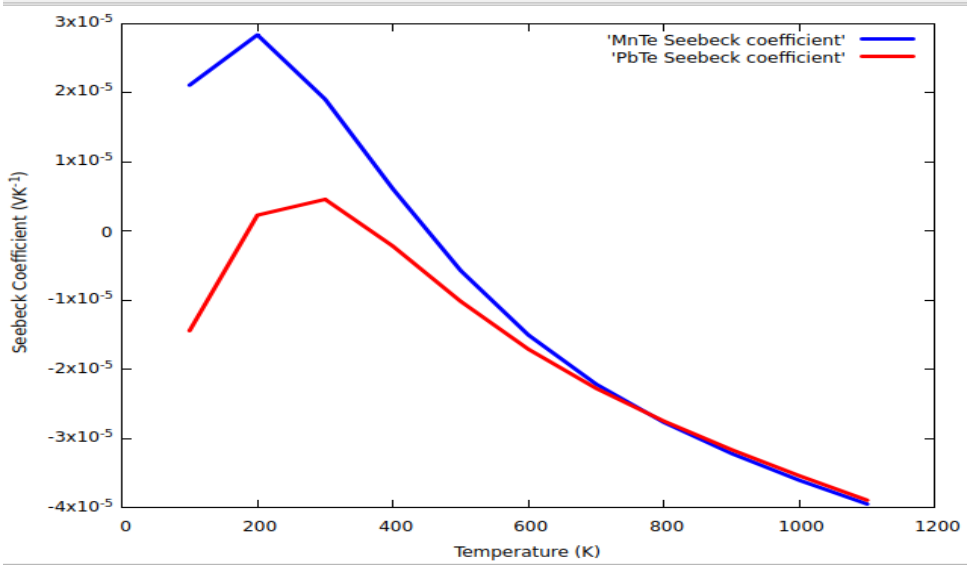

Figure 1: Seebeck Coefficient

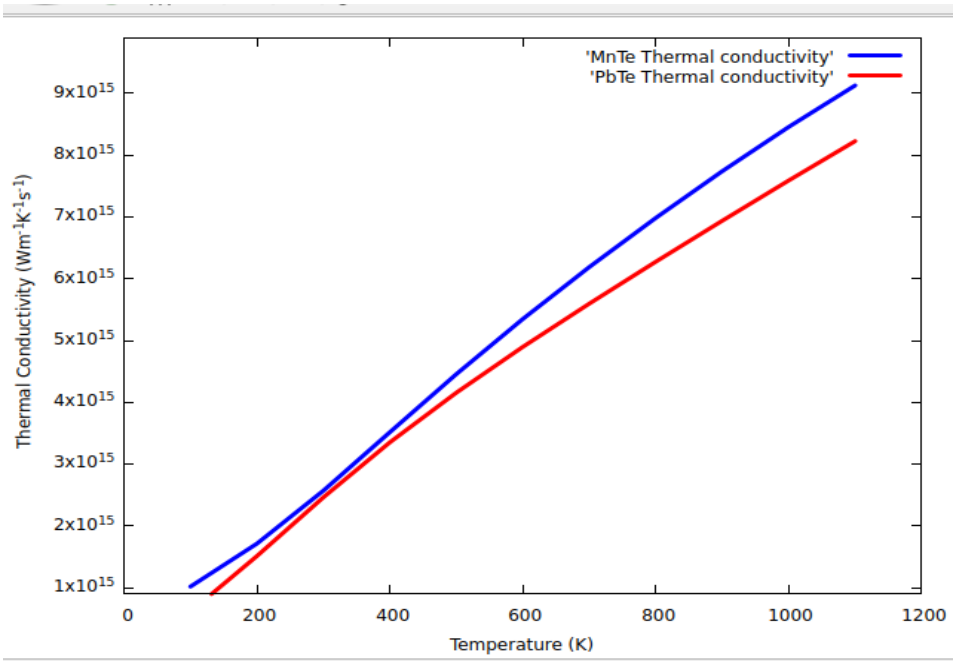

Figure 2 : Thermal CondFigureuctivity

3.3 Electrical Conductivity

Electrical conductivity is the measure of the materials ability to conduct electricity, looking at figure 3, we noticed that there is widegap between the conductivity of MnTe and PbTe this can be attributted to the fact that PbTe has a band band gap of 0.8eV and MnTe has band gap of 0.0eV in their cubic structure respectiviely, the metallic nature of MnTe (Mu, *et al. (*2019) could be the reason why its conductivity is higher than that of PbTe which exhibit band gap (Folley, *et al. (*1977), even though (Tonga and Baro (2022) and (Baro and Tonga (2022) reported in their work that materials can exhibit different band gap when studied in different structures. Our interest is to study these chalcogenides and provide and insight into their thermolectric properties. Our results show that MnTe can conduct better at higher temperatures. We observed that for these two chalcogenide, they at

higher temperatures show constant electrical conductivity which made us to conclude that the materials do not show changes in their electrical conductivity when exposed to high temperatures and extreme conditions.

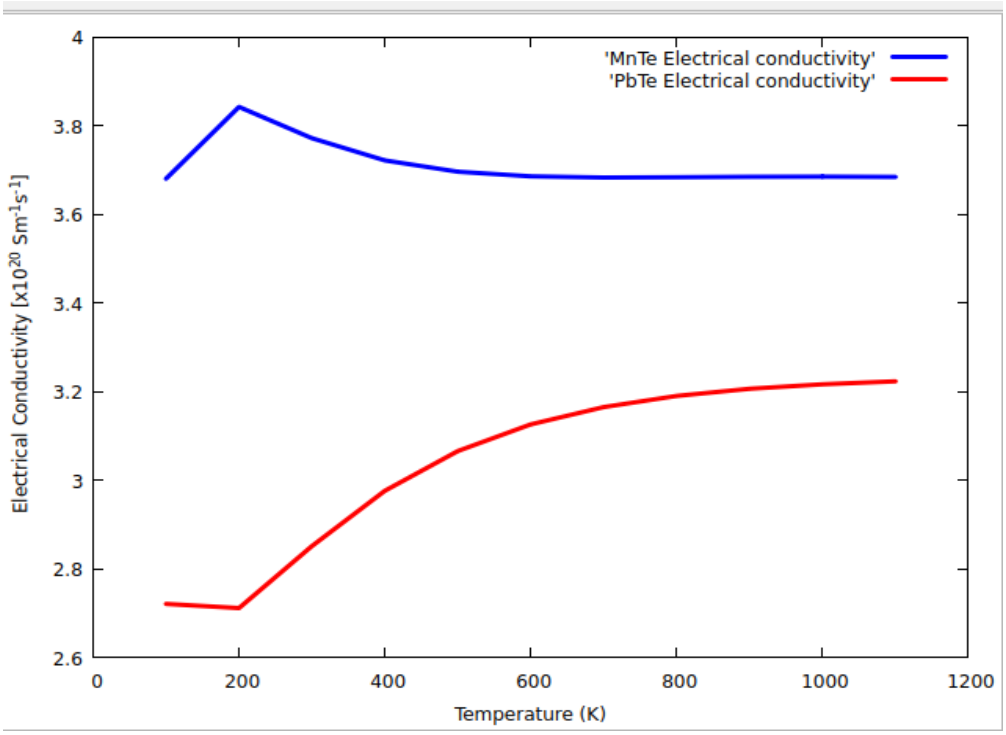

Figure 3: Electrical conductivity

3.4 Power Factor

The power factor of a material is the measure of the material's efficiency in converting thermal energy to electricity. This parameter depend on the seebeck coefficient, electrical conductivity and temperature difference. So if our material show a high or good power factor it means the material will be effective in converting waste heat to electricity. Mathematically the it is given by

$$PF = S^2\sigma \quad (1)$$

Where S is the Seebeck coefficient and σ is the electrical conductivity.

From our results in figure 4, at 200K, MnTe has a power factor of $3.2\text{x}10^{11}$ while PbTe has zero. This effect can be as a result of the nature of PbTe, we earlier stated that it has a band gap, we can therefore say that it requires more than 200K to excite the electrons to move to the conduction band. Since power factor is responsible for converting heat which is as result of temperature difference across a material to electricity, we therefore noted that for this material it requires more heat to convert excesses to electricity. For MnTe, we noticed an instability in its power factor between 0 to 400K which contradicts the work of (Hooshmand Zaferani, *et al.* (2021). Interestingly the power factor for both materials begin to rise at a temperature above 400K and it increases in a proportional manner. The increase in the power factor at higher temperatures means that the two materials can convert heat to electricity at higher temperature which confirms to us that they are good TE materials and can be used for any TE related applications.

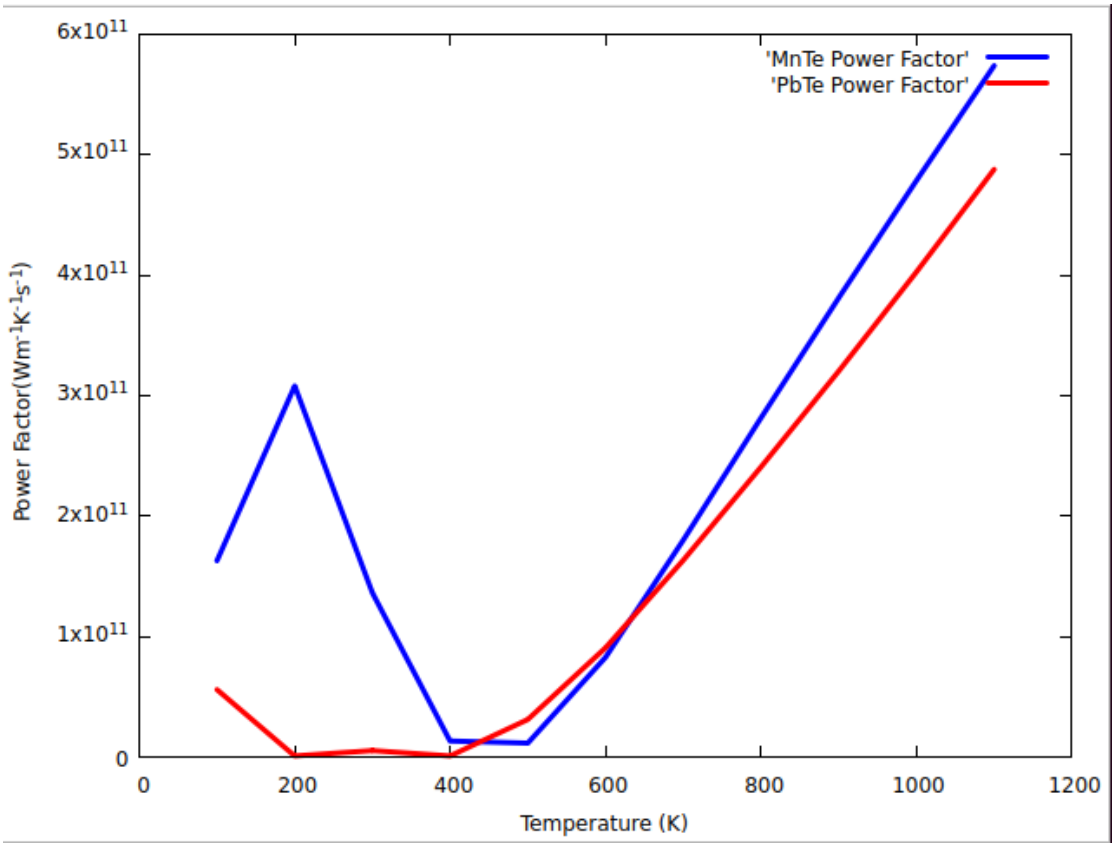

Figure 4: Power Factor

Conclusion

In this study, the thermoelectric properties of MnTe and PbTe were studied, the parameters that are indicators of a material's ability to convert heat to electricity i.e., Seebeck's coefficient, thermal conductivity, electrical conductivity and power factor revealed to us that, the two material at some higher temperature exhibit similar thermoelectric properties except for the electrical conductivity that show a different trend and we have noted that the disparity could be as a result of the nature of their band gap. In conclusion the two materials are said to have similar properties especially at higher temperature and they can also be used for any TE related applications, for example thermoelectric materials are used in the manufacture of sensors and can be used to cool electronic devices due to their high temperature gradient.

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Disclosure statement: *Conflict of Interest:* The authors declare that there are no conflicts of interest.

Compliance with Ethical Standards: This article does not contain any studies involving human or animal subjects.

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