

equal to or greater than $\nu = 0.25$ [29]. The calculated results of $\nu = 0.25 \sim 0.24$ for PtTe₂ and PtSe₂ suggest marginal ionic bonding.

Table 2. Elastic constants C_{ij} (GPa), elastic bulk moduli B_V (GPa), shear moduli G (GPa), Young's moduli E (GPa), Poisson's ratio and for of PtTe₂ and PtSe₂.

		C_{11}	C_{12}	C_{13}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	B_V	E	G	ν
PtTe ₂	PBEsol	170	53	42	170	67	45	45	58	68	105	42	0.24
	vdW-D2	200	62	55	200	83	65	65	68	84	129	52	0.24
	vdW-D3	175	52	48	175	77	49	49	61	74	111	44	0.25
	vdW-TS	169	52	42	169	69	42	42	58	68	103	41	0.24
PtSe ₂	PBEsol	197	67	41	197	51	40	40	64	66	102	41	0.24
	vdW-D2	262	83	62	262	94	69	69	89	101	157	63	0.24
	vdW-D3	202	63	41	202	61	43	43	69	71	111	45	0.24
	vdW-TS	183	59	41	183	62	38	38	61	68	102	40	0.25

3.3. Dynamical stability

In order to test the dynamic stability of the PtTe₂ and PtSe₂, their underlying phonon dispersion relations were calculated. Since PBEsol gave the best lattice parameters, it was used in the computations of the phonon structure. The phonon band structure and density of states for PtTe₂ and PtSe₂ are presented in Figure 3 and Figure 4 respectively. The phonon frequencies are in the range of 0 – 6 THz for PtTe₂ and 0 – 7 THz for PtSe₂. The reduction in the range can be attributed to the relative atomic weights of Te and Se. All the phonon frequencies are positive, which indicates that the structure of PtTe₂ and PtSe₂ are dynamically stable, thereby satisfying one of the necessary conditions for crystal stability.

The primitive cell of PtTe₂ and PtSe₂ contains three atoms and therefore there are nine phonon modes for each wave vector, three acoustic modes and six optical modes. The highest frequencies of the acoustic modes, defined here as the acoustic cutoff, are approximately 3.44 THz and 4.58 THz for PtTe₂ and PtSe₂, respectively.

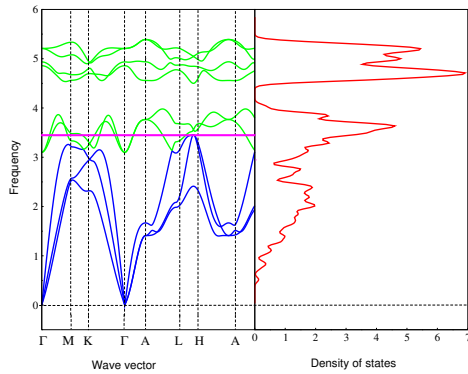


Figure 3. Phonon dispersion and DOS for PtTe₂.

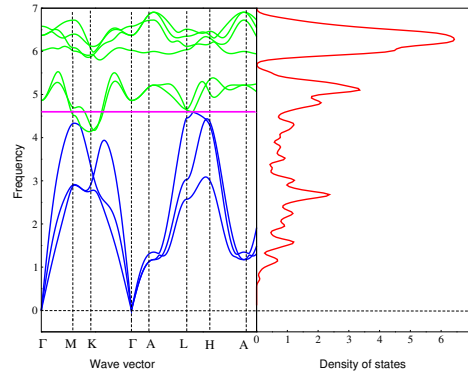


Figure 4. Phonon dispersion and DOS for PtSe₂.

3.4. Lattice thermal conductivity

The lattice thermal conductivity of PtTe₂ and PtSe₂ was calculated using the single-mode relaxation-time approximation to the linearized phonon Boltzmann equation [19]. The calculated lattice thermal conductivities of PtTe₂ and PtSe₂ in the range 0 to 1000 K are shown in Figure 5 and Figure 6 respectively, while the average of the cumulative thermal conductivities, as function of frequency at 300 K, are shown in Figure 7 and Figure 8 respectively. We note that the lattice thermal conductivity is highly anisotropic, with the thermal conductivity in the plane of the layers much higher than in the cross-plane direction.

Using Mattheissens rule [30] the average lattice thermal conductivity of PtTe₂ and PtSe₂ is 3.49, and 4.28 Wm⁻¹K⁻¹ respectively. The lattice thermal conductivities of these compounds is therefore small, which makes these compounds potential good thermoelectric materials.

We also estimated the contribution to the thermal conductivity from the acoustic modes at 300 K. We found that the in-plane acoustic mode contribution is 88.36% and 87.63% and cross-plane 71.34% and 68.00% for PtTe₂ and PtSe₂ respectively. This is in clear contrast to the conventional understanding, especially in the cross-plane direction, that the acoustic modes dominate thermal conductivity [30].

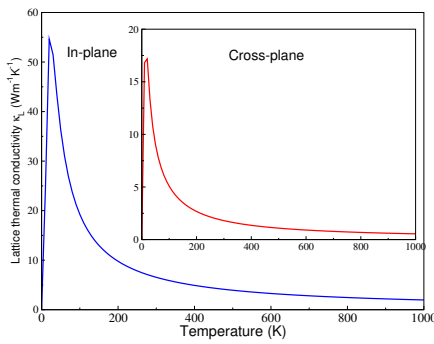


Figure 5. Lattice thermal conductivity Wm⁻¹ K⁻¹ $\kappa_L(T)$ for PtTe₂.

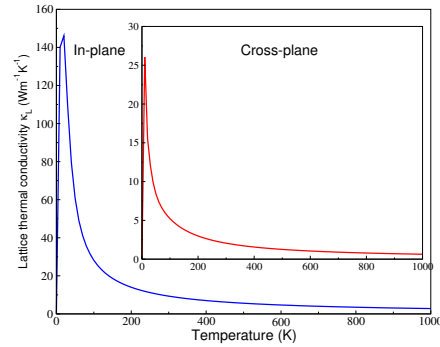


Figure 6. Lattice thermal conductivity Wm⁻¹ K⁻¹ $\kappa_L(T)$ for PtSe₂.

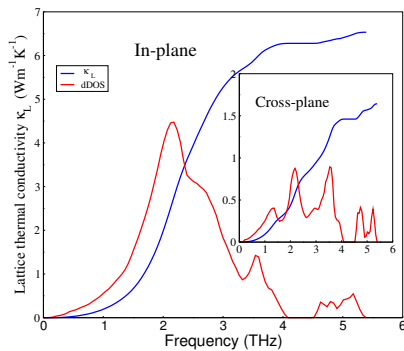


Figure 7. Average cumulative lattice thermal conductivity and derivative density $\kappa_L(\omega)$ for PtTe₂.

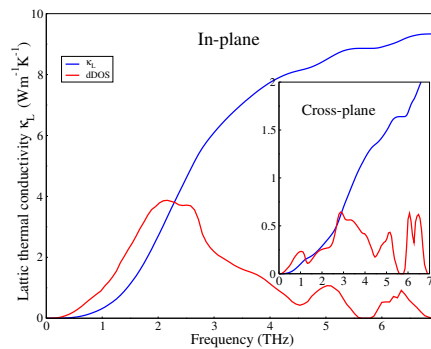


Figure 8. Average cumulative lattice thermal conductivity and derivative density $\kappa_L(\omega)$ for PtSe₂.

4. Conclusion

We have investigated the structural, mechanical and dynamical properties as well as the lattice thermal conductivity of bulk PtTe₂ and PtSe₂ from a first principles Density Functional Theory approach. Furthermore, we showed that the thermal conductivity of bulk PtTe₂ and PtSe₂ is highly anisotropic with the in-plane thermal conductivity much higher than the cross-plane thermal conductivity. The low value of the lattice thermal conductivity in the out-of-plane direction for both structures suggests that these materials are good candidates for thermoelectric applications.

Acknowledgements

We would like to acknowledge the financial support received from Shendi University, Shendi, Sudan. We also wish to acknowledge the Center for High Performance Computing (CHPC), Cape Town, South Africa, for providing us with computing facilities.

References

- [1] Holgate T C, *et al* 2013 *J. Elec. Mater.* **42** 1751–1755.
- [2] Mahan G D 1979 *Solid State Phys.* **51** 81–157.
- [3] Terasaki I, Sasago Y and Uchinokura K 1997 *Phys. Rev. B.* **56** R12685.
- [4] Yoffe A D 1983 *Solid State Ion.* **9** 59–69.
- [5] Hor S and Cava J 2009 *Mater. Res. Bull.* **44** 1375–1378.
- [6] Chen X, Wang M, Mo C and Lyu S 2015 *J. Phys. Chem. C* **119** 26706–26711.
- [7] Yan M, *et al* 2017 *Nat. Commun.* **8** 257.
- [8] Zhang K, *et al* 2017 *Phys. Rev. B* **96** 125102.
- [9] Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758.
- [10] Kresse G and Furthmüller J 1996 *Comput. Mater. Sci.* **6** 15–50.
- [11] Perdew P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865.
- [12] Ruzsinsky A, Csonka G I and Vydrov O A 2008 *Phys. Rev. Lett.* **100** 136406.
- [13] Monkhorst J and Pack D 1976 *Phys. Rev. B* **13** 5188.
- [14] Bucko T, Hafner J, Lebegue S and Ángyán J G 2010 *J. Phys. Chem. A* **114** 11814–11824.
- [15] Moellmann J and Grimme S 2014 *J. Phys. Chem. C* **118** 7615–7621.
- [16] Bučko T, Lebègue S, Ángyán J G and Hafner J 2014 *J. chem. phys.* **141** 034114.
- [17] Togo A, Chaput L and Tanaka I 2015 *Phys. Rev. B* **91** 094306.
- [18] Togo A, and Tanaka I 2015 <http://phonopy.sourceforge.net>.
- [19] Togo A and Tanaka I 2015 *Scr. Mater.* **108** 1–5.
- [20] Murnaghan D 1944 *Proc. Natl. Acad. Sci.* **30** 244–247.
- [21] Lamfers J, Meetsma A, Wieggers A and De Boer L 1996 *J. Alloys Compd.* **241** 34–39.
- [22] Zappa D 2017 *Materials.* **10** 1418.
- [23] Furuseth S, Selte K and Kjekshus A 1965 *Acta Chem. Scand.* **19** 257.
- [24] Thomassen L 1929 *J. Phys. Chem.* **2** 349–379.
- [25] Mouhat F and Coudert X 2014 *Phys. Rev. B.* **90** 224104.
- [26] Luo J and Stevens R 1996 *J. Appl. Phys.* **79** 9057–9063.
- [27] Hill R 1952 *J. Proc. Phys. Soc.* **65** 349.
- [28] Hopcroft M A, Nix W D and Kenny T W 2010 *J. Microelectromech. S* **19** 229–238.
- [29] Bouhemadou A, *et al* 2009 *Comput. Mater. Sci.* **45** 474–479.
- [30] Kittel C 2005 *Introduction to solid state physics* (USA: John Wiley and Sons, Inc).