DFT Approach into the Physical Properties of MTe_3(M=Hf, Zr): A Comprehensive Study

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INTRODUCTION

- **Transition-metal trichalcogenide compounds, MTe_3 (M=Hf, Zr) have recently piqued interest due to its mechanical, chemical and dynamical stability and also their prospective applications in various electronic and optoelectronic devices.**
- **The appearance of superconductivity with ~ Tc = 2 K of $HfTe_3$ has been confirmed experimentally.**
- **These compounds have a great prospect as a coating materials due to its high value of reflectivity.**

Theoretical Methodology

- DFT calculations are performed using the Cambridge Serial Total Energy Package (CASTEP).
- The generalized gradient approximation (GGA) is used for electron exchange correlation function with the Perdew-Burke-Ernzerhof (PBE) type to perform geometry optimization. Elastic constants were calculated by the 'stress-strain' method using CASTEP program.
- The bulk modulus, B, shear modulus G and Young modulus, Y were obtained from the calculated elastic constants C_{ij}.

Structural Properties

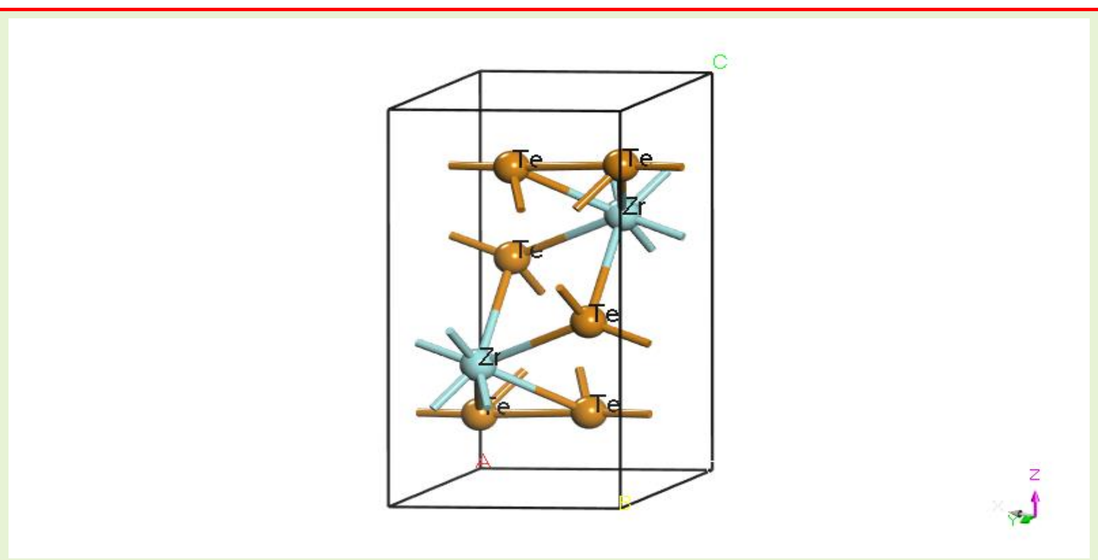

Fig. 1: Optimized crystal structure of MTe_3(M= Hf, Zr)

Optimized parameters	a	b	c	V	Ref.
$HfTe_3$	5.883	3.988	10.649	247.882	This
	5.8845	3.9026	10.0551	228.70	Ref. 1
$ZrTe_3$	5.89480	3.926400	10.1040	231.62421	This
	5.1339	3.6363	9.0032	……	Ref. 2

Table 1: Optimized lattice parameters, *a*, *b* and *c* (Å), unit cell volume *V* (Å^3) of MTe_3 (M =Hf and Zr) compounds

- The obtained structural parameters, such as lattice parameters, angles, and volume, agree with the previous study.
- The crystal system is monoclinic with space group P_{21}/m (No. 11)

Electronic Properties

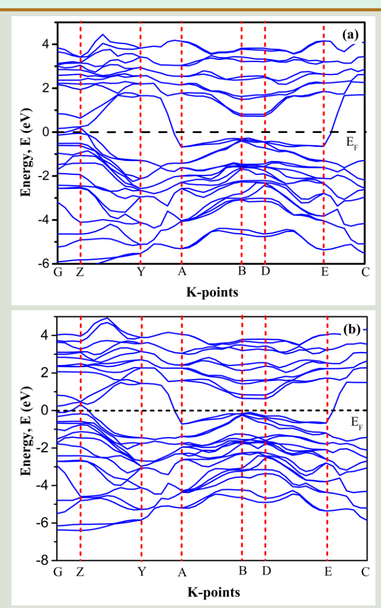

Fig 2. Calculated electronic band structure of (a) $HfTe_3$ (b) $ZrTe_3$ along the high symmetry directions in the Brillouin zone at ambient conditions.

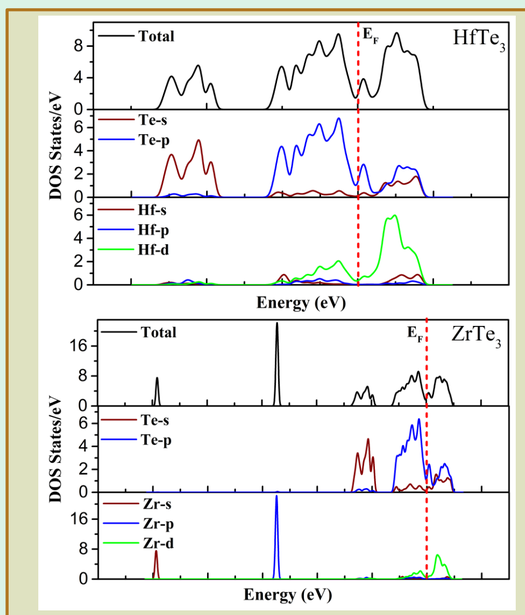

Fig 3. The total and partial energy density of states of (a) $HfTe_3$ (b) $ZrTe_3$.

- ✓ Electronic band structure profile demonstrates that the studied compounds are metallic in nature.
- ✓ The Partial density of states (PDOS) confirms that the prime contribution to the conductivity comes from the Te-*p* orbital electrons.

Mechanical Properties

Compounds	C_{11}	C_{12}	C_{13}	C_{23}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	CP
$HfTe_3$	94	94	11	18	87	41	28	16	22	66
$ZrTe_3$	105	16	14	17	82	49	34	9	22	-18

Table 2: The calculated single crystal elastic constants Cij (GPa) and Cauchy pressure (CP) for MTe_3 (M =Hf and Zr).

Compounds	B	G	Y	G/B	υ
$HfTe_3$	28	21	50	0.74	0.20
$ZrTe_3$	35	22	55	0.63	0.23

Table 3 :The calculated bulk modulus, B (GPa), shear modulus, G (GPa), Young's modulus, Y (GPa), Pugh ratio G/B, and Poisson ratio, νfor MTe_3 (M =Hf and Zr).

- The title compounds are mechanically stable, which is confirmed from the stiffness constants.
- The value of Pugh's ratio (ratio of shear and bulk modulus) indicates that $ZrTe_3$ is less brittle in nature compared to $HfTe_3$.
- The title compounds are predicted to be highly soft and anisotropic in nature.

References
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2. D. S. Muratov, V. O. Vanyushin, N.S. Vorobeva, P. Jukova, A. Lipatov, E. A. Kolesnikov, D. karpenkov, D. V. Kuznetsov, and A. Sinitskii J. Alloys Compd.815, 152316 (2020)

Conclusions

- The obtained structural parameters, such as lattice parameters, angles, and volume, agree with the previous study.
- Electronic band structure demonstrates that there are no band gaps between the valence and conduction bands, making the material metallic.
- The mechanical properties that are technologically important (stiffness constant, elastic moduli, brittle/ductile behavior, Poisson's ratio, anisotropy, and hardness) are thoroughly examined and addressed. When compared to $HfTe_3$, the value of Pugh's ratio (ratio of shear and bulk modulus) indicates that $ZrTe_3$ is less brittle in nature. The title compounds are projected to be highly soft and anisotropic in nature.