Theoretical study of the electronic structure of Sn_4Ge using first-principles

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Background

- The first-principle calculations are a powerful tool to predict the electronic properties of solids.
- It was recently predicted[1] that the tetragonal structure of Ge_5 and Sn_5 as topological semi-metal and topological insulators, respectively, using first-principles calculations.
- As Ge and Sn both have the same valency, it is likely to have similar (topological) properties in the tetragonal allotropes of compounds made up of Ge and Sn. Subsequently, we studied the electronic properties of the new Sn_4Ge.

AIM

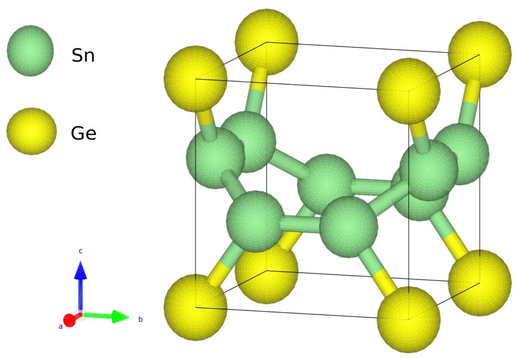
- The main aim of this work is to study the electronic properties of Sn_4Ge.
- The stability of the system is confirmed by calculating the formation energy of Sn_4Ge.
- Spin-orbit interaction (SOI) plays a significant role in heavy elements. Therefore we also consider SOI while performing the electronic structure calculations.

Methodology

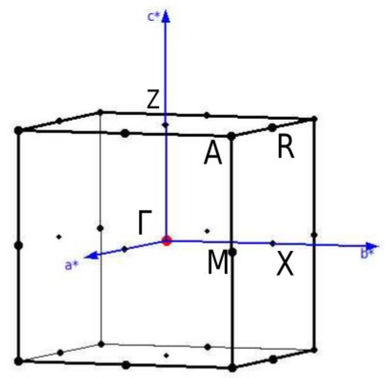
- Geometry optimization and self-consistent calculations are performed using density functional theory as implemented in Quantum Espresso[2].
- The Projector Augmented Wave (PAW) pseudopotential: Scalar relativistic (without SOI) and fully relativistic (with SOI) with PBE exchange-correlation functional.
- We used 80 Rydberg kinetic energy cut off with Monkhorst Pack k-point mesh of 18×18×18.

Results & discussion

Optimized Structure



(1) Primitive unit cell

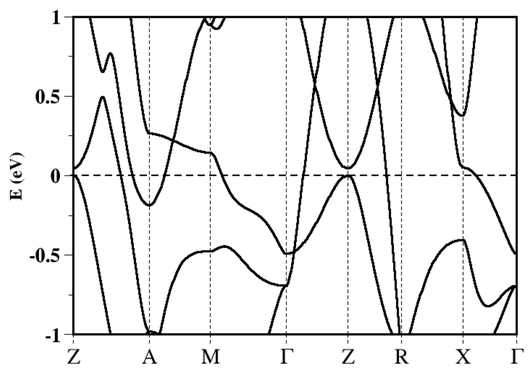


(2) Primitive Brillouin zone

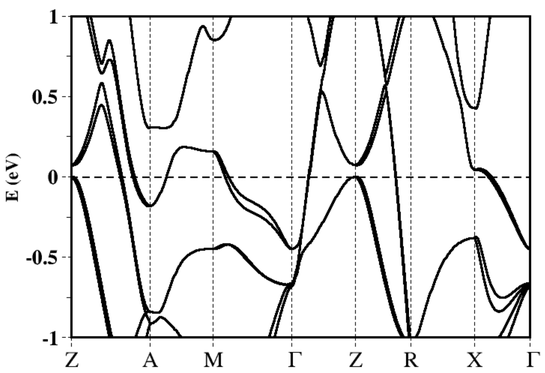
- Tetragonal crystal structure with space group $P\bar{4}M2$ (No. 115).
- Primitive unit cell contains four Sn atoms and one Ge atom with Wyckoff positions 4j (0.0000, 0.2731, 0.3190) and 1a (0.0, 0.0, 0.0), respectively.
- Formation energy of Sn_4Ge is calculated to be -4.17 eV.

Electronic Properties

Band structure of Sn_4Ge with and without spin-orbit interaction (SOI)



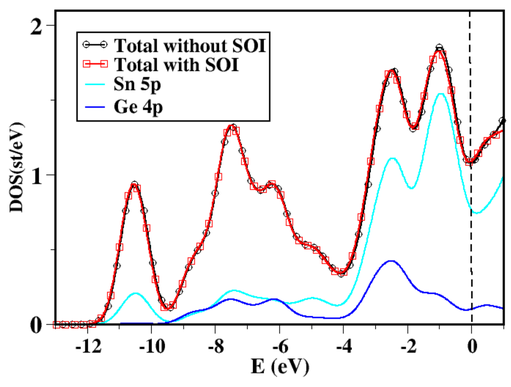
(3) Without SOI



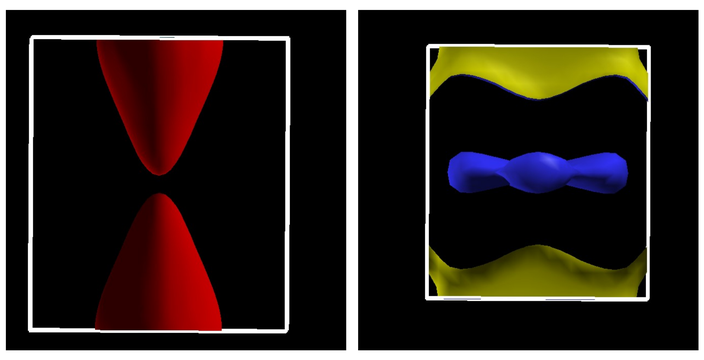
(4) With SOI

- Sn_4Ge is metallic, and significant band splitting due to SOI is observed along M-Γ path.

Electronic Properties



(5) Projected density of states of Sn_4Ge



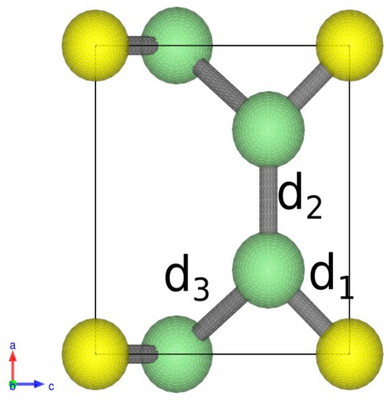
(6) The Fermi surface of Sn_4Ge

- Spin-polarized calculation confirms the non-magnetic nature of Sn_4Ge.
- There is no significant change in the total density of state due to spin-orbit interaction.
- There is a strong hybridization between Ge 4p and Sn 5p orbitals in the energy range -4 to -2 eV.
- Fermi surface (left panel in Fig. 6) has a typical Dirac cone shape with a gap at the Γ point.

TABLE 1. Bond lengths and lattice parameters comparison in the unit of Å

Structure	a	c	d_1	d_2	d_3
Ge_5	5.63	5.23	2.53	2.50	2.54
Sn_5	6.49	5.99	2.91	2.89	2.93
Sn_4Ge	6.42	5.63	2.51	2.92	3.21

(7) Ge_5 and Sn_5 data taken from Ref. 1



Summary

- The ground state of newly predicted Sn_4Ge was found to be metallic and non-magnetic in nature.
- The inclusion of spin-orbit interaction leads to a significant band-splitting along M-Γ.
- The Fermi surface plot of one of the bands shows the typical Dirac cone with a gap at the Γ point.

Acknowledgment

• The first author acknowledges UGC for financial support.
• The authors acknowledge IIT BOMBAY and CDAC PUNE for the computational facility.

References

1. Chengyong Zhong, Front. Phys. 16(6), 2021.
2. Paolo Giannozzi *et al.*, J. Phys.: Condens. Matter 21, 2009.