بسم الله الرحمن الرحيم
الجامعة الإسلامية للتكنولوجيا
UNIVERSITÉ ISLAMIQUE DE TECHNOLOGIE
ISLAMIC UNIVERSITY OF TECHNOLOGY
DHAKA, BANGLADESH
THE ORGANIZATION OF THE ISLAMIC CONFERENCE

First-Principles Study On Structural, Electronic and Optical Properties of a Novel Janus Material Al_2S_2SiGe

A Dissertation Submitted in Partial Fulfillment of Requirement for the Degree of Bachelor of Science in Electrical and Electronic Engineering

Submitted By:

Md.Shartaz Malik (180021216)

Ahsan Ali (170021182)

Supervised By:

Nishat Tasnim Hiramony
Lecturer
Department of Electrical and Electronic Engineering

First-Principles Study On Structural, Electronic and Optical Properties of a Novel Janus Material Al_2S_2SiGe

By

Md.Shartaz Malik (180021216)

Ahsan Ali (170021182)

A Thesis Submitted to the Academic Faculty in Partial Fulfillment of the Requirements for the Degree of
BACHELOR OF SCIENCE IN ELECTRICAL AND ELECTRONIC ENGINEERING

Department of Electrical and Electronic Engineering
Islamic University of Technology
Gazipur, Bangladesh

June2023

Declaration of Candidate

It is hereby declared that this thesis or any part of it has not been submitted elsewhere for the award of any Degree or Diploma.

Nishat Tasnim Hiramony
Lecturer
Department of Electrical and Electronic Engineering
Islamic University of Technology
Date:

Md.Shartaz Malik
Student no. 180021216
Academic Year:

Ahsan Ali
Student no. 170021182
Academic Year:

ACKNOWLEDGEMENTS

Foremost, we would like to express our sincere gratitude and gratefulness to Allah Almighty, for without His graces and blessings, this study would not have been possible.

Acknowledging all who helped us to complete this work, we wish to compliment the significant role of the university and the department that has been very amiableto us during the entire period of our research.

We are indebted to our honorable supervisor Nishat Tasnim Hiramony madam for his selfless support, his motivation, patience, enthusiasm and extensive knowledge of the relevant fields. His continuous guidance and detailed supervision kept us going even during the hardest of hours. We could not have imagined a better mentor for our thesis work.

Lastly, our warmest tribute to our parents, friends and families, whose moral support and well wishes benefitted us spiritually in achieving our goals.

ABSTRACT

The main purpose of this thesis is to make a novel janus material.The band structure and the density of state give us the result of the material. Basically we found the material as a semi-conductor or insulator.As phonon calculation gives us the electronic properties of the material. In the context of density functional theory, we have utilized first-principles computations. The material's band gap is the difference in energy between the highest occupied and lowest unoccupied band. This is a crucial characteristic for both electrical transport and a variety of spectroscopies. Around the Fermi energy, we saw that the system had an area without states. Therefore, there is a bang-gap. Possible materials include insulators (big band-gap) and semi-conductors (modest band-gap).

Contents

List of Figures

List of Tables

CHAPTER 1

INTRODUCTIION

Literature Review of Structural properties of the compounds LnAl2X2 (Ln=Eu,Yb, X=Si, Ge).We have also explored many materials from computational 2D Materials Database(C2DB)We got the monolayers of Al2S2Si2 and Al2S2Ge2 and they both are dynamically stable.We predicted a novel Janus material (Al2S2SiGe) from these two pure monolayers.We have run phonon calculation of our material to see if it comes out stable. In the result, our material contained no negative frequency confirming the dynamic stability.In our thesis we want to see the properties of our novel janus material. The band gaps,Fermi energy levels,Electronic ans electrical properties etc.

Thesis Objective

The main purpose of our thesis is to predict a novel Janus material. We have used first-principles calculations within the context of density functional theory. The structure is modeled with Quantum Espresso.Then we have found the dynamic stability by phonon calculation. Finding the band structure of our novel Janus material and finding the density of states (DOS). The density of states (DOS) is essentially the number of different states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy. The density of states for silicon was calculated using the program Quantum Espresso. Notice that the bandgap is too small. This commonly occurs for semiconductors when the bandstructure is calculated with density functional theory. The charge density difference and optical properties of the material are the important objectives of this thesis Choose a suitable substrate for the material. And finally the last objective is to explore how strain application affects electronic properties.

Chapter 2

THEORETICAL BACKGROUND

A computation in physics is referred to by the terms "from first principles, if it begins at the level of established physical laws and makes no assumptions, such as using an empirical model or fitting parameters. Methods of computation based on quantum mechanics do not rely on measuring parameters from research or base any conclusions on anything. They are totally dependent on physics laws. They are referred to as First Principle (ab initio) Methods as a result. As a result of its background in quantum physics, the density functional theory of physics (DFT) is also known as first principles theory. We shall briefly cover the theoretical foundations of DFT in this chapter.

2.1 Density Functional Theory (DFT)

Density functional theory (DFT) has shown to be one of the most effective and alluring approaches to material modeling issues in solid-state and condensed matter physics. DFT calculations performed using ab initio (from basic principles) allow for the prediction and calculation of material behavior based on considerations related to quantum mechanics. This theory states that a functional (function of a function) of the ground state density can be

used to describe the characteristics of a system of interfering particles. This method has been found to provide reasonable findings in a range of systems, allowing the investigation of real systems with small or even enormous numbers of atoms. The main goal of DFT is to assess observables like the equilibrium position of the atoms in a molecule, equilibrium bond length and angles, vibrational frequencies and phonons, forces on atoms, bulk modulus, excited states, optical absorption, electron energy loss spectrum, superconductivity, etc. Due to these factors, DFT has recently emerged as the method of choice for computations involving electronic structures.

2.2 Density of States (DOS)

The number of independent states that electrons are permitted to occupy at a specific energy level is known as the density of states (DOS), or the number of electron states per unit volume per unit energy. The electrical properties of materials can be accurately determined using DOS. It is directly connected to how the system properties are dispersed. If the DOS is large for a particular energy level, then many states are open for occupancy, but if the DOS is zero then no states are open for occupation. In contrast to the bands, where it has a finite value, a material's DOS is nothing at the bandgap. The density of states is calculated using the program *Quantum Espresso*. The bandgap can be too small some times. When the bandstructure is determined using density functional theory, this frequently happens for semiconductors.A common

solution to the small bandgap issue is to simply raise the energy of the states in the conduction band until the bandgap is the proper size. This procedure is sometimes called a scissors cut. The density of states is cut in the bandgap and pushed apart until the bandgap is correct.

2.3 2D Group IV Materials

Graphene, silicene, and other group IV elements are discussed, as well as phosphorene, transition metal dichalcogenides, and monochalcogenide-monolayers. The resemblances and distinctions between families are highlighted. We begin by giving a brief overview of crystallography and diffraction, emphasizing its use as a foundation for comprehending the primary characteristics of charge-carrier propagation. Then, we look at the theoretical instruments, such as Dirac and Weyl materials, required to model the electrical properties. The significance of free-electron bands in describing interactions between graphene and substrates and polar liquids like water is also discussed. Such tools allow one to describe a new playground for observing exotic matter phases, such as Kekulé patterns, moiré patterns, graphene over graphene at magic angles, mixed Dirac–Schrödinger electronic spectrum, and topological insulator states.

2.4 Janus Materials

Most impressive applications have recently been discovered for Janus (type) materials, which are particles with at least two separate anisotropically released properties on the surface. The term “Janus” originates from the roman God Janus. Who has a head with two faces looking in opposite directions to the future and past. “Janus” material was first used by Casagrande in 1989 to describe spherical glass particles with hydrophobic/hydrophilic hemispheres and became more and more popular after the Nobel Prize lecture by Pierre-Gilles de genes entitle “Soft Matter”. The Janus family of two-dimensional (2D) materials, such as Janus graphene, Janus transition metal chalcogenides, etc., has attracted a lot of interest lately. The concept of Janus materials with asymmetric facial features and substantial study on graphene and graphene derivatives with various asymmetric chemical groups as functional groups have contributed to this. According to both experimental and theoretical data, Janus 2D materials have unique properties like an out-of-plane piezoelectric polarization and a strong Rashba effect because of their out-of-plane asymmetry. In our thesis we predicted a novel Janus material (Al2S2SiGe) from these two pure monolayers.

CHAPTER 3

METHODOLOGY

3.1 COMPUTATIONAL DETAILS

3.1.1 Simulation Tools

At the heart of all the calculations carried out here lies a code capable of ab initio calculations. The code used here *is Quantum Espresso*, which is based on density functional theory (DFT), plane waves and pseudopotentials.

3.1.2 Simulation Parameters

Parameter	Value
Total energy convergence threshold	7.349E-8 Ry
Force convergence threshold	3.889E-4 Ry/Bohr
Energy cutoff	500 eV
Pseudopotential	PAW
K-point grid dimension	
K-path for bands	

Table-1:Simulation parameters

We have used these parameters. Total energy convergence threshold which value was 7.349E-8 Ry. Force convergence threshold. Which value was 3.889E-4 Ry/Bohr . Energy cutoff value was 500eV.

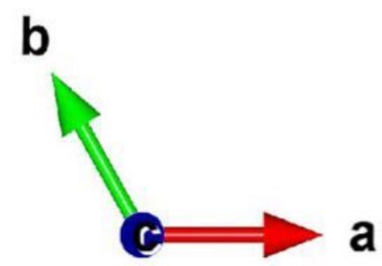
3.1.3 Value of Fermi energy for different elements

Element	Fermi Energy eV
Li	4.74
K	2.12
Na	3.24
Cs	1.59
Rb	1.85
Ag	5.49
Cu	7.00
Be	14.3
Au	5.53
Ca	4.69
Mg	7.08
Ba	3.64
Sr	3.93
Fe	11.1
Nb	5.32
Zn	9.47
Mn	10.9
Hg	7.13
Cd	7.47
Al	11.7
Ga	10.4
In	8.63
Tl	8.15
Sn	10.2
Pb	9.47
Bi	9.90
Sb	10.9

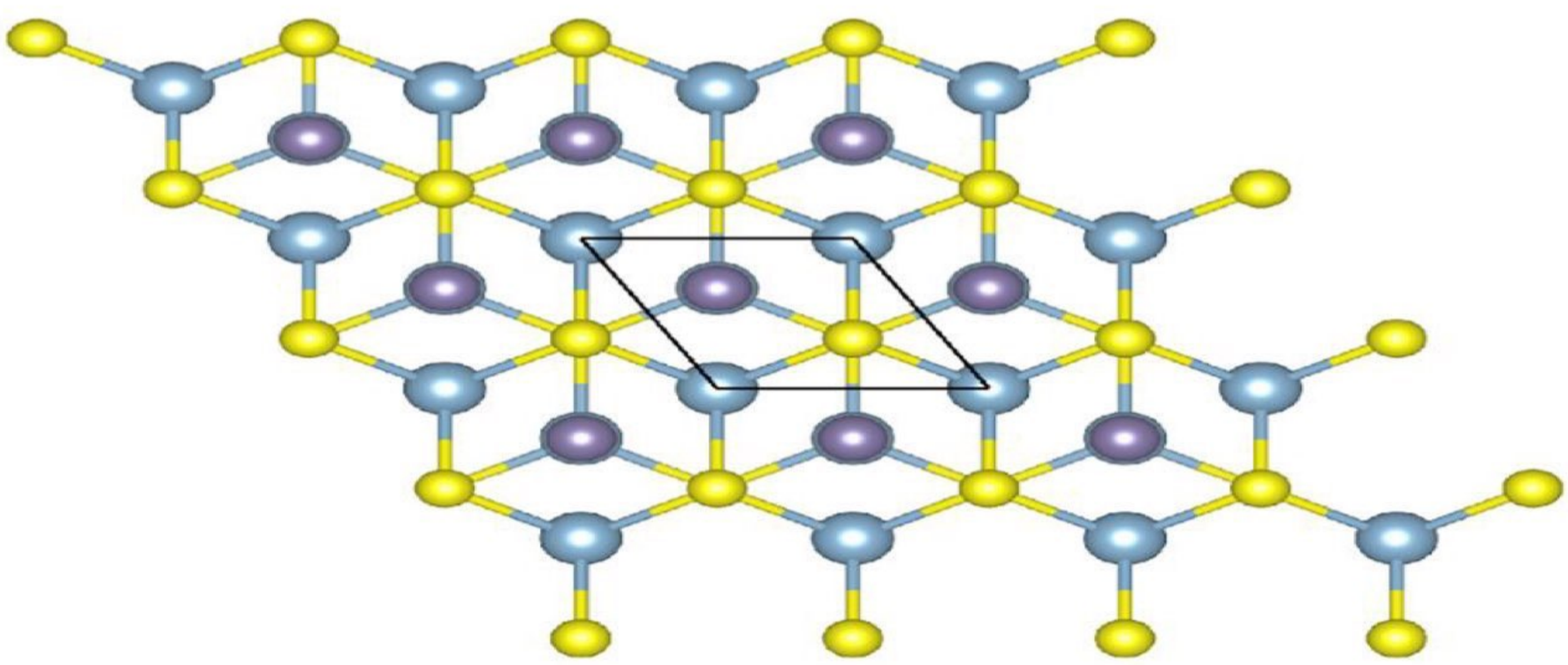
CHAPTER 4

RESULTS AND DISCUSSION

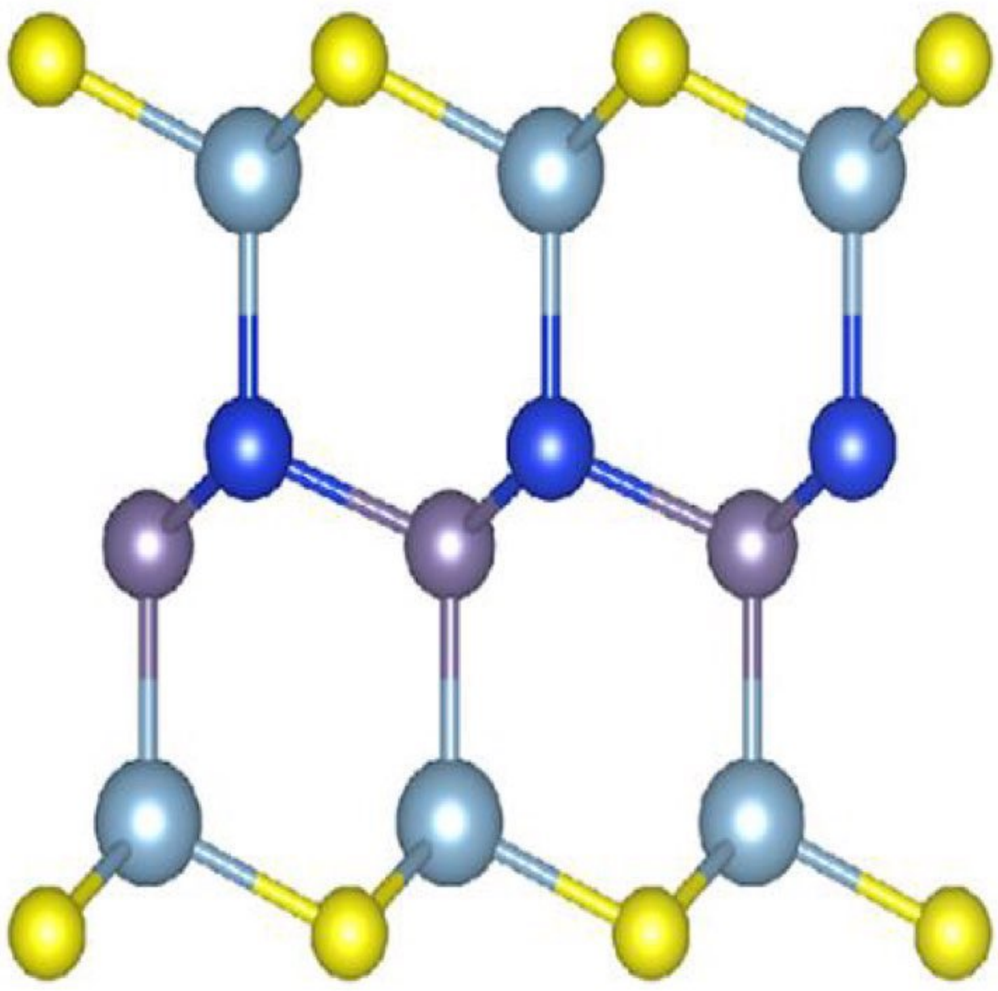
4.1 View of Our Structure (Al2S2SiGe)



Top View:



Side View:



4.2 Dynamic Stability of the Structure

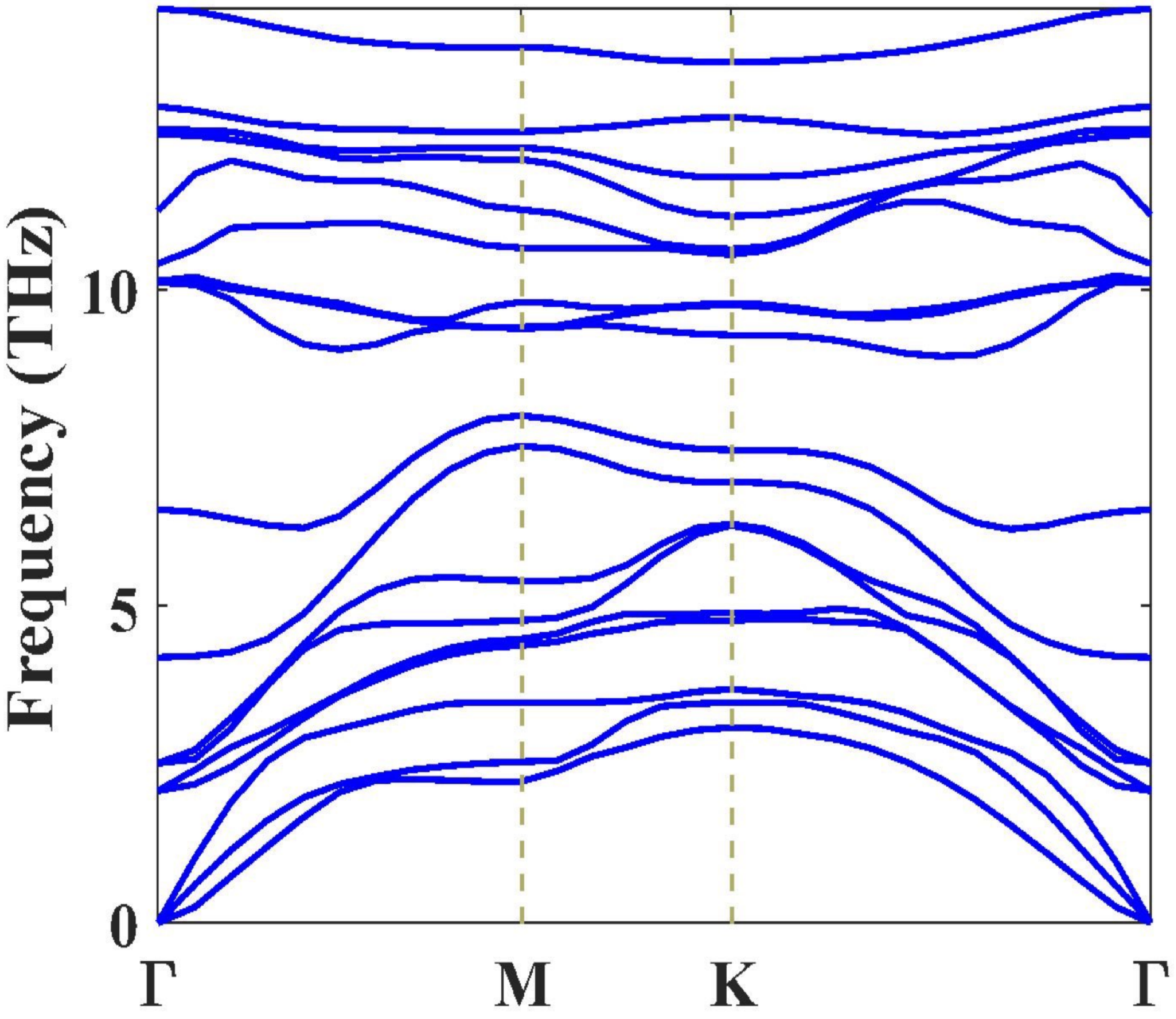
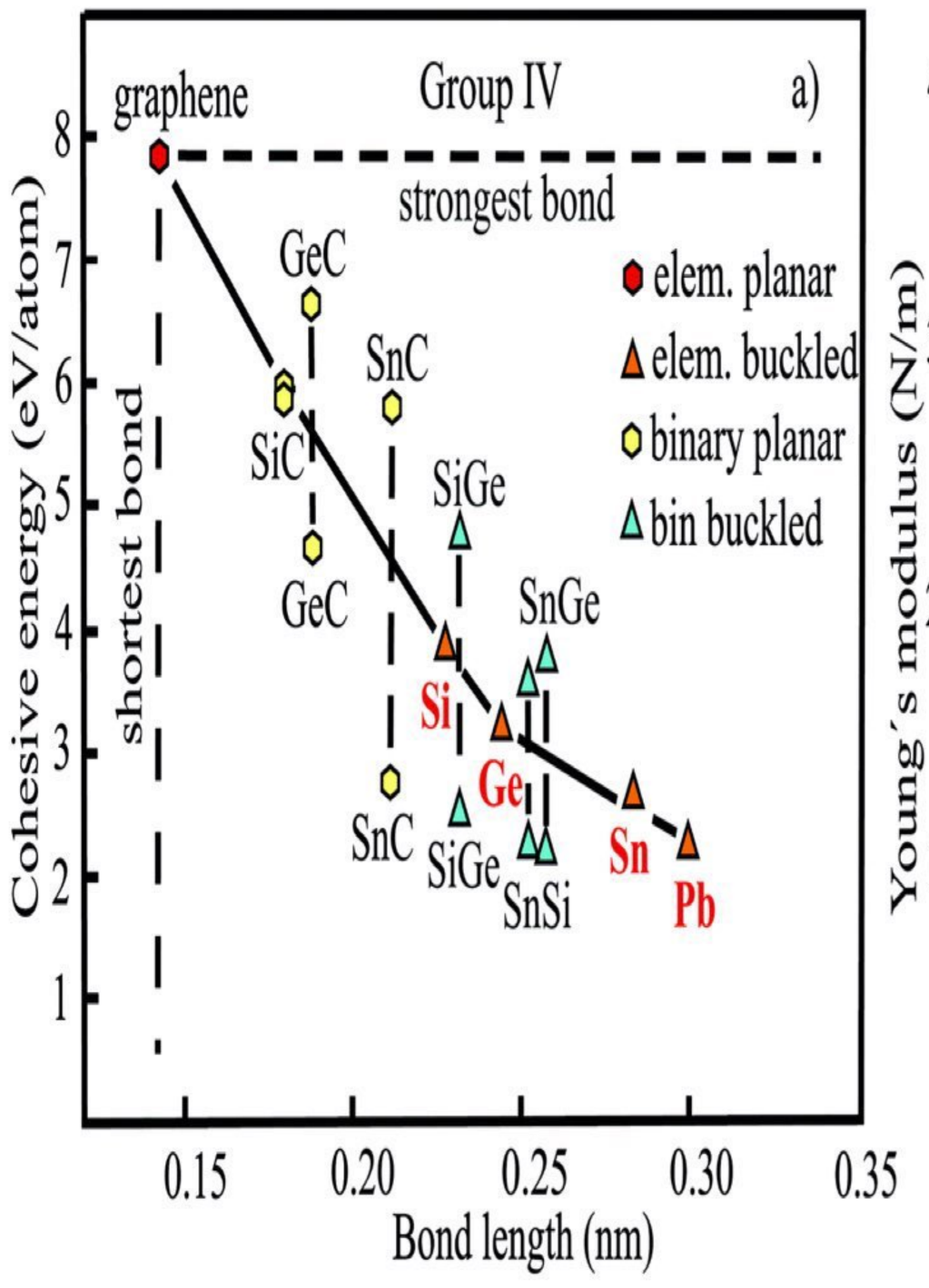


Figure: Phonon Band Structure

Fundamental principles The planar honeycomb phase of indiene, which acts like a metal, and the buckled graphene-like allotrope, an indirect semiconductor that changes to a metal under compressive and tensile strain, are the two dynamically stable phases of the material, according to DFT-PBE simulations. The cohesive energy governs the mechanical stability of the entire network and specifies how an atom interacts with the atoms in its 2D environment. The greatest bond length, which denotes the bond with the lowest critical fracture strength, is typically used in the case of corrugated monolayers, and for the significant differences of some puckered phases, the mean value is used. Included for comparison is graphene, which possesses the longest bond and highest cohesive energy of any uniform single-atomsheet.



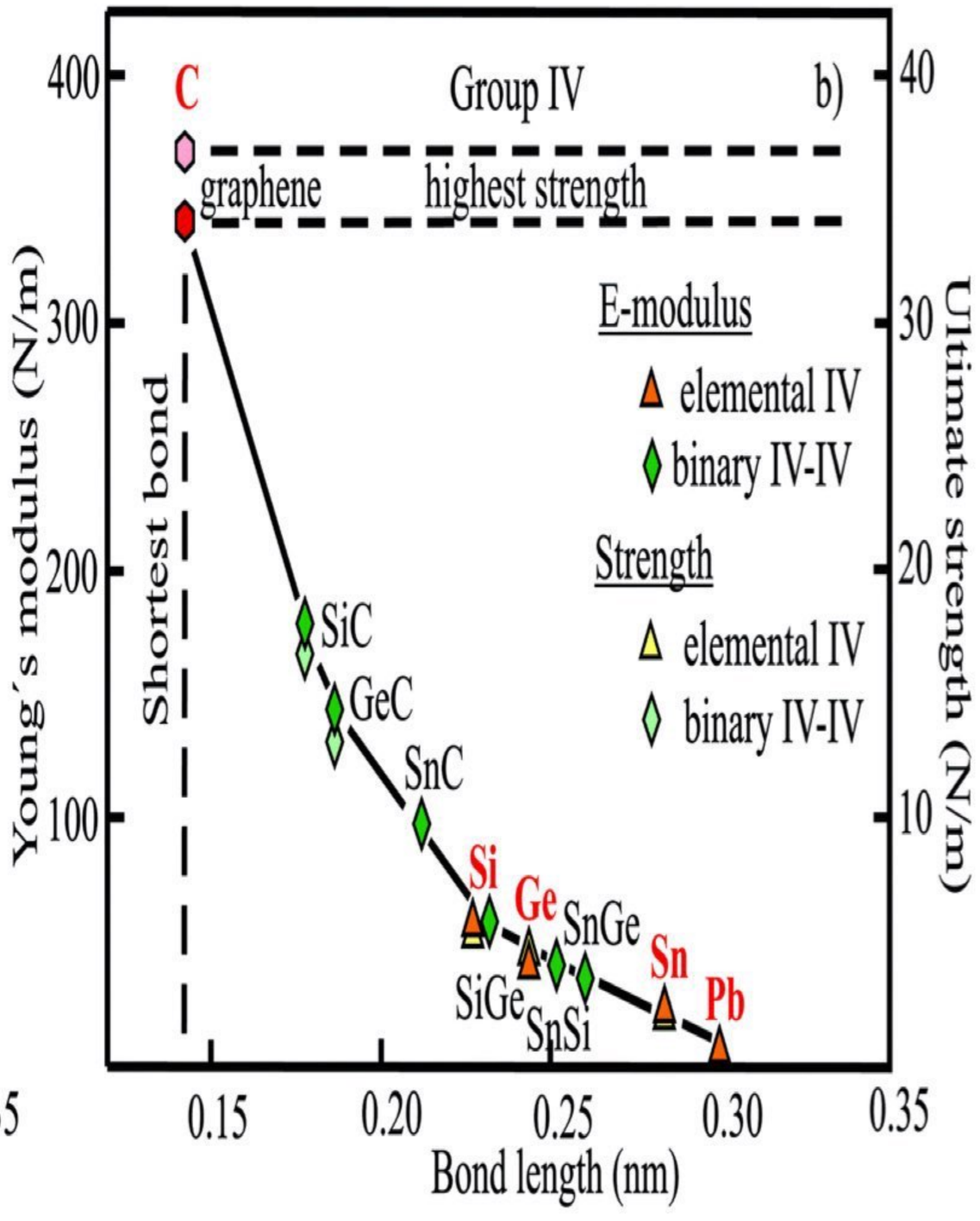


Fig: (a) Plot of cohesive energy versus bond length of elemental and binary group IV monolayers in comparison to graphene.
(b) Young's modulus and ultimate strength of elemental and binary group IV monolayers versus bond length in comparison to graphene.

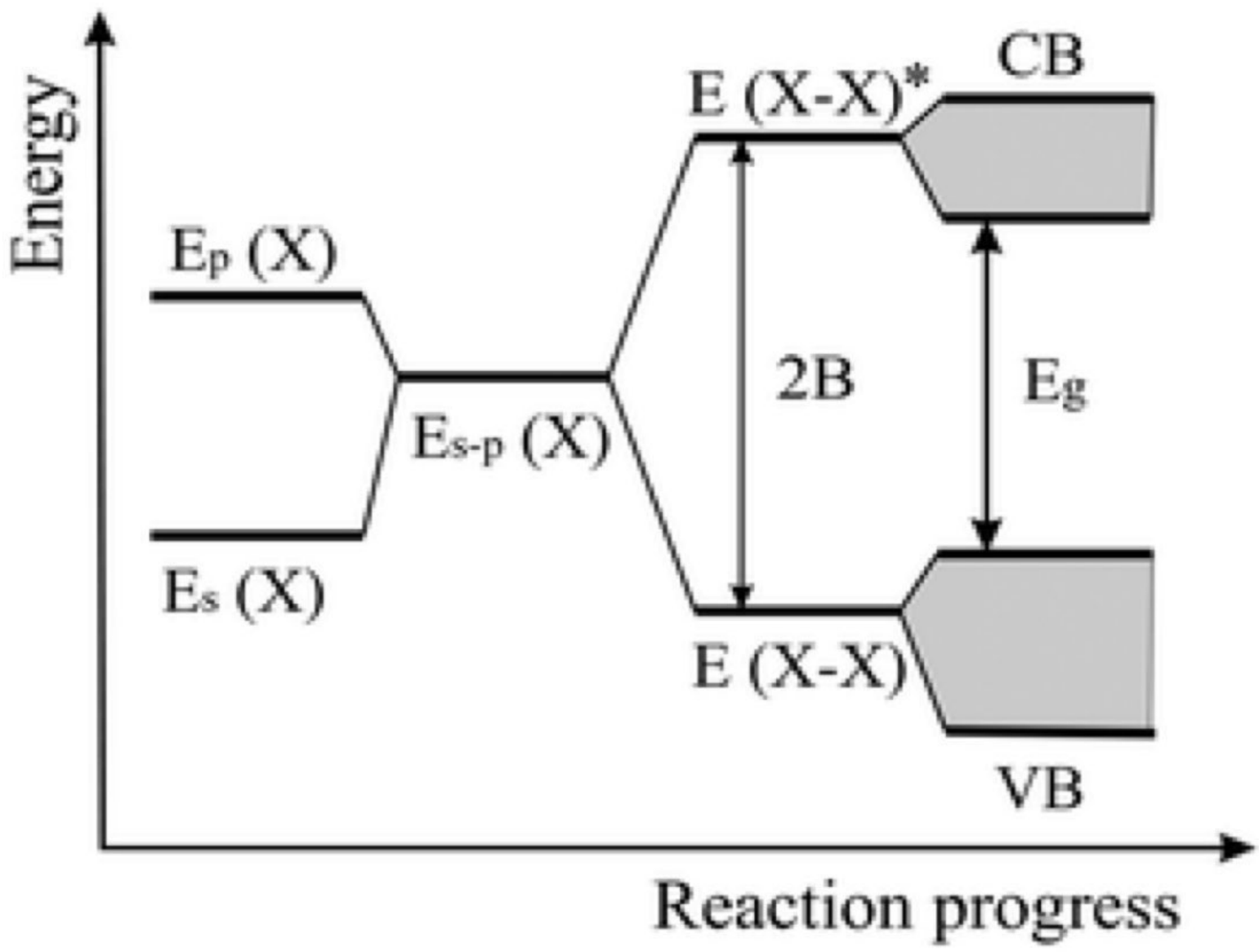


Fig: Energy levels of hybridized s and p orbitals, reacting to molecular bonding and antibonding levels with level broadening and band formation of a monolayer.

4.3 Band Structure of Al2S2SiGe

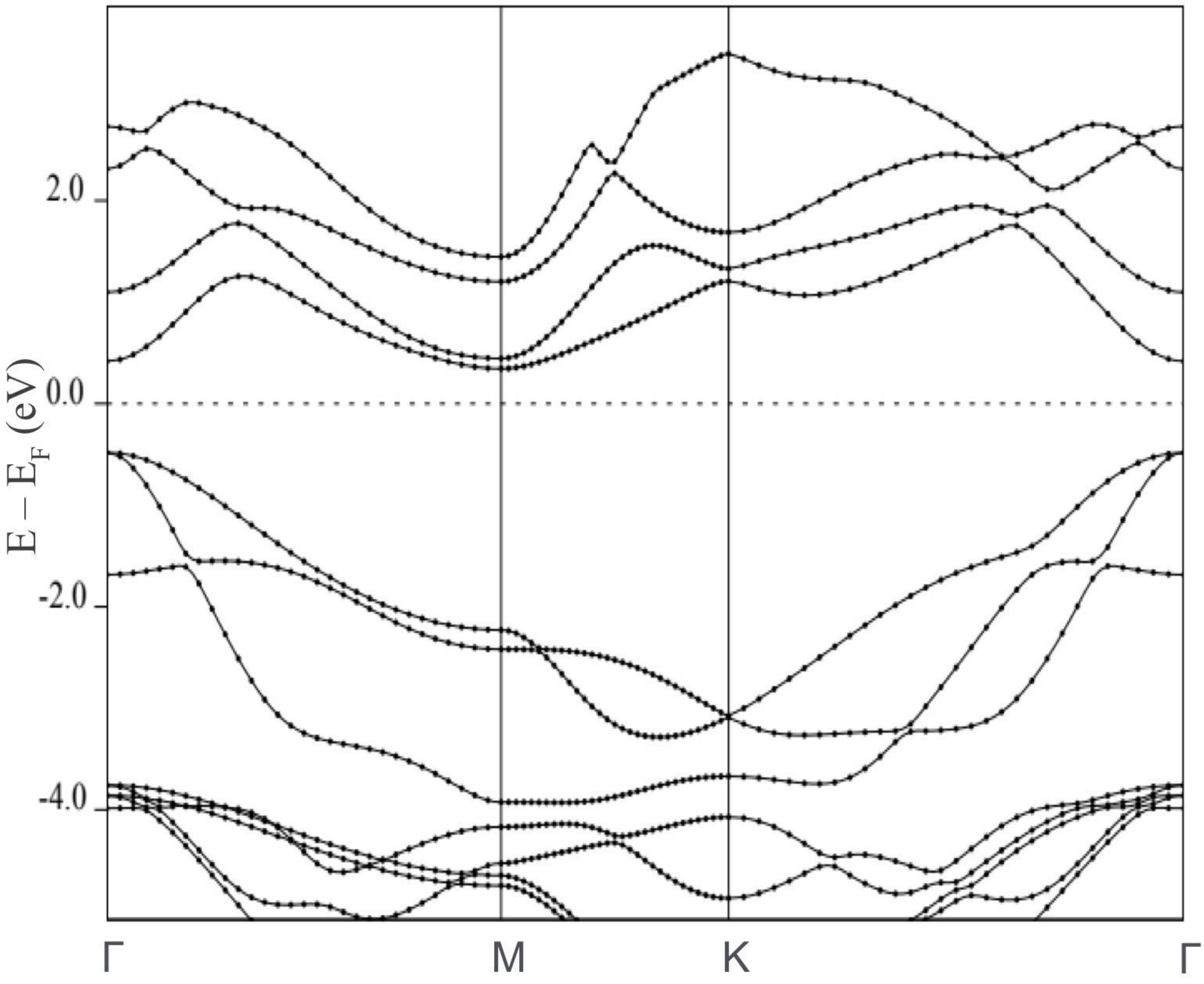


Fig: Band structure of our material

It is for the explanation of the electrical properties of a material. Bloch's theorem introduces a wavevector **k** .

• It can always be confined to the 1st BZ (any **k** outside the 1st BZ can be mapped back into it).

• The band index appears in Bloch's theorem for each **k** there are many solutions.

$$H\Psi n.k = En,k\Psi n,k$$

This leads to a description of the energy levels of electrons in a periodic potential in terms of a family of continuous functions E n,k. This is the *band structure* of the solid.

In Castep we use an accurate plane wave basis set. Castep Input Files:
Can control k-points used in band structures by several cell keywords

- *bs_kpoints_list*
- *bs_kpoints_path*
- *bs_kpoints_mp_grid*

Controlled by param keyword task
- task : BandStructure

For Silicon band structure:

```
%block lattice_cart
2.7 2.7 0.0
2.7 0.0 2.7
0.0 2.7 2.7
%endblock lattice_cart
%block positions_frac
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
%endblock positions_frac
%block bs_kpoints_path
```

0.0 0.0 0.0
0.5 0.0 0.5
0.5 0.5 0.5
0.0 0.0 0.0
%endblock bs_kpoints_path
Symmetry_generate

The k values corresponding to high symmetry points (such as Γ, X, U, L) which we need to label in our band diagram, can be found in the post-processing output file (si_bands_pp.out).

Bandgap value can be determined from the highest occupied, lowest unoccupied level values printed in scf calculation output.

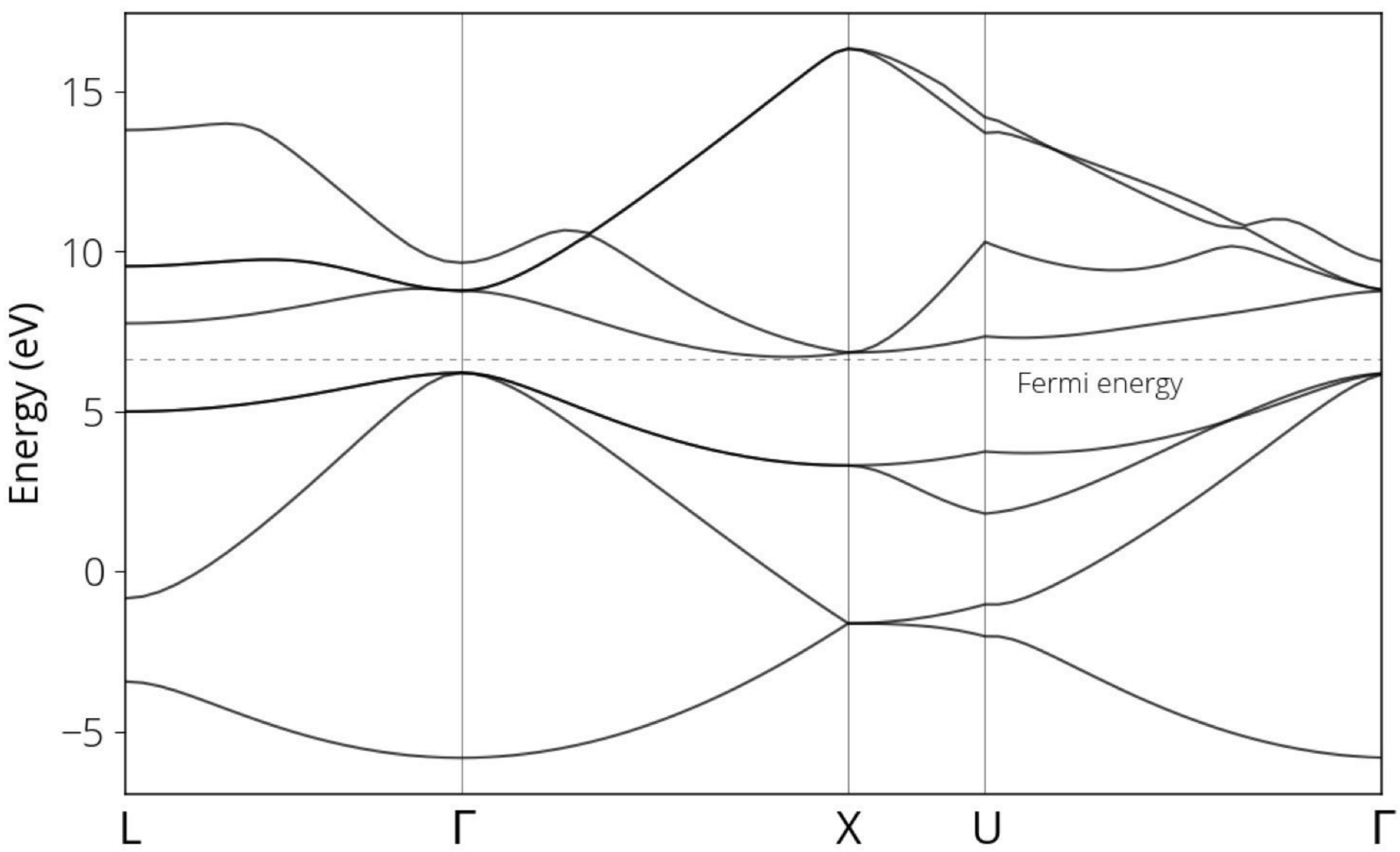


Fig: Band structure of Silicon

4.4 Density of States of Al2S2SiGe

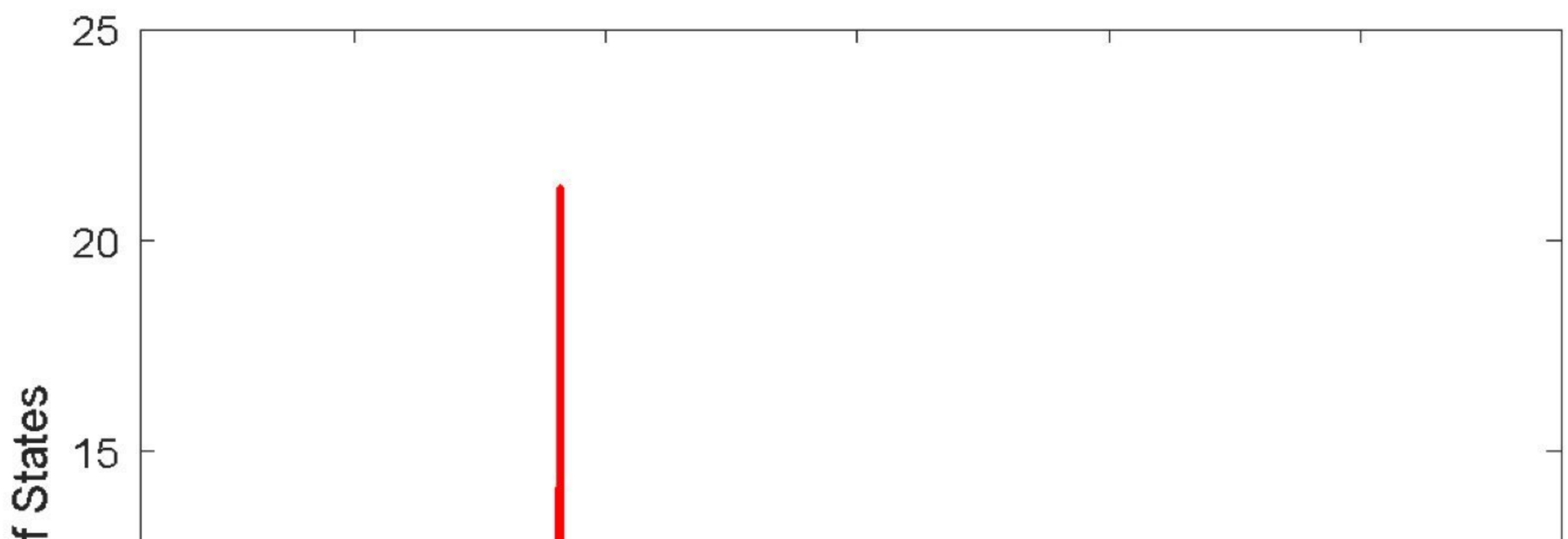


Fig: DOS of our novel jonus material.

It is calculated for lattice vibrational mode. The difference in energy between the highest occupied and the lowest unoccupied band is the material's band – gap. This is an important properties for a range of spectroscopies as well as electronic transport. Here we noticed the system has a region around the Fermi energy with no states. So, there is a bang –gap. Possibly the material is a semi-conductor (modest band-gap) or insulator (large band-gap).

Here the energy scale has been shifted so that the Fermi energy lies at zero. It is clear that there are a large number of states near Fermi energy. We compute using DFT in the CASTEP program.

REFERENCES

1. Stability and electronic structure of 2D allotropes of group-IV materials (physical review) 29 July 2018
2. Graphene-based 2D Janus materials (NPG Asia Materials) October 2018
3. Recent progress in solution assembly of 2D materials for wearable energy storage applications (Journal of energy chemistry) 1 March 2021
4. Structure and Properties of the compounds LnAl2x2 (Ln=Eo, Yb, x=Si, Ge) (Elsevier solid state sciences) 23 February 2000
5. A 2DSiGeO monolayer with high electron mobility and negative poisson's ratio (Journal of physics)1 January 2004
6. Crystal chemistry and thermoelectric transport of layered AM2X2 compunds (The Royal society of chemistry) 9 April 2018
7. A review on mechanics and mechanical properties of 2D materials-graphene and beyond. (Extreme Mechanics Letters) 20 January 2017
8. Progress, Challenges and Opportunities for 2D material based photodetectors (advanced functional materials) 2018
9. A perspective on the application of specially resolved ARPES for 2D materials (MDPI/journal/nanomaterials) 27 April 2018
10. Solid-State energy storage devices based on two-dimensional Nano-materials (Energy storage materials) 25 November 2018
11. Recent progress on two=-dimensional Nano flake ensembles for energy storage application (Nano-Micro lett) 20 august 2018
12. 2D materials chemistry (chemical reviews) 11 July 2018
13. Bonding, structure, and mechanical stability of 2D materials: the predictive power of the periodic table. Institute of Physical Chemistry, INF 253, University of Heidelberg, 69120 Heidelberg, Germany.