

**Structural, Electronic, Magnetic, Mechanical and Optical Properties of
RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) Half-Heusler Compounds for
Possible Spintronics and Optoelectronics Applications: First-Principles
Calculations**



Adem Beriso Bejo

**A Dissertation Submitted to the Department of Applied Physics
College of Applied Natural Sciences**

**Presented in a Partial Fulfillment of the Requirements for the Degree of
Doctor of Philosophy in Applied Physics (Specialization in Material
Physics)**

**Office of Graduate Studies
Adama Science and Technology University**

**June, 2025
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Declaration

I declare that this dissertation entitled “**Structural, Electronic, Magnetic, Mechanical and Optical Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) Half-Heusler Compounds for Possible Spintronics and Optoelectronics Applications: First-Principles Calculations**” is my own work and has not been submitted to any university for a similar purpose. The references used in this dissertation are duly recognized by proper citations.

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Approval of Board of Examiners

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DEDICATION

I dedicate this dissertation to the loving memory of my dear mother, Tayibe Bedane, father, Beriso Bejo and senior brother, Aman Bunta, who left this world before witnessing the completion of this work. Their unwavering love, sacrifices and prayers have been the foundation of my journey. Though they are no longer with me, their guidance and values continue to inspire and strengthen me every day.

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Contents

Contents	vii
List of Figures	viii
List of Tables	viii
Acronyms and Abbreviations	viii
Abstract	viii
1 Introduction	1
1.1 Background of the Study	1
1.2 Statement of the problem	4
1.3 Research Questions	5
1.4 Objectives	6
1.4.1 General Objective	6
1.4.2 Specific Objectives	6
1.5 Significance of the study	6
1.6 Scope of the study	7
1.7 Organization of the Dissertation	7
2 Literature Review	9
2.1 Introduction to Half-Heusler (HH) Compounds	9
2.2 Properties of Half-Heusler compounds	10
2.2.1 Structural Properties	11
2.2.2 Mechanical properties	14
2.2.3 Electronic properties	17
2.2.4 Optical properties	18
2.2.5 Magnetic properties	22
2.3 Applications of HH Compounds	25
2.3.1 Optoelectronic applications	25
2.3.2 Spintronic applications	27
2.4 Density Functional Theory (DFT)	30
2.4.1 The Hohenberg-kohn Theorems	31
2.4.2 The Kohn-Sham Assumptions	32
2.4.3 The Exchange-Correlation Function	35
2.4.4 An Instrument for DFT Calculations: Quantum ESPRESSO (QE) . . .	38
2.4.5 Periodic Boundary Conditions	39

3	Materials and Methods	41
4	Results and Discussion	45
4.1	Structural Properties of RhYZ (Y =Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Compounds	45
4.1.1	Lattice Parameters and Structural stability	46
4.1.2	Formation Energy and Thermodynamic stability	47
4.1.3	Phonon Dispersion and Dynamical Stability	51
4.2	Mechanical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Com- pounds	56
4.2.1	Elastic Properties	56
4.2.2	Debye Temperature and Sound Velocity	58
4.3	Electronic Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds	60
4.3.1	Band Structure and density of states of RhZrZ (Z = Li, As Si, Sb) HH compounds	60
4.3.2	Band Structure and density of states of RhNbZ (Z= Li. As, Si, Sb) HH compounds	67
4.3.3	Band Structure and density of states of RhIrZ (Z = Li, As, Si, Sb) HH compounds	74
4.4	Optical Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds	81
4.4.1	Optical Properties Analysis of RhZrZ (Z = As, Li, Si, Sb) HH Compounds	82
4.4.2	Optical Properties Analysis of RhNbZ (Z = As, Li, Si, Sb) HH Compounds	88
4.4.3	Optical Properties Analysis of RhIrZ (Z = As, Li, Si, Sb) HH Compounds	95
4.5	Magnetic Properties of RhYZ (Y =Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Compounds	99
5	Conclusions and Recommendations	103
5.1	Conclusions	103
5.2	Recommendations	104
	List of Publications	106
	References	108

Acronyms and Abbreviations

BFGS	Broyden-Fletcher-Goldfarb-Shanno
CBM	Conduction Band Minimum
CIF	Crystallographic Information File
CP	Cauchy's Pressure
DFT	Density Functional Theory
DFPT	Density Functional Perturbation Theory
E_F	Fermi Energy
FCC	Face-Centered Cubic
GGA	Generalized Gradient Approximation
HEG	Homogeneous Electron Gas
HH	Half-Heusler
HPC	High-Performance Computing
LDA	Local Density Approximation
LEDs	Light-Emitting Diodes
MRAM	Magnetoresistive Random Access Memory
MTJs	Magnetic Tunnel Junctions
NIR	Near-Infrared
PAW	Projector Augmented Wave
PBE	Perdew-Burke-Ernzerhof
PDOS	Partial Density of States
PV	Photovoltaic
QE	Quantum ESPRESSO
SCF	Self-Consistent Field
SHE	Spin Hall Effect
SIT	Spin Injection and Transport
SOC	Spin-Orbit Coupling
SP	Slater-Pauling
SPT	Spin-Polarized Tunneling
STT	Spin-Transfer Torque
SpinFETs	Spin Field-Effect Transistors
TDOS	Total Density of States
XC	Xchange-Correlation
U	Hubbard Potential
VASP	Vienna Ab initio Simulation Package
USPP	Ultrasoft Pseudopotential

UV	Ultraviolet
VBM	Valence Band Maximum
VEC	Valence Electron Count

Abstract

Half-Heusler (HH) compounds have attracted considerable interest for various advanced technological applications owing to their adjustable properties. The ability to fine-tune their properties through compositional variation makes them ideal candidates for use in spintronic and optoelectronic devices. The aim of this work was to investigate the structural, mechanical, electronic, optical and magnetic properties of $RhYZ$ ($Y = Zr, Ir, Nb$; $Z = Li, As, Si, Sb$) HH compounds by using first-principles calculations based on density functional theory (DFT) as implemented in the QUANTUM ESPRESSO (QE) package. For electronic and magnetic properties, both the Generalized Gradient Approximation (GGA) and GGA+U (U is the Hubbard potential) were employed. Structurally, most compounds are stable in type I atomic configuration, except $RhIrZ$ ($Z = As, Si, Sb$), which prefer type II. Negative formation energies in their stable configurations indicate thermodynamic stability for most compounds, while $RhIrLi$ shows positive formation energy, suggesting thermodynamic instability. Phonon dispersion calculations confirm dynamical stability for all compounds through the presence of positive phonon frequencies across the Brillouin zone. Mechanical stability is also confirmed by satisfying Born and Huang stability criteria. Electronic property analysis shows that $RhZrZ$ ($Z = As, Sb$) and $RhNbSi$ are semiconductors, making them promising for optoelectronic applications. $RhNbZ$ ($Z = As, Sb$) compounds are half-metallic, indicating potential for spintronic devices. All other HH compounds remain metallic under both methods. Partial density of states (PDOS) reveals that transition metal atoms (Rh, Zr, Nb, Ir) dominate the electronic states, while contributions from Li, As, Si, and Sb are less significant. The semiconductor compounds exhibit favorable optical properties, including high real dielectric constant (ϵ_1), strong absorption coefficient (α) and low energy loss (L) in the low photon energy range, further supporting their suitability for optoelectronic devices. Half-metallic compounds also show promising optical features for spin-light interaction applications. In contrast, metallic HH compounds show negative ϵ_1 in the low energy range, making them less ideal for traditional optoelectronics but potentially suitable for plasmonic applications. Magnetic analysis under GGA shows most compounds are non-magnetic, except $RhNbSb$ and $RhIrZ$ ($Z = As, Si, Sb$). The inclusion of U enhances magnetic response in several systems, particularly $RhNbZ$ ($Z = Li, As$) and $RhIr$ -based compounds. Comparison with the Slater-Pauling (SP) rule reveals agreement in half-metallic systems, while deviations appear in others.

Keywords: *HH compounds, first-principles calculations, DFT, electronic properties, optical properties, magnetic properties, spintronics, optoelectronics, plasmonics, GGA+U, formation energy*

Introduction

1.1 Background of the Study

The discovery of Heusler compounds dates back to the early 20th century when Fritz Heusler, in 1903, observed that Cu_2MnAl exhibited ferromagnetic behavior despite none of its constituent elements being intrinsically ferromagnetic (Graf et al., 2011; Tavares et al., 2023). This pioneering finding transformed the understanding of magnetic materials (Hayashi et al., 2020) and led to the identification of a large family of compounds, known as Heusler compounds that display diverse electronic, magnetic, optical, thermal and mechanical properties (Felser and Parkin, 2022; Zahir et al., 2022). Continued research uncovered compounds like TiNiSn , a semiconductor composed of metallic elements, reflecting the unconventional nature of this class (Berry et al., 2017). Over time, scientists developed a structural classification for Heusler compounds (Wu et al., 2019). Full-Heusler compounds (X_2YZ) possess ordered structures and often exhibit strong magnetic and electronic properties (Jin and Jung, 2022). HH compounds (XYZ) show semiconducting, metallic or half-metallic behavior due to their partially filled atomic sites (Kawasaki et al., 2022). Inverse-Heusler compounds (X_2YZ), with swapped X and Y atom positions, exhibit modified magnetic and electronic properties (Aryal et al., 2020). Quaternary-Heusler compounds ($\text{XX}'\text{YZ}$) introduce further tunability via an additional compositional degree of freedom (Gencer et al., 2021). This structural and electronic flexibility makes Heusler compounds promising candidates for next-generation materials. As a result, they remain a focus of intense research, with experimental and theoretical efforts aiming to explore their potential in magnetic storage, spintronic devices, topological insulators and high-efficiency energy conversion systems (Patel et al., 2020; Wederni et al., 2024).

Intermetallic compounds, especially HH types, are increasingly important for next-generation technologies due to their structural and electronic versatility (Feng et al., 2014; Kervan and Kervan, 2017). They adopt a face-centered cubic (FCC) structure with one vacant atomic site, allowing chemical flexibility and precise tuning of mechanical, optical, magnetic and electronic properties (Özdemir et al., 2022; Jafari et al., 2022). Their ability to exhibit metallic, semiconducting or half-metallic behavior is governed by atomic radii, electronegativity, hybridization and spin-orbit coupling (SOC) which makes them ideal for applications in spintronics and optoelectronics (Sun et al., 2020; He et al., 2022). Alongside electronic and magnetic tunability, HH compounds offer mechanical stability and adaptable band topologies. Their spin-polarized states enable spintronic and quantum computing applications (Chen et al., 2020). Additionally,

their tunable optical behavior supports use in infrared detectors, LEDs, and solar cells (Ciftci and Evecen, 2018; Abubakr et al., 2021).

Advancements in computational and experimental techniques in the late 20th and early 21st centuries have significantly deepened our understanding of the electronic, structural, magnetic, optical, thermal and mechanical behavior of HH materials (Gzyl et al., 2020). Tools like DFT, Boltzmann transport theory and machine-learning-based materials design have accelerated the discovery of high-performance HH compounds (Filanovich et al., 2023), while experimental methods such as synchrotron spectroscopy and electron microscopy have revealed critical insights into their structural and interfacial properties (Zhang et al., 2024). Owing to their tunability and multifunctionality, HH compounds are often termed “designer materials” (Mohamed et al., 2020), with promising applications in spintronic memory, quantum computing and green energy technologies like solar cells (Levin et al., 2017). With continued progress in modeling, synthesis and fabrication, HH materials are set to play a transformative role in future high-performance and sustainable technologies (Patel et al., 2022).

Materials with half-metallic or semiconducting behavior are crucial for spintronic and optoelectronic applications due to their distinct electronic and transport properties (Galanakis, 2023; Lim et al., 2021). Half-metals conduct electrons of one spin while blocking the other, yielding 100% spin polarization which makes them ideal for spintronic devices like magnetic tunnel junctions (MTJs) and spin filters (Faleev et al., 2023; Baral and Chakrabarti, 2019). Though perfect polarization can be affected by disorder and thermal effects (Hoang et al., 2022), research continues to enhance their stability (Ding et al., 2022). Semiconductors, with adjustable conductivity and defined band gaps, underpin modern electronics and optoelectronics (Khandy and Chai, 2021). Their tunable properties make them essential for transistors, LEDs and solar cells, where optimized band structures improve carrier mobility (Azouaoui et al., 2023; Feng et al., 2020; Jia et al., 2020). Given their structural and electronic flexibility, HH compounds are capable of showing semiconducting, half-metallic or metallic behavior which make strong candidates for multifunctional, next-generation devices (Parvin et al., 2021).

The electronic band structure of HH compounds is central to their electronic and magnetic behavior (Anissa et al., 2022). Their band gaps can be tuned via doping, strain or elemental substitution, enabling transitions among semiconducting, metallic and half-metallic states (Huang et al., 2020). Half-metallicity, offering 100% spin polarization at the Fermi level (E_F), which is ideal for spintronic devices like MTJs, spin valves and filters. Though full polarization is yet to be experimentally confirmed, high spin polarization is still observed (Guo et al., 2022). This arises from their unique spin-dependent band structure, with one spin channel metallic and the other semiconducting (Candan and Kushwaha, 2021), supporting low-power and high-speed

spintronic technologies (Husain et al., 2023). In HH compounds, the interplay between the DOS near the E_F and magnetic moments is crucial (Ti et al., 2022). In RhYZ systems, combinations of Li, As, Sb, Si with Zr, Ir, and Nb introduce diverse electronic configurations and magnetic interactions, allowing systematic exploration of spin polarization, magnetic ordering and Curie temperature, key for spintronic applications.

Materials with strong optical properties, such as high absorption coefficients, tunable band gaps and powerful photoluminescence are vital to optoelectronics, which bridges light and electronic devices (Djelti et al., 2020). Many HH compounds are suitable for photodetectors, LEDs and solar cells due to their semiconducting nature with direct or indirect band gaps in the visible to infrared range (AlShaikh Mohammad et al., 2024). A key advantage is their tunable optical behavior, achieved by modifying elements at the Y and Z sites to shift the band gap (Mesbah et al., 2021). Their typically low defect densities and high carrier mobility further enhance performance in optoelectronic applications. First-principles simulations aid in designing HH compounds with targeted optical functions (Essaoud et al., 2023). For RhYZ systems, varying Y and Z elements helps explore trends in optical absorption, reflectivity and refractive index, offering valuable insights for device development.

Mechanical properties such as hardness and elastic constants are critical for integrating HH compounds into practical devices (Rasul et al., 2024). Their intrinsic strength and resistance to deformation stem from the $F\bar{4}3m$ cubic symmetry, making them suitable for demanding environments like high-temperature spintronic and optoelectronic systems (El-Khouly et al., 2021). Their ability to endure lattice strain ensures structural integrity under varying conditions (Wafula, 2023). First-principles calculations enable detailed analysis of mechanical parameters like elastic moduli and Poisson's ratio (Dey et al., 2021).

Extensive theoretical and experimental studies have explored Rh-based HH compounds. For instance, DFT analysis of RhVZ ($Z = P, As, Sb$) revealed half-metallicity and low-energy optical activity, making them promising for spintronic and optoelectronic applications (Ahmad and Mehmood, 2018). Benzoudji and his co-workers reported that MRhSb ($M = Ti, Zr, Hf$) HH compounds were mechanically stable, ductile and semiconducting, suitable for optoelectronics (Benzoudji et al., 2019). Jaishi with his colleagues used DFT and Boltzmann transport theory on RhTiZ ($Z = P, As, Sb, Bi$), identifying indirect band gaps with strong UV-visible absorption (Jaishi et al., 2021). Meenakshi with his Collaborators found half-metallicity in RhFeSn and RhFeGe, indicating their potential in spintronic devices (Meenakshi et al., 2021).

Despite progress in understanding HH compounds, several RhYZ combinations remain unexplored. While some properties of RhZrSb (Benzoudji et al., 2019), RhZrAs (Manzoor et al., 2024) and RhNbSi (Ahmed et al., 2024) have been studied, other RhYZ compounds under cur-

rent work lack theoretical and experimental investigation. This gap is surprising given their potential for unique structural, electronic, magnetic, optical and mechanical behaviors. Rh and Y atoms are known to enable semiconducting, half-metallic or metallic properties, key for spintronic, optoelectronic and other applications, while the Z atom often stabilizes the structure. This work aimed to contribute to addressing that gap by using first-principles DFT calculations to investigate RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds. QE, known for its accuracy and efficiency in simulating material properties, was employed to investigate their structural, mechanical, electronic, magnetic and optical properties, highlighting their potential in advanced technologies.

1.2 Statement of the problem

The development of advanced functional materials remains a key objective in modern materials science, particularly for applications in spintronics and optoelectronics (Chiker et al., 2022). Among the most promising material classes are HH compounds, which offer a simple ternary crystal structure, high thermal and mechanical stability and remarkable tunability of structural, electronic, magnetic and optical properties (Benyoussef et al., 2024). These compounds, generally formulated as XYZ, typically adopt a cubic $C1_b$ structure and have demonstrated a wide range of phenomena including semiconducting, half-metallic, metallic, semi-metallic and topological insulators. The ability to engineer such properties by tailoring elemental composition makes HH compounds especially attractive for next-generation technologies requiring both spin-polarization and electronic band control (Guillemard et al., 2020; Quinn and Bos, 2021).

Within this class, Rhodium-based HH compounds, in particular RhYZ (Y = Zr, Ir, Nb; Z = Li, Si, As, Sb), are of special interest due to the unique role of Rhodium (Rh). As a 4d transition metal, Rh contributes strong d–d orbital hybridization and significant SOC, which can induce complex and useful physical properties. These include narrow or tunable band gaps, magnetic ordering and potentially topologically non-trivial states. Additionally, the diversity of Y and Z elements in the RhYZ system provides further degrees of freedom to modulate key properties relevant to spintronic devices (such as half-metallicity and spin polarization) and optoelectronic systems (such as optical absorption and electronic transition energies).

Despite their potential, Rh-based HH compounds remain significantly under-investigated. Compared to the extensively studied Co-, Fe-, and Ni-based HH counterparts (Samanta et al., 2020), RhYZ compounds have received relatively little attention. A review of existing literature indicates that only a few members, such as RhZrAs, RhZrSb, and RhNbSi (Gurunani and Gupta, 2024a; Manzoor et al., 2024), have been partially explored, primarily in the context of structural and thermoelectric properties, while lacking in-depth analysis of their electronic, magnetic or

optical behavior. More critically, several other compositions within this family have not been studied at all, either theoretically or experimentally. This uneven coverage has resulted in a fragmented understanding of the property trends across the RhYZ series and has left substantial gaps in knowledge regarding their potential functionalities.

Addressing these gaps is crucial for advancing the design of new materials for emerging technologies. A systematic and comprehensive investigation of RhYZ compounds using first-principles calculations can uncover structure and property relationships, clarify stability conditions and predict key mechanical, electronic, optical and magnetic behaviors. By identifying which compositions exhibit semiconducting, half-metallic or metallic properties along with suitable mechanical and optical properties, this research can significantly contribute to the discovery and rational design of materials tailored for spintronic and optoelectronic applications. Ultimately, filling these knowledge gaps will not only expand the scientific understanding of Rh-based HH systems but also contribute the broader goal of developing efficient, multifunctional materials for advanced technological applications.

1.3 Research Questions

This study seeks to answer the following research questions based on first-principles calculations:

- What are the equilibrium lattice parameters, formation energies, and structural stabilities of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds?
- What are the electronic band structures and density of states of RhYZ compounds, and do they exhibit semiconducting, metallic, or half-metallic behavior?
- How do the magnetic moments and spin-resolved electronic structures of RhYZ compounds correlate with their potential for spintronic applications?
- What are the elastic constants and mechanical parameters (e.g., bulk modulus, shear modulus, Poisson's ratio), and what do they reveal about the mechanical stability and ductility of the studied compounds?
- How do the optical properties (e.g., dielectric function, reflectivity, and absorption coefficient) of RhYZ compounds vary, and which are suitable for optoelectronic applications?
- Which RhYZ compositions offer a desirable combination of electronic, magnetic, and optical properties for potential multifunctional applications?

1.4 Objectives

1.4.1 General Objective

- This research aims to investigate the structural, electronic, magnetic, mechanical and optical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds using first-principles DFT calculations to assess their potential for optoelectronic and spintronic applications.

1.4.2 Specific Objectives

The purpose of this research is to achieve the following specific objectives:

- to determine structural properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds.
- to calculate electronic properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds.
- to analyze magnetic properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds.
- to calculate mechanical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds.
- to examine optical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) half-Heusler compounds.
- to compare the obtained results with the desired properties of materials intended for spintronic and optoelectronic applications.

1.5 Significance of the study

Investigating properties of Heusler compounds is the first step to avail them for practical applications. RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) HH compounds are of interesting because of their potential uses in optoelectronics and spintronics. This research contributes to the development of materials for next-generation technologies by offering a thorough understanding of their structural, electronic, magnetic, mechanical and optical properties through the use of first-principles simulations. Some of these compounds' optical tendencies make them appropriate for cutting-edge optoelectronic applications like LEDs and photodetectors, while magnetic

qualities of others' offer promise for effective spintronic devices. Furthermore, these materials' mechanical stability guarantees their durability for useful gadget integration. This theoretical analysis not only advances our theoretical knowledge of Rh-based HH compounds but also provides information that could guide and assist future practical endeavors to synthesize and customize these materials for high-performance and environmentally friendly technology uses. In general, despite the fact that the lack of previous studies highlights the uniqueness and importance of our work, this work is the first theoretical investigation for most of these compounds and lays the groundwork for future experimental and theoretical research on these materials.

1.6 Scope of the study

This study is limited to the use of first-principles computations to thoroughly examine the structural, electronic, magnetic, mechanical and optical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) HH compounds. QE simulation code based on DFT were employed for the calculation. Its main objective is to assess these materials' stability and compatibility for possible employment in optoelectronics and spintronics. To comprehend their performance in cutting-edge technologies, the study examines their band gaps, optical responses, magnetic behaviors, elastic constants and crystalline structures. By investigating these characteristics, the study hopes to enable the experimental realization and incorporation of Rh-based HH compounds into future devices by offering a theoretical framework and predictive insights.

1.7 Organization of the Dissertation

This dissertation covers different properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) HH Compounds. As a result structural, mechanical, electronic, optical and magnetic properties of the compounds were thoroughly investigated for possible spintronics and optoelectronics applications. This dissertation is structured as follows: it starts with a general introduction, reviews relevant literature, materials and methods, presents the findings and ends with conclusions and recommendations. The introduction (Chapter 1) focuses on the background, rationale, research questions, objectives and it explains the general framework of the dissertation. Chapter 2 (literature review), emphasizes research strategy as well as the sequential and coherent description of the backgrounds of the subjects of this study. It also stresses the technological applications of materials under study, future prospects and research directions of these materials computationally. The methods employed in this study are briefly and exhaustively described in Chapter 3. In this sense, it describes the fundamentals of DFT in this research, as well as the exchange correlational functions that are employed, software, pseudopotentials and the theoretical physics that supports it. Chapter 4 discusses the results obtained using the DFT approach with different

functionals in QE. This presents the major effects of chemical substitution on structural, mechanical, electronic, optical and magnetic properties in RhYZ compounds. The conclusion and recommendations for further study are included in Chapter 5.

Literature Review

2.1 Introduction to Half-Heusler (HH) Compounds

HH compounds, a key subgroup within the Heusler family, have become a major focus in materials science due to their wide range of physical properties, including structural, mechanical, electronic, optical, magnetic and even topological properties (Hoat, 2019; Huang et al., 2016). These materials crystallize in a non-centrosymmetric cubic structure (space group $F\bar{4}3m$, space group number 216), which is a derivative of the full-Heusler structure. The general formula XYZ allows for significant chemical flexibility, enabling researchers to substitute different elements and thereby tune the material's properties. This adaptability has led to the discovery of HH compounds with behaviors ranging from semiconducting (Everhart and Newkirk, 2019), metallic (Wafula et al., 2022) and half-metallic (Wen et al., 2019) to superconducting (Chatterjee et al., 2021) and even topologically non-trivial states (Huang et al., 2016). As a result, they continue to attract interest for a variety of potential technological applications. Possible combination of elements in the formation of Heusler compounds including HH type is indicated in Figure 2.1.

HH compounds based on Rhodium (Rh) have attracted a lot of interest lately because of their exceptional structural, electronic, magnetic, mechanical, optical and thermal properties, which make them extremely promising for a range of technological and industrial uses. The electronic and magnetic behavior of these materials is largely determined by their crystallization in the $C1_b$ structure, a FCC lattice with one unoccupied sublattice site (Gurunani and Gupta, 2024a). They are appropriate for demanding industrial and aerospace applications because of the strong chemical link that exists between Rh and its constituent elements, which guarantees great structural stability even in the face of harsh environmental factors like high temperatures and mechanical stress (Wei et al., 2023). The strong chemical stability of Rh and its capacity to produce intermetallic compounds with a broad variety of transition metals (Y) and main group elements (Z) are two of the main benefits of Rh-based HH compounds (Dixit et al., 2024). As a result, materials with superior mechanical hardness, desired electronic, optical and magnetic properties can be created by fine-tuning electronic band structures, magnetic interactions and mechanical properties (Dubey et al., 2024). Depending on the atomic arrangement and valence electron count (VEC), Rh-containing HH compounds can exhibit either semiconducting, half-metallic or metallic behavior, providing substantial potential for application in optoelectronic and spintronic devices (Almaghbash et al., 2021).

Group→	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
↓Period																		
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

Figure 2.1: The periodic table of chemical elements. Different colors indicate the elements, appropriate combination of which can form a Heusler compound (Marchenkov et al., 2022).

2.2 Properties of Half-Heusler compounds

The exceptional crystal structure of HH compounds and the large number of constituent elements they can contain result in a wide range of properties (Joshi et al., 2019). Their usual crystal structure is the $C1_b$ structure, which is a defect-ordered form of the $L2_1$ structure that is present in full Heusler compounds and has an empty atomic site. In order to determine their other features, this structural feature is essential (Ciesielski et al., 2020a). HH compounds can be semiconducting, metallic, semi-metallic, half-metallic (with one spin orientation acting as a semiconductor and the other as a metal). For applications using spintrons, half-metallicity is especially appealing. In terms of mechanical strength, many HH compounds are very strong and can be fairly hard, which is crucial for real-world applications. Their optical properties can be adjusted by altering their composition, which makes them appropriate for a range of optoelectronic uses. Because of the way these properties interact, HH compounds provide a flexible framework for investigating basic physics and creating new technologies (Min et al., 2022). Magnetically, they can display a range of magnetic behaviors, ranging from ferromagnetism to ferrimagnetism. Although HH compounds are more widely recognized for their semiconducting and half-metallic ferromagnetic properties, they can also display ferrimagnetism and

antiferromagnetism. Atomic ordering, electron filling and elemental content all affect how HH compounds behave magnetically (Kamlesh et al., 2021b). In general, properties of HH compounds are influenced by various intrinsic and external factors. For example, elemental substitution, along with variations in size and electronegativity, can significantly impact their properties in various ways. Further more, the total number of VEC in HH compounds is a strong predictor of whether the material will be metallic, semiconducting, or half-metallic, but other factors like atomic ordering, crystal symmetry and electron correlations can also influence the electronic properties (Majumder et al., 2019).

2.2.1 Structural Properties

Since their discovery in 1903, Heusler compounds drew great attention by scientific community, even though three decades were needed until their crystal structure was determined to be ordered with a FCC lattice (Aulakh, 2017). HH compounds are ternary intermetallic materials with the general formula XYZ, where X is transition metal, Y can be transition metal or rare-earth element whereas Z is a main-group element which is non-magnetic (Chen et al., 2021). They crystallize in a structure similar to that of full-Heusler compounds but display unique properties due to a vacant atomic site. The typical HH structure adopts the cubic $C1_b$ structure, corresponding to space group $F\bar{4}3m$ (space group number 216) (Xia et al., 2021). They can have different types of atomic configuration, namely type I (α phase), type II (β phase), type III (γ phase) etc. In one of their atomic arrangements, say type I, the X atoms occupy the Wyckoff position 4a (1/4, 1/4, 1/4), the Y atoms are placed at the 4b (1/2, 1/2, 1/2), the Z atoms are located at 4d (0, 0, 0), and the remaining 4c (3/4, 3/4, 3/4) position is vacant which differentiates them from full-Heusler compounds (Yazdani-Kachoei et al., 2023). Table 2.1 and Figure 2.2 illustrate crystal structure of HH compounds with comparison to other Heusler compounds.

Studying compounds like $RhYZ$ ($Y = Zr, Ir, Nb$; $Z = Li, As, Si, Sb$) in different atomic arrangements (phases) provide valuable insights into their structural stability, electronic behavior and functional properties. Investigating various phases helps identify the most structurally, thermodynamically and dynamically (geometrically) stable configuration while also revealing potential phase transitions under different pressure and temperature conditions. Structural variations significantly impact the electronic band structure, enabling band gap tuning for optoelectronic and spintronic applications, while certain phases may exhibit metallic or half-metallic behavior, making them promising for spintronic devices (Meghoufel et al., 2021). Additionally, different atomic arrangements influence magnetic properties, mechanical stability and optical absorption, further broadening their technological potential. Moreover, understanding the effects of atomic swapping aids in experimental synthesis, defect engineering and doping strate-

gies, optimizing HH compounds for practical applications in optoelectronics, spintronics and energy conversion (Araújo et al., 2024).

The Birch-Murnaghan equation of state, a widely established method, was utilized to compute the equilibrium lattice constant (a_0), minimum volume (V_0), minimum energy (E_0), bulk modulus (B) and its pressure derivative (B') for the three distinct atomic arrangements of RhYZ ($Y = \text{Zr, Ir, Nb}$; $Z = \text{Li, As, Si, Sb}$) HH compounds which is given as (Katsura and Tange, 2019)

$$E_{tot} = E_0(V) + \frac{BV}{B'(B' - 1)} \left[B \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B'} \right] \quad (2.1)$$

was used. Here E_{tot} is the total energy at instantaneous volume (V).

Table 2.1: Structural prototypes of Heusler compounds (Li et al., 2019).

Type	Formula	Crystal Structure	a	b	c	d	Key features
Half-Heusler	XYZ	$\text{Cl}_b(\text{F43m})$	X	Y	-	Z	one site vacant
Full-Heusler	X_2YZ	$\text{L2}_l(\text{F3m3})$	X	Y	X	Z	Complete
Inverse-Heusler	X_2YZ	$\text{XA}(\text{F43m})$	X	X	Y	Z	X-Y swap order
QuaternaryHeusler	$\text{XX}'\text{YZ}$	Y (Modified L2_l)	X	Y	X'	Z	different X atom added

One of the most important thermodynamic parameter that affects a HH compound's phase stability, synthesizability and structural preference is its formation energy (Bartel et al., 2020). It is the energy difference between the total energy of the HH compound and the sum of the energies of its constituent elements in their most stable reference states. The following equation provides the formation energy per formula unit (Ward et al., 2017):

$$E_f = E_{HH} - (E_X + E_Y + E_Z) \quad (2.2)$$

where E_f and E_{HH} are the formation energy and energy of the HH compound and E_X , E_Y and E_Z are the total energies of the component elements in their ground-state reference phases. A positive formation energy implies that the material is metastable or unstable under normal circumstances, whereas a negative formation energy indicates that the HH compound is thermodynamically stable and can be experimentally synthesized (Wang et al., 2022c).

Elemental composition, atomic size matching, chemical bonding and competing phases are some of the important aspects that affect the formation energy of HH compounds. Since HH compounds with 18 valence electrons per formula unit often have lower formation energies and are hence more stable, the VEC is one of the most important variables (Komaiko and McClements, 2016). For example, materials with negative formation energies, such as ZrNiSn and TiCoSb are thermodynamically stable semiconductors. Negative formation energy of a

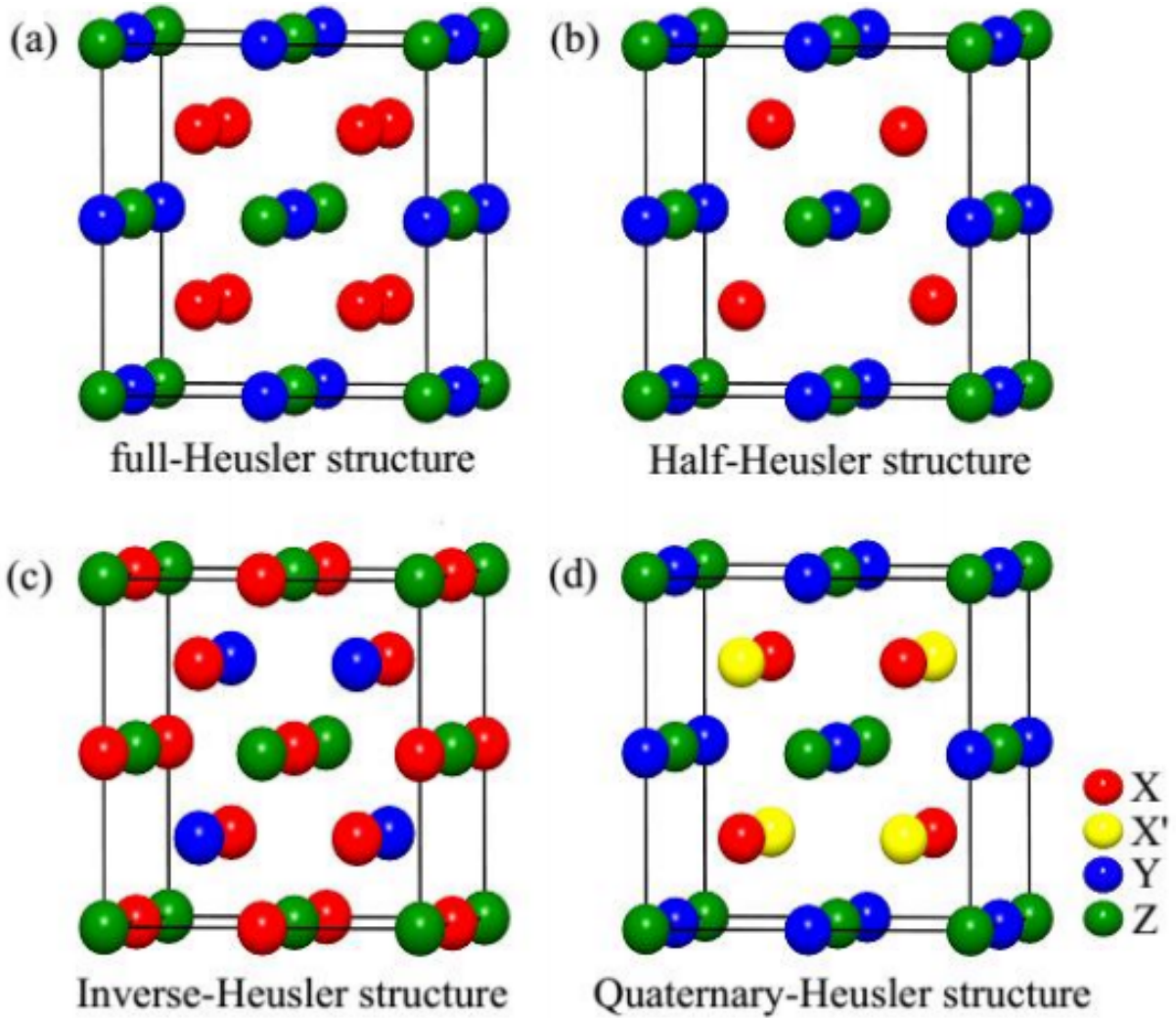


Figure 2.2: Types of Heusler structures. Full-Heusler (a), Half-Heusler (b), InverseHeusler (c), and Quaternary-Heusler structures (d) (Yun et al., 2016)

material indicates that it can be experimentally synthesized under normal condition. Since large differences in atomic radii between constituent elements can cause lattice strain, which raises the formation energy and decreases stability, atomic size compatibility is another crucial consideration (Sin et al., 2020). Furthermore, stability is largely determined by hybridization between X-Y and Y-Z atoms, with strong covalent bonds in semiconducting HH compounds assisting in lowering the formation energy. Additionally, the formation energy may be affected by the presence of competing binary (such as NiSn, TiSb) or full-Heusler (X_2YZ) phases, since the HH phase may be less likely to develop due to the favoring of alternative phases with lower energy (Shang et al., 2016). Designing HH compounds with desired electronic and magnetic

properties requires an understanding of and attention to these parameters. In general, one of the most important indicator of the stability and synthesizability of HH compounds is formation energy (Yang and Yakobson, 2018).

2.2.2 Mechanical properties

The mechanical properties of HH compounds, including hardness, elasticity and fracture toughness play a crucial role in assessing their potential for high-performance applications such as in optoelectronic and spintronic (Li et al., 2024). In order to discuss the mechanical stability of HH compounds, the value of elastic constants must be determined first (Rogl et al., 2016). The elastic properties of a material are indicative of its mechanical stability and are therefore significant for diverse practical applications. For simple geometrical system (cubic crystals) like HH compounds, three independent elastic constants, C_{11} , C_{12} and C_{44} , are sufficient even though we can have many of these elastic constants in tensor form for other more complicated geometry. The mechanical stability can be assessed from Born and Huang stability criteria for cubic structure which is given as follows (Uto et al., 2022).

$$C_{11} > 0 \quad (2.3)$$

$$C_{44} > 0 \quad (2.4)$$

$$C_{11} - C_{12} > 0 \quad (2.5)$$

$$C_{11} + 2C_{12} > 0 \quad (2.6)$$

$$C_{12} < B < C_{11}. \quad (2.7)$$

These elastic constants give valuable information about the mechanical behavior (stability, elasticity, ductility, anisotropy, etc.) of a given HH compound. After stability is determined, anisotropy, Cauchy's pressure, bulk modulus, shear modulus etc can be applied to further see the mechanical properties of a given HH compound (Adebambo et al., 2022). These mechanical parameters can be readily obtained from the three elastic constants. Anisotropy deals with the micro-cracks and defects in the material as it varies from the equilibrium value ($A=1$) and is calculated by applying the following equation (Wang et al., 2022a):

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \quad (2.8)$$

As the value of the anisotropy (A) increases above 1, the possibility of cracks and defects increase. The atomic bonding among the materials can be illustrated by Cauchy's pressure (CP)

formula which is given as (Gabal et al., 2022):

$$CP = C_{12} - C_{44}. \quad (2.9)$$

CP helps us to see whether the character of the atomic bond is fragile or ductile in a given compounds. If CP has positive value, then the material is ductile in nature otherwise it becomes fragile. Many other parameters that describe the mechanical properties of a given compound are collectively given below (Kadri et al., 2022; Atli and Karaman, 2023).

$$B = \frac{C_{11} + 2C_{12}}{3} \quad (2.10)$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (2.11)$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{3(C_{11} - C_{12}) + 4C_{44}} \quad (2.12)$$

$$G = \frac{G_V + G_R}{2} \quad (2.13)$$

$$Y = \frac{9BG}{3B + G}. \quad (2.14)$$

Here B, G, G_V , G_R and Y stand for bulk, shear, Voigt's shear, Reuss's shear and young moduli of a given compound. The bulk modulus(B) measures the resistance of a given compound towards the fracture, while the shear modulus (G) measures the resistance of the compound to plastic deformation. Young modulus predicts the extension or contraction of a given material under tension and compression, respectively, which is used to measure the stiffness of the material. Higher value of Y indicates that the given material is inflexible (Kadri et al., 2023).

Other important parameter which determines atomic bonding in a given material is the Poisson's coefficient (ratio), ν . It explains the ratio of relative contraction to relative expansion. For most materials the value of ν ranges from 0.0 to 0.5. If $\nu \sim 0.1$ the material is covalently bonded, if $\nu \sim 0.25$ the material is ionically bonded whereas if $\nu \sim 0.33$ the material is metallically bonded. This parameter is defined as (Abd El Aal et al., 2022):

$$\nu = \frac{3B - 2G}{2(3B + G)}. \quad (2.15)$$

The hardness of a material is important for practical applications and can be predicted by using

the following equation (Pintaude, 2023):

$$H_V = 2 \left(\left(\frac{G}{B} \right)^2 G \right)^{0.585}. \quad (2.16)$$

The Debye temperature (θ_D) is crucial for assessing heat transport properties since it is closely connected to thermal conductivity and lattice vibrations and thus, it reflects the thermal stability of a material. Mathematically, it can be quantified using the subsequent equation (Yang et al., 2021):

$$\theta_D = \frac{h}{k_B} \left(\frac{3nN_A\rho}{4\pi M} \right)^{\frac{1}{3}} v_a \quad (2.17)$$

where h , k_B , ρ , N_A , v_a , M , n are respectively Plank's constant, Boltzmann constant, mass density, Avogadro's number, average elastic wave (sound) velocity, molecular weight and number of atoms in the given compound. Elastic velocities (v_a , v_t and v_l) aid in evaluating mechanical stiffness and rigidity of a material. The average sound velocity of material can be expressed as (Wang et al., 2022b);

$$v_a = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{-\frac{1}{3}} \quad (2.18)$$

where v_t and v_l stand for the transverse and longitudinal sound velocity, respectively, and can be obtained from

$$v_t = \left(\frac{G}{\rho} \right)^{1/2} \quad (2.19)$$

$$v_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2}. \quad (2.20)$$

The melting (fusion) temperature, which signifies the solid-to-liquid phase transition of a compound and is a critical parameter for materials employed in heating systems, can be theoretically predicted as a function of the elastic constant, C_{11} according to the following equation (Andharia et al., 2022):

$$T_m(K) = \left[553 + \left(\frac{5.911C_{11}}{\text{GPa}} \right) \right] K \pm 300K. \quad (2.21)$$

B/G is the Pugh's ratio and it describes the brittleness and ductility in a material that rely upon its equilibrium value (1.75). The greater B/G deduces the ductile character and the smaller value indicates brittle character of the material, which shows the low malleability of the crystals (Huang et al., 2024).

2.2.3 Electronic properties

HH compounds, with their distinctive crystal structure and varied composition, display a wide range of electronic properties, making them ideal candidates for optoelectronic and spintronic applications (Nenuwe and Omugbe, 2023). The electronic nature of a HH compound, whether it exhibits semiconducting, conducting (metallic), half-metallic, semi-metallic, insulating or topological insulating behavior, is largely governed by the total count of its valence electrons (Toboła and Pierre, 2000). The case of 18 valence electrons is especially important in HH compounds, as this electron count corresponds to a stable and balanced electronic configuration, which often results in semiconducting behavior. If the total number of valence electrons in HH compounds is not equal to 18, the compounds will incline to become metal or magnetic materials (Phuc et al., 2023). Examples are NiMnSb and PtMnSb, which are known as half-metallic ferromagnets (Yang et al., 2022a). According to different spin directions, these half-metals can exhibit both metal and insulator properties in the same material. The presence of strong covalent and metallic bonding interactions within their $C1_b$ structure results in a unique electronic band structure, allowing for high carrier mobility and tunable band gaps (Chibani et al., 2018). For full Heusler to be a semiconductor, the total number of valence electrons should be equal to 24, so that the outermost electron layer can reach a full shell state. The best example is Fe_2VAl (Berarma et al., 2023). When the total number of valence electrons is not equal to 24, there will appear ferromagnetism, ferrimagnetism or anti-ferromagnetism and therefore, the compound has magnetic character (Elphick et al., 2021).

In conductor, the conduction and the valence bands overlap, so that the electrons can move easily in the bands (Sattar et al., 2018). In insulator, the gap between conduction and valence bands is large. Topological insulator also has huge band gap comparable to the insulator, but in this case the topological surface state allows electron conduction (Bouldiab et al., 2021). In semiconductor, the band gap is less than that of insulator, so electrons can jump from the valence band to the conduction band at higher temperatures (Dehghan and Davatolhagh, 2021). In semimetals, the bottom of conduction band and the top of valence band just meet at a point, as shown in Figure 2.3e, so it can conduct electricity even if it is at very low temperature (Ram et al., 2020).

Rh-based HH compounds have become one of the most promising materials among HH compounds because of their exceptional thermoelectric qualities and stable semiconducting nature (Paul et al., 2024). With band gaps that usually range from 0.5 eV to 1.2 eV, these compounds, e.g., RhTiSb, RhZrSn, and RhHfSn make promising choices for optoelectronic and high-efficiency thermoelectric applications (Xing et al., 2024). Strong hybridization between the Rh d-orbitals and the Y and Z elements results in distinct valence and conduction bands with

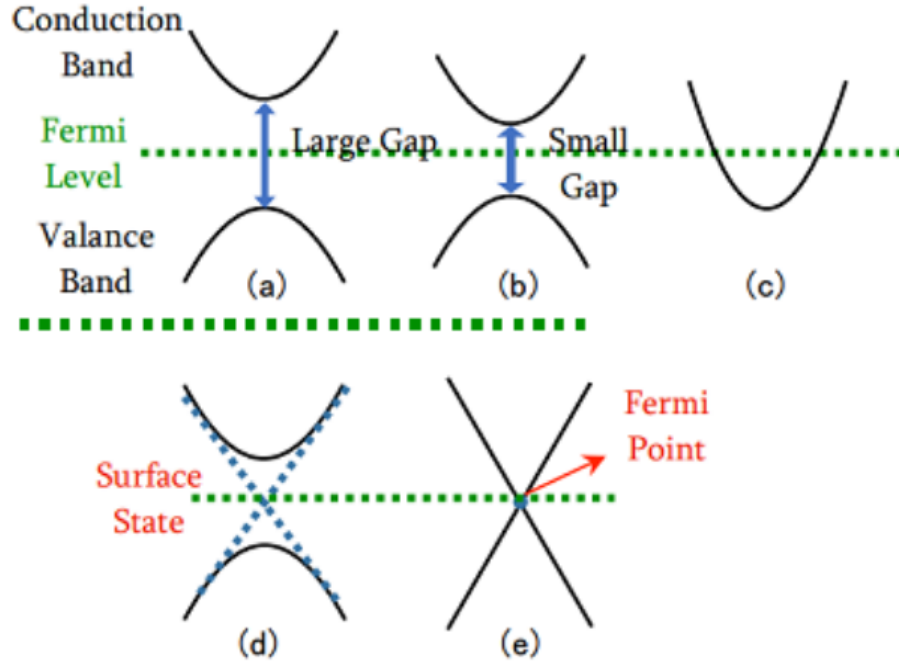


Figure 2.3: Band structure of different materials: (a) insulator; (b) semiconductor; (c) conductor; (d) topological insulator; (e) semimetal (Lin, 2020).

comparatively low effective masses, improving the carrier transport characteristics. Rh-based HHs exhibit low formation energies and high power factors, which are further supported by computational investigations employing DFT (Abir et al., 2022).

Rh-based HH compounds' potential as topological materials is an additional intriguing feature. The bulk of some Rh-based systems, such RhPbBi and RhPtBi, is expected to remain insulating while conducting surface states form as a result of high SOC. This is known as topological insulating behavior. Because spintronic devices and quantum computers require stable, spin-polarized surface states, this property is especially helpful (Kalita and Saxena, 2021). Topological insulators are characterized by considerable band inversion, which is caused by the strong SOC in Rh-based HH compounds. Rh-based HH compounds are extremely adaptable due to their electronic properties, which may find use in spintronics, topological quantum materials and next-generation thermoelectrics (Maji, 2023).

2.2.4 Optical properties

The optical properties of a material are of significant interest due to their direct correlation with the diverse ways in which it interacts with electromagnetic radiation of varying energies (Kars Durukan and Oztekin Ciftci, 2021; Forozani et al., 2020). Interaction of photons with electrons within a material give rise to some optical properties of the material that may in-

clude absorption, transmission and scattering (Jubair et al., 2021). Dielectric constant (real and imaginary), electron energy loss, refractive index, extinction coefficient, absorption coefficient, reflectivity, optical conductivity (real and imaginary) are some key optical parameters that may well describe optical properties of a given material (Satyam and Saini, 2021). A material appropriate for optoelectronic or photovoltaic application must have high absorbance, high refractive index and low emissivity of light. Moreover, high dielectric constant, high optical conductivity and reflectivity are prerequisites for a good optical material (Knyazev et al., 2024; El Krimi et al., 2020).

Many HH compounds, especially those with 18 valence electrons per formula unit, exhibit semiconducting behavior with direct or indirect band gaps, making them suitable for optoelectronic and photovoltaic applications (Mehmood et al., 2017). The optical response of HH compounds is primarily characterized by their optical band gap, absorption coefficient, refractive index, dielectric function and reflectivity, all of which are vital for understanding their potential in photodetectors, solar cells and infrared (IR) devices (Wei and Wang, 2018). The band gaps of HH compounds typically range from 0.1 eV to 2 eV, allowing them to absorb light in the visible to infrared regions, depending on their elemental composition. The high absorption coefficient of HH compounds, especially in the visible and ultraviolet (UV) regions, is one of the main features of their optical behavior. Materials with substantial optical absorption, such as ZrNiSn, TiCoSb and Rh-based semiconductor HH compounds, for instance, are interesting options for thermophotovoltaic and solar energy harvesting systems (Verma et al., 2022). The absorption spectra of HH compounds show a strong rise near the band edge, which is a feature of direct-gap semiconductors. Furthermore, HH compounds with high SOC, such as RhPtBi, show distinctive optical transitions that may find use in spintronic as well as optoelectronic devices and infrared sensors (Missoum et al., 2022). The optical sensitivity of HH compounds is also significantly influenced by their refractive index and dielectric function. In optoelectronic applications, the high static real part of dielectric constant of certain HH compounds improves their capacity to screen charge carriers (Mehta and Saini, 2024). While the imaginary component of the dielectric function explains the material's absorption properties, the real part provides information about the material's capacity to store electromagnetic energy (Benyettou et al., 2024). Moreover, transparent conductive films and coatings are best suited for HH compounds with strong optical conductivity and low reflection (Toual et al., 2024). Researchers can create HH compounds with specific optical properties for high-performance optoelectronic devices, infrared detectors and photovoltaics by adjusting composition and doping amounts (Jabar et al., 2025).

Dielectric function is the most fundamental optical properties from which other optical pa-

rameters can be calculated (Bhavani, 2021). It gives linear response of a system to an external electromagnetic field and has two parts: real and imaginary parts. The real part is related to the stored energy within the medium and the imaginary part is to the dissipation of energy within the medium. This complex dielectric function is mathematically given by the Ehrenreich and Cohen equation (Zhu et al., 2017):

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \quad (2.22)$$

where ε_1 is the real part and ε_2 is the imaginary part of the dielectric function. The dielectric function, $\varepsilon(\omega)$ has two primary contributions: interband transitions and intraband transitions. In this case, we disregard the indirect interband transitions, which involve phonon scattering and are anticipated to contribute only minimally to $\varepsilon(\omega)$ (Naderizadeh et al., 2012). The imaginary part of the dielectric function, $\varepsilon_2(\omega)$ is given as

$$\varepsilon_2(\omega) = \frac{\nu e^2}{2\pi\hbar m^2 \omega^2} \int d^3k \sum_{k,k'} [|\langle kn|\mathbf{p}|kn'\rangle|^2 \times f(kn)(1 - f(kn'))\delta(E_{nk} - E_{n'k} - \hbar\omega)] \quad (2.23)$$

where $\hbar\omega$ is the energy of the incident photon, $\mathbf{p}$ is the momentum operator, $\frac{\hbar}{i} \frac{\partial}{\partial x'}$, $|kn\rangle$ is the eigenfunction with eigenvalue E_{nk} and $f(kn)$ is the Fermi distribution function (Aly, 2023). The real part of the dielectric function, $\varepsilon_1(\omega)$ is obtained from the Kramers-Kronig relation (Hilfiker and Tiwald, 2018):

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon_2(\omega')\omega'}{\omega'^2 - \omega^2} d\omega'. \quad (2.24)$$

The complex refractive index characterizes the propagation of light through a medium, encompassing both the changes in amplitude and phase as the light interacts with the material. It is denoted as $\tilde{n}$ and mathematically expressed as (Zhang et al., 2020):

$$\tilde{n} = n + ik. \quad (2.25)$$

The real part of the refractive index, n , determines the speed of light in the material and the extent to which light is bent (refracted) when entering the medium. The imaginary part, k (also known as the extinction coefficient), describes the absorption of light within the material. It quantifies the rate at which the amplitude of the light wave decreases as it propagates through

the medium. They are given by the following relations (Sorensen et al., 2019):

$$n(\omega) = \frac{1}{\sqrt{2}} \left[(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega))^{\frac{1}{2}} + \varepsilon_1(\omega) \right]^{\frac{1}{2}}. \quad (2.26)$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left[(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega))^{\frac{1}{2}} - \varepsilon_1(\omega) \right]^{\frac{1}{2}}. \quad (2.27)$$

Reflectivity, (R) provides a quantitative measure of the proportion of incident photon energy that is reflected by a material, thereby indicating its opacity to electromagnetic radiation at a given energy (Mostari et al., 2020). It is given by the following relation (Tarekuzzaman et al., 2024):

$$R(\omega) = \left[\frac{\sqrt{\varepsilon(\omega)} - 1}{\sqrt{\varepsilon(\omega)} + 1} \right]^2. \quad (2.28)$$

Absorption coefficient, α results from the interaction between electrons and photons as well as due to interband and intraband transitions. It can be used as a basic optical parameter to identify whether the material is optically active or optoelectronic material (Kumar and Chand, 2023). It is given by the following relation (Mekki et al., 2023)

$$\alpha(\omega) = \sqrt{2}\omega \left[(\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega))^{\frac{1}{2}} - \varepsilon_1(\omega) \right]^{\frac{1}{2}}. \quad (2.29)$$

Electron energy loss, (L) is a phenomenon resulting from the inelastic scattering of incident external radiation by valence electrons within a material (Mehta and Saini, 2023). This significant optical parameter quantifies the energy dissipated by a fast electron as it traverses the material (El Yousfi et al., 2023) and it is given by the following equation:

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}. \quad (2.30)$$

Optical conductivity is a key parameter in the study of the interaction between electromagnetic radiation and the charge carriers in a material. It characterizes how a material responds to an applied electric field, particularly in the infrared and visible regions of the spectrum (Hong et al., 2016). In solid-state physics, the optical conductivity is closely related to the electronic structure of a material, as it reflects the transitions between different energy states under an external electromagnetic field. The real part of the optical conductivity provides insights into the absorption of light and the response of free charge carriers, while the imaginary part is connected to the material's dielectric function (Naseri and Hoat, 2019). In materials like HH compounds, which exhibit unique electronic and magnetic properties, understanding the optical

conductivity is crucial for evaluating their potential in optoelectronic applications, such as in LEDs, photovoltaic devices and other optical sensors. Analyzing the spectral distribution of optical conductivity can offer valuable information about the band structure, carrier dynamics, and the material's overall suitability for these technologies (Bouhadjer et al., 2024). The optical conductivity of a material is derived from its complex dielectric function, specifically its real and imaginary parts, as described by the following equations (Uğur et al., 2021).

$$\sigma_1 = \frac{\omega}{4\pi} \varepsilon_2(\omega) \quad (2.31)$$

$$\sigma_2 = \frac{\omega}{4\pi} (1 - \varepsilon_1(\omega)) \quad (2.32)$$

where σ_1 and σ_2 are the real and imaginary parts of optical conductivity.

2.2.5 Magnetic properties

Heusler compounds are known to follow the Slater-Pauling (SP) behavior (rule), which posits that the total magnetic moment is equivalent to the number of uncompensated electron spins (Ahmed et al., 2019). This behavior is observed in both half- and full-Heusler compounds, for which the total magnetic moment can typically be approximated by the following expressions (Zheng and Jin, 2012):

$$M_t = Z_t - 18 \quad (2.33)$$

$$M_t = Z_t - 24. \quad (2.34)$$

In these expressions, M_t denotes the total magnetic moment and Z_t the total number of valence electrons, with the constants 18 and 24 representing twice the number of minority band electrons for half- and full-Heusler compounds, respectively. Inverse Heusler compounds, where the second X atom shifts to the third lattice position, adopting the XA structure with $F\bar{4}3m$ symmetry, also adhere to the SP rule. However, their lack of a consistent number of fully occupied minority bands leads to a range of potential equations, a few examples of which are presented below (Parzer et al., 2024):

$$M_t = \begin{cases} Z_t - 18, & \text{X = V, Sc, Ti} \\ Z_t - 24, & \text{X = V, Cr, Mn} \\ Z_t - 28, & \text{X = CR, Mn and Y = Cu, Zn.} \end{cases} \quad (2.35)$$

The inversion of the second X atom's position in the lattice of inverse Heusler compounds causes the Y atom to become involved in the material's SP behavior. Similarly, quaternary

Heusler compounds ($XX'YZ$), exemplified by CoFeMnSi and LiMgPdSb (exhibiting a valence order of $X > X' > Y$), adhere to the same SP relationship as their full-Heusler counterparts, as defined in eq.(2.34) (Ghellab et al., 2024).

Electrons show not only charge property but also spin property. Electron spin produces spin magnetic moment whereas electrons orbiting the nucleus produce orbital magnetic moment. The combination of these moments makes the given material magnetic. It is these magnetic moments that determine the magnetic nature of the material (Idrissi et al., 2019). HH compounds with the XYZ stoichiometry exhibit a single magnetic sublattice, a consequence of localized magnetic moments on the octahedral sites, as depicted in Figure 2.4a. For example, the magnetic of MnNiSb HH compound exist only for $X = \text{Mn}$ and Rare Earth (RE) because of the localized nature of the four 3d electrons of Mn^{3+} and the 4f electrons, respectively, which carry the magnetic moment (Rogl and Rogl, 2023). HH compounds containing manganese frequently exhibit half-metallic ferromagnetism coupled with high Curie temperatures. By contrast, in full-Heusler (X_2YZ) compounds, the occupation of tetrahedral sites by two X atoms facilitates magnetic interaction and the formation of a second, more delocalized magnetic sublattice, as depicted in Figure 2.4b. Because of these two different magnetic sublattices, the full-Heusler compounds (e.g., Co_2MnSn) mostly can show all kinds of magnetic phenomena like ferromagnetism, ferrimagnetism and half-metallic ferromagnetism (Wakeel et al., 2021). HH compounds often preferred for spintronic devices due to their potential as spin gapless semiconductors, offering high spin polarization and tunable band gaps whereas full-Heusler compounds widely used in magnetoresistive devices and permanent magnets due to their high magnetic moments and robust ferromagnetic behavior (Wen et al., 2018).

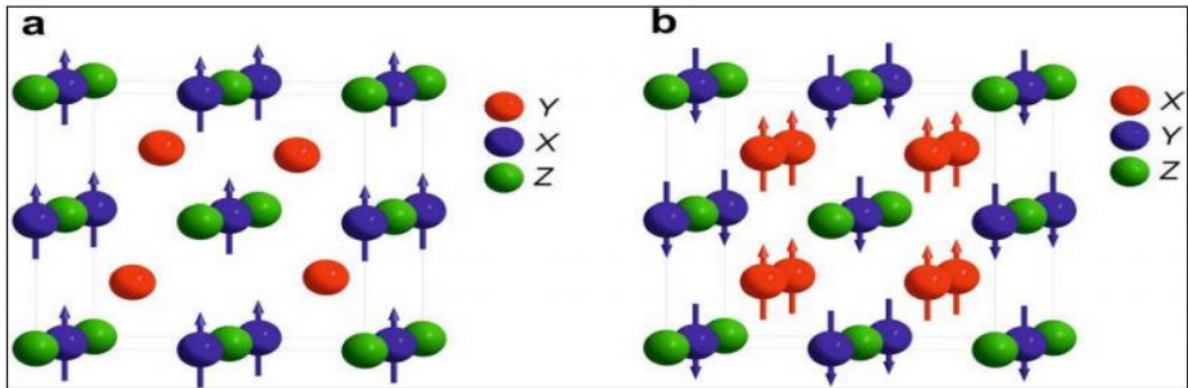


Figure 2.4: Magnetic sublattices in (a) XYZ HH (one sublattice) and (b) X_2YZ full-Heusler (two sublattices with potential ferro- or antiferromagnetic coupling).

The spin-polarization property at the E_F of a material can be calculated by using the density

of states at the E_F for the corresponding spin and mathematically defined as (Dutta et al., 2023):

$$P = \frac{\rho \uparrow (E_F) - \rho \downarrow (E_F)}{\rho \uparrow (E_F) + \rho \downarrow (E_F)}. \quad (2.36)$$

In this context, $\rho \uparrow (E_F)$ and $\rho \downarrow (E_F)$ denote the density of states at the E_F for the spin-up and spin-down channels, respectively. Complete (100%) spin polarization occurs when the density of states for one spin channel at the E_F is zero. The spin polarization (P) is found to be high for materials with predominantly d-like orbital character at the E_F , but low for those with s-like or mixed s+d-like character (Liu et al., 2024).

Depending on their elemental makeup, atomic arrangement and VEC, HH compounds can display a variety of magnetic behaviors, including as ferromagnetism, ferrimagnetism, antiferromagnetism and spin-gapless semiconducting states (Vishali and John, 2022). The magnetic interactions in HH compounds are mostly determined by the presence of transition metal elements (X, Y) with unpaired d-electrons and substantial hybridization effects between X–Y and X–Z atoms (Song and Zhang, 2018). The $C1_b$ cubic structure's absence of an inversion center affects the exchange interactions as well, producing intricate magnetic characteristics that can be adjusted for topological, magnetocaloric and spintronic uses. Half-metallic ferromagnetism, in which one spin channel acts metallically while the other stays semiconducting, results in 100% spin polarization at the E_F and is one of the most well-studied magnetic properties in HH compounds. Because of this characteristic, HH compounds are great choices for spintronic devices like MTJs and spin injectors (Mukhopadhyay et al., 2019). Examples are NiMnSb and CoMnSb, which are suited for high-temperature spintronic applications due to their virtually perfect spin polarization and high Curie temperatures ($> 600K$) (Mandal et al., 2022; Pokar et al., 2022). Certain HH compounds exhibit ferrimagnetic behavior, where magnetic moments from various sublattices are antiparallel but uneven, resulting in a net magnetization. Examples of these compounds include CoFe(Ti)Sb and Mn-based HH compounds (MnNiSb, MnCoSb, etc.). Because of their prospective uses in antiferromagnetic spintronics and exchange bias systems, antiferromagnetic HH compounds are also quite interesting. The non-magnetic Z-site element mediates superexchange interactions that result in antiferromagnetic ordering in several Mn-based HH compounds, including MnVSb and MnVSn (Musa Saad H.-E and Al-sobhi, 2023). Furthermore, many HH compounds exhibit spin-gapless semiconducting (SGS) behavior, which allows for high-mobility spin-polarized carriers by allowing the valence and conduction bands to meet at a single point (Saib et al., 2020). This shows promise for high-speed spintronic applications, especially in Mn-based HHs such as MnCrSb and CoFe(Mn)Si. The adaptability of HH compounds in contemporary magnetic and quantum technologies is

further increased by their capacity to modify the magnetic moment, Curie temperature and spin polarization via elemental substitution, strain engineering and external forces (Ahmad et al., 2019).

2.3 Applications of HH Compounds

Due to their many interesting physical properties, such as their intrinsic spin polarization, strong mechanical strength, tunable electronic structure and high thermoelectric efficiency, HH compounds have garnered a lot of interest in condensed matter physics and materials research. The broad and varied range of features of HH compounds, which make them appropriate for a variety of technological applications, are a result of their non-centrosymmetric crystal structure (Anand et al., 2019). The ability of HH compounds to behave half-metallic or semiconducting, depending on the constituent composition selected, is one of their most remarkable properties. Because of this tunability, scientists can design materials with specialized optical, magnetic and electronic properties for particular uses (Poon, 2018). Because HH compounds can be altered by chemical substitution, strain engineering or doping, their band gap which normally falls between 0.1 eV and 2 eV makes them extremely versatile for a variety of device functions. Furthermore, some HH compounds are better suited for applications needing effective charge transport and spin manipulation due to their strong SOC and high carrier mobility (Zhang et al., 2017). The semiconducting conductivity and spin-polarized transport features of HH compounds are among their most potential uses in optoelectronics and spintronics, where they are essential to device performance. For applications in photodetectors, solar cells, LEDs and laser diodes, where effective light absorption and emission are essential, HH compounds with direct or near-direct band gaps were being investigated in optoelectronics. Their mechanical stability and excellent absorption coefficient further increase their potential for long-term use in challenging conditions (Ciesielski et al., 2020b; Xiong et al., 2022a).

2.3.1 Optoelectronic applications

HH compounds' superior mechanical and thermal durability, high absorption coefficients and variable band gaps have made them interesting materials for optoelectronic applications (Jolayemi and Babalola, 2023). They can operate in a broad spectrum, from visible to mid-infrared, which makes them useful in a range of optoelectronic devices, including lasers, photodetectors, LEDs and solar cells (Kamlesh et al., 2021a). The band gap of HH compounds drives their very variable semiconducting activity. Thus, these compounds are appropriate for particular optoelectronic applications because the band gap can be precisely controlled by substituting atoms at the X, Y or Z sites in the XYZ structure (Kamlesh et al., 2022). For example, HH com-

pounds, such as CoTiSb, that have band gaps between 1.0 and 2.0 eV are perfect for applications using visible light (Nenuwe and Omagbemi, 2022). Near-infrared applications can benefit from the tunable band gaps of Rh-based compounds, such as RhTiZ ($Z = \text{P, As, Sb, Bi}$) which fall between 0.7 and 1.2 eV. Effective light absorption is also made possible by these compounds even in thin-film geometries by their high optical absorption coefficients. Computational studies have demonstrated that these compounds have significant absorption in the infrared spectrum, which makes them ideal candidates for thin-film and multi-junction solar cells (Jaishi et al., 2021). HH compounds with narrow band gap of 0.333 eV such as RhBiHf, are especially well suited for thermal imaging and mid-infrared photodetection systems. Narrow band gap high sensitivity IR photodetection is possible with these compounds, which can be used for thermal imaging and optical communication. For infrared LEDs, these compounds are perfect because of their strong optical transitions and narrow band gaps. These substances can be utilized in optical communication systems, which frequently use infrared LEDs. Their dependability in high-power mid-IR lasers is guaranteed by their mechanical and thermal stability. Gas sensing, environmental monitoring and industrial processes all make use of these lasers (Wei et al., 2023).

Furthermore, HH compounds are gaining attention as strong rivals for next-generation photovoltaic (PV) applications, owing to their adjustable band gaps, excellent mechanical, thermal and chemical resilience and reliable electronic properties. HH compounds exhibit semiconducting behavior when appropriately configured, especially when the system maintains an 18 VEC. Their compositional flexibility allows for tuning the band gap into the ideal range of 1.0–1.5 eV, suitable for effective solar absorption and aligned with the Shockley–Queisser efficiency limit for single-junction cells. Additionally, certain HH compounds display strong SOC, which can enhance interactions with light, while their compatibility with thin-film deposition techniques and heterojunction structures makes them well-suited for device fabrication. Research has revealed that specific HH semiconductors, such as CoHfZ ($Z = \text{As, Bi}$), possess high absorption coefficients in the visible light range, positioning them as promising absorber materials for solar cells (Gurunani and Gupta, 2025a). Furthermore, first-principles studies suggest that HH materials can form favorable band alignments with conventional buffer and window layers in photovoltaic architectures (Menaria et al., 2025). Collectively, these features make HH compounds attractive for developing efficient, stable, and scalable solar energy devices.

HH compounds can also find applications in conjunction with conventional semiconductor materials. For example, ternary copper-based chalcopyrite semiconductors like p-type CuInSe₂ (CISE) or Cu(In, Ga)Se₂ (CIGSe) are highly effective light-absorbing materials for cost-efficient thin-film solar cell technologies. In standard chalcopyrite solar cells, a CdS buffer layer with

a thickness of approximately 50 nm were employed between the light absorber and the n-type ZnO window layer to improve device efficiency. Record efficiencies of 19.9% have been reported for the ZnO/CdS/Cu (In, Ga)Se₂ heterojunction (Belmiloud et al., 2016). To have a good solar-cell performance, a precise design of the heterojunction between absorber and buffer layer is crucial. The buffer layer material must avoid unnecessary absorption losses and its crystal structure should ensure a good contact between absorber and buffer layer. It is desirable to have an inverted interface (conduction band of the absorber close to the Fermi E_F at the interface) and to avoid a barrier reduction at the interface in order to minimize recombination. CdS can meet these conditions, but unfortunately it is very toxic and hence, much research activity is undertaken to replace CdS by a less toxic buffer layer material (Solet et al., 2022).

HH compounds are the best candidates to solve this problem due the following reason: The crystalline structure, being rather loosely packed and similar to chalcopyrite, suggests that good interfacial contact between the two materials can be expected if their lattice constants are of a similar magnitude. Compounds of special interest are I-II-V, in which the component elements X, Y and Z have 1, 2 and 5 valence electrons, respectively. One example is LiZnP, for which the crystalline structure and electronic properties have been predicted with the help of local-density approximation (LDA) calculations before they were analyzed experimentally. Raman scattering indicated a strongly ionic bond between Li and P and a covalent bond between Zn and P. The system may be viewed as a (ZnP)⁻ zinc-blende lattice partially filled with Li⁺ ions. With the extra electron, the (ZnP)⁻ sublattice is similar to the III-V semiconductor GaP and, indeed, LiZnP is semiconducting (Kaur et al., 2023).

A good buffer layer material must meet several demands with respect to its electronic structure, the interaction with the adjacent materials, the electron affinity and other aspects to reasonably replace CdS. Here we can select two primary criteria which should be fulfilled by a good substitute for CdS. The first criteria is that the band gap of the buffer material should not be smaller than 2 eV for a reasonably small absorption loss, and the second criteria is that the lattice constant should be around 5.9Å for a good lattice matching with the absorber material (Menaria et al., 2024).

2.3.2 Spintronic applications

A new science called spintronics, or spin electronics, uses electrons' inherent spin in addition to their charge to create sophisticated electronic devices. This area has the potential to completely transform technologies including memory devices, logic circuits and data storage by providing quicker and more energy-efficient substitutes for traditional semiconductor devices (Dehghan and Davatolhagh, 2019). HH compounds, especially those in the Rh-based group, are great can-

didates for spintronic applications because of their distinct electronic and magnetic properties. Some applications in spintronic may include spin injection and transport(SIT), spin-polarized tunneling (SPT), magnetic properties and ferromagnetism, spin torque and magnetic switching, topological effects and SOC. It has been demonstrated that Rh-based HH compounds, like RhVZ (Z = P, As, Sb) (Ahmad and Mehmood, 2018) and RhFeZ (Z = Sn, Ge) (Meenakshi et al., 2021) have strong spin polarization due to their half-metallic behavior. Because of its distinct electronic structure, rhodium plays a major role in spin polarization at the E_F . Thus, these substances are perfect for spintronic applications that require high spin-polarized currents. These HH compounds can facilitate effective spin transfer because of their half-metallic composition and adjustable electronic properties. The scattering mechanisms in the material affect the spin relaxation time, which determines how long a spin maintains its orientation. They can enable extended spin diffusion lengths, which are necessary for effective spin transport in devices like spin transistors, because to their favorable electron mobility and decreased scattering rates. Long spin diffusion lengths for effective spin transport, high electronic conductivity with little scattering and high spin polarization from the transition metal Rh are some of the benefits of spin injection and transport in spintronic applications (Rai, 2020).

MTJs and spin-valve devices use SPT, a fundamental feature in spintronics. In these devices, the relative alignment of the spins in the two ferromagnetic layers that are separated by an insulating barrier determines the tunneling current. The materials utilized in the device have an impact on the spin polarization of SPT. Since HH compounds, notably Rh-based HH compounds, can show high spin polarization at the E_F , they can be utilized as the materials in one of the layers of MTJs. MTJ's spin-polarized current tunneling through the insulating barrier is extremely sensitive to the ferromagnetic layers' magnetization, which is reliant on the HH materials' spin-polarization. The relative alignment of the spins in the ferromagnetic layers determines the resistance of spin-valve devices, which are utilized in data storage and magnetic sensors. The SPT properties of these devices could be improved by including these HH compounds, which would result in improved read-out speed and sensitivity. These HH compounds are perfect for effective tunneling in MTJs and spin-valves because of their high spin polarization, adjustable spin-polarization levels through changes in material composition and structure, and potential for lower power consumption (Al-Douri and Ameri, 2024).

For many spintronic applications, such as magnetic memory and data storage, ferromagnetism, the alignment of electron spins in the same direction, is crucial. Ferromagnetism can be improved or induced in materials used for spintronic devices through substitution, doping or structural changes. Certain Rh-based HH compounds, such as RhCrZ(Z=Si, Ge), have been shown or anticipated to behave ferromagnetically because of the interactions with the transition

metal (like Cr) and the particular arrangement of the Rh atoms. For devices where controlling magnetization is essential, such as spin valves and MTJs, this ferromagnetism is advantageous. The directional dependency of the material's magnetic characteristics, known as magnetocrystalline anisotropy, can be seen in Rh-based HH compounds. In spintronic systems, high anisotropy is preferred because it improves control over the magnetization orientation, which is essential for data storage and magnetic sensor functionality. It is possible to engineer the exchange contacts in Rh-based HH compounds by applying external magnetic fields or substituting by other elements. These interactions can be used to improve the material's magnetic characteristics, which makes it appropriate for use in spintronic memory systems like Magnetoresistive Random Access Memory (MRAM). Certain Rh-based HH compounds exhibit ferromagnetic behavior, which makes them ideal for spintronic applications. They also have strong magnetocrystalline anisotropy, which improves control over magnetic domains and tunable exchange interactions, which improve magnetic stability and speed up switching (Mehmood et al., 2017).

When a spin-polarized current applies a torque to a ferromagnetic layer's magnetization, it causes the layer to change direction, a phenomenon known as spin torque. MRAM and other spintronic devices use this effect to store data and perform logic operations. Strong spin polarization and ferromagnetic characteristics make Rh-based HH compounds suitable for application in Spin-Transfer Torque (STT) based devices like MRAM. The application of a spin-polarized current in MRAM switches the magnetization of a free layer. High spin polarization and effective spin transport in Rh-based HH materials allow for quick and low-energy switching of the magnetization of the free layer, improving MRAM device performance (Brito et al., 2024). It is possible to incorporate Rh-based HH compounds into MRAM systems' free magnetic layers. In comparison to traditional memory technologies, MRAM devices may have better storage densities, faster switching speeds and lower power consumption due to the combination of strong spin polarization, programmable magnetic characteristics and effective spin transport. For sophisticated spintronic memory devices like MRAM, Rh-based HH compounds are perfect due to their effective STT, high spin polarization for low-energy switching and the possibility of increased data storage capacity and device downsizing (Mouchou et al., 2024).

A key component of topological spintronic devices is SOC, which is the relationship between an electron's mobility in an electric field and its spin. Strong SOC materials can produce spin currents without the need for an external magnetic field, among other unique spintronic effects (Gurunani and Gupta, 2025b). The Rashba effect, or the splitting of spin states in the presence of an electric field, can be seen in Rh-based HH compounds because of their crystal symmetry and strong spin-orbit interactions. Spin-polarized currents can be produced in

spintronic devices by taking use of this effect, particularly in topological insulators and spin field-effect transistors (SpinFETs). Rh-based HH compounds may help create topological insulators, which have surface states with strong spin-polarized currents, when combined with other materials. These topological materials show promise for usage in cutting-edge spintronic applications, including quantum computing and low-power logic circuits (Karimullah and N, 2024). Rh-based HH compounds are perfect for advanced topological spintronics because of their strong SOC, which allows for effective spin manipulation without magnetic fields, the Rashba effect, which generates spin currents and the possibility of integration into topologically protected devices with improved robustness against defects (Benabdellah et al., 2024).

2.4 Density Functional Theory (DFT)

A detailed investigation into the ground state properties of quantum mechanical systems is inherently complex. Unlike the analytically solvable hydrogen atom (a two-body problem), the helium atom presents a much greater challenge. Small quantum systems can be solved numerically, for instance, through matrix diagonalization. However, because the dimension of the underlying parameter space grows dramatically with the system size, computational limits are rapidly encountered (Orio et al., 2009). In his Nobel Prize lecture, Walter Kohn, one of the pioneers of DFT, estimated that the parameter space needed for a system of 100 interacting particles would far surpass the number of baryons in the universe. He referred to this phenomenon as the "exponential wall." Thus, solving complex many-body systems, such as solids, necessitates the use of different methods. One of the most prominent techniques is DFT (Hohenberg and Kohn, 1964a).

DFT represents a prevalent computational quantum mechanical approach within physics, chemistry and materials science for the investigation of the electronic structure of many-body systems, notably atoms, molecules and solids (Lee, 2021). It is distinguished by its optimal balance of accuracy and computational efficiency, making it an essential tool for researchers in these disciplines. At its foundation, DFT relies on the principle that the properties of a many-electron system can be derived from the electron density (ρ) instead of the many-body wave function (Verma and Truhlar, 2020). This method significantly simplifies computations by transforming the complex many-body problem into a functional of the electron density. As it was developed by Hohenberg and Kohn in 1964, it is an exact framework for describing an interacting electron gas in an external potential. For a solid or a molecule, the external potential is the Coulomb potential of the nuclei, which are treated as fixed according to the Born-Oppenheimer approximation (Yang et al., 2022b). The Hamiltonian of the many-electron

system can then be expressed as (Baptista et al., 2021):

$$\hat{H} = -\frac{1}{2} \sum_i \Delta_i^2 + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_i V_{\text{ext}}(\mathbf{r}_i) + E_{nn}. \quad (2.37)$$

The first term represents the kinetic energy, the second term accounts for the Coulombic repulsion between electron pairs and the third term corresponds to the energy of the electrons in the external potential. E_{nn} signifies the classical interaction between the nuclei and encompasses all other energy contributions that are independent of the electronic degrees of freedom. The stationary solution of the N-electron Schrödinger equation takes the form $\Psi(r_1, \dots, r_N)$. The electron density, $\rho(\mathbf{r})$ is expressed as the expectation value of the density operator $\hat{\rho}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$:

$$\rho(\mathbf{r}) = \frac{\langle \Psi | \hat{\rho}(\mathbf{r}) | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (2.38)$$

The total energy is defined by the expectation value of the Hamiltonian (Singh and Harbola, 2021):

$$E = \langle \hat{H} \rangle = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \quad (2.39)$$

2.4.1 The Hohenberg-kohn Theorems

The Hohenberg-Kohn theorems serve as the foundation of DFT, a powerful method in quantum mechanics for investigating the electronic structure of many-body systems. Introduced by Pierre Hohenberg and Walter Kohn in 1964, these theorems establish the theoretical basis for DFT. They are stated as follows (Hohenberg and Kohn, 1964b):

Theorem I: The ground-state particle density $\rho_0(\mathbf{r})$ uniquely determines the external potential $V_{\text{ext}}(\mathbf{r})$, except for an additive constant, for any system of interacting particles. Since the Hamiltonian is fully defined apart from a constant energy shift, the many-electron wavefunctions are also uniquely determined. Consequently, the entirety of the system's properties is dictated by the ground-state density $\rho_0(\mathbf{r})$.

Theorem II: A universal functional $E[\rho]$, formulated as a function of the electron density $\rho(\mathbf{r})$, can be defined and possesses validity for any arbitrary external potential $V_{\text{ext}}(\mathbf{r})$. Given a specific external potential $V_{\text{ext}}(\mathbf{r})$, the exact ground-state energy of the system is obtained at the global minimum of the energy functional. The electron density $\rho(\mathbf{r})$ that minimizes this functional is the exact ground-state density $\rho_0(\mathbf{r})$. Thus, the energy functional $E[\rho]$ is sufficient to uniquely determine both the exact ground-state energy and the exact ground-state electron density. In other words, the implication of this theorem provides a variational principle that allows one to compute the ground state energy by searching for the density that minimizes the

functional energy.

In short, the Hohenberg-Kohn theorems assert that there is a unique relationship between the ground-state density and the ground-state potential. As a result, the ground-state density corresponds to the global minimum of the energy functional $E[\rho]$, which can be found through a variational calculation.

Similar to the many-body Hamiltonian (Equation (2.37)), the total energy functional $E_{HK}(\rho)$ proposed by Hohenberg and Kohn is as follows:

$$E_{HK}[\rho] = T[\rho] + E_{int}[\rho] + \int V_{ext}(\mathbf{r})\rho(\mathbf{r}) d(\mathbf{r}) + E_{nn}. \quad (2.40)$$

Here, $T[\rho]$ represents the electron kinetic energy, and $E_{int}[\rho]$ refers to the interaction energy among the electrons. These terms can be combined into a universal functional of the density, meaning one that applies to all electron systems:

$$F_{HK}[\rho] = T[\rho] + E_{int}[\rho]. \quad (2.41)$$

$F_{HK}[\rho]$ is the total energy functional that describes the kinetic energy and interaction energy of the system of electrons, and it is valid for any electron system, independent of the external potential V_{ext} . It is a key part of the energy functional used in DFT to compute the total energy of the system. Provided this functional were known, the ground state of the system could be determined by performing a minimization of the total energy with respect to the electron density $\rho(\mathbf{r})$.

It is straightforward to generalize this to spin-polarized systems. A Zeeman term is introduced into the Hamiltonian, which differentiates between spin-up and spin-down electrons when a magnetic field is applied. In this event, two separate densities are defined, one for each spin, and each satisfies the Hohenberg-Kohn theorems independently. The density is given by $\rho(\mathbf{r}) = \rho(\mathbf{r}, \uparrow) + \rho(\mathbf{r}, \downarrow)$, and the spin density is expressed as $s(\mathbf{r}) = \rho(\mathbf{r}, \uparrow) - \rho(\mathbf{r}, \downarrow)$.

2.4.2 The Kohn-Sham Assumptions

The DFT, as proposed by Hohenberg and Kohn, has two major limitations: First, the functional F_{HK} is generally unknown, making a straightforward variational approach to determine the ground-state density unfeasible. Second, while there is a unique relationship between the ground-state density and the properties of the system, there is no known method for extracting these properties directly from the density (De Queiroz et al., 2021).

In 1965, Kohn and Sham suggested replacing the full interacting many-body problem with a simpler, non-interacting auxiliary system (Kohn and Sham, 1965). Their approach is based

on the assumption that the ground-state density of the interacting system can be represented by the ground-state density of an appropriately chosen non-interacting system. The central idea is to reintroduce orbitals for non-interacting electrons and express the many-body problem in terms of an exchange-correlation functional of the density. In this manner, the Hohenberg-Kohn functional, F_{HK} is reduced to the kinetic energy of the non-interacting fictitious electrons. The auxiliary Kohn-Sham Hamiltonian, which replaces Equation (2.37), is defined as follows (Aouina et al., 2023):

$$H_{\text{KS}}^\sigma = -\frac{1}{2}\nabla^2 + V_{\text{KS}}^\sigma(\mathbf{r}). \quad (2.42)$$

The spin index is denoted by σ . The N electrons, composed of $N_\uparrow$ spin-up and $N_\downarrow$ spin-down electrons, occupy the orbitals $\psi_i^\sigma(r)$ associated with the lowest eigenvalues, as governed by the Schrödinger-like Kohn-Sham equations:

$$(H_{\text{KS}}^\sigma - \varepsilon_i^\sigma) \psi_i^\sigma(\mathbf{r}) = 0 \quad (2.43)$$

here ε_i represent associated Kohn-Sham eigenvalues. The density of the Kohn-Sham system can be expressed as:

$$\rho(\mathbf{r}) = \sum_{\sigma} \sum_{i=1}^{N^\sigma} |\psi_i^\sigma(\mathbf{r})|^2 \quad (2.44)$$

and the Kohn-Sham kinetic energy can be expressed as:

$$T_s = \frac{1}{2} \sum_{\sigma} \sum_{i=1}^{N^\sigma} |\nabla \psi_i^\sigma(\mathbf{r})|^2. \quad (2.45)$$

The classical electrostatic interaction energy arising from the Coulombic repulsion of the electron density with itself is termed as the Hartree energy,

$$E_{\text{Hartree}}[\rho] = \frac{1}{2} \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'. \quad (2.46)$$

Using these components, the Hohenberg-Kohn total energy functional, Equation (2.40) can be expressed as:

$$E_{\text{KS}}[\rho] = T_s[\rho] + E_{\text{Hartree}}[\rho] + \int V_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}) d\mathbf{r} + E_{\text{nn}} + E_{\text{xc}}[\rho]. \quad (2.47)$$

All unquantified contributions arising from interactions and correlations are encapsulated in the so-called exchange-correlation functional $E_{\text{xc}}[\rho]$. In simple terms, $E_{\text{xc}}[\rho]$ accounts for all the errors introduced by approximating the system as non-interacting, except for the classical

Coulomb interaction between the electrons. The Kohn-Sham potential $V_{\text{KS}}^\sigma(r)$ can be written in terms of variations with respect to the density as:

$$V_{\text{KS}}^\sigma(\mathbf{r}) = V_{\text{ext}}(\mathbf{r}) + \frac{\delta E_{\text{Hartree}}}{\delta \rho(\mathbf{r}, \sigma)} + \frac{\delta E_{\text{xc}}}{\delta \rho(\mathbf{r}, \sigma)} = V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{xc}}^\sigma(\mathbf{r}). \quad (2.48)$$

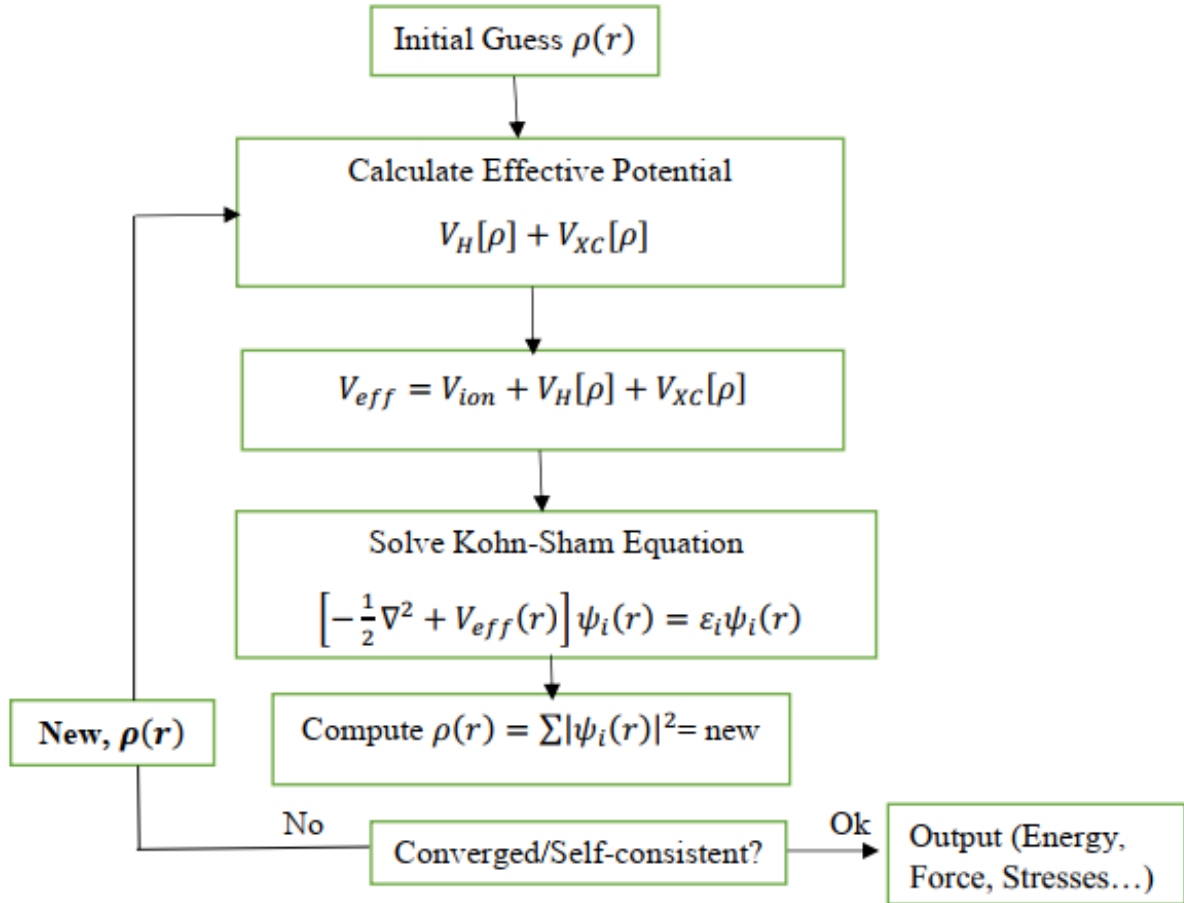


Figure 2.5: Schematic representation of the iterative algorithm used to solve the Kohn-Sham equations.

Since Equation (2.48) relies on the density obtained from the solution of Equation (2.43), the equations must be iterated to achieve self-consistency, beginning with an initial guess (such as a superposition of atomic densities). The primary algorithm commonly used in the QE package is illustrated in Figure 2.5. The Figure elaborates the self-consistent field (SCF) algorithm used in Kohn-Sham DFT calculations to determine the ground-state properties of a quantum system. The process begins with an initial guess of the electron density, $\rho(r)$. Using this guess,

the effective potential is calculated, which consists of the Hartree potential ($V_H[\rho]$) representing electron–electron repulsion and the exchange-correlation potential ($V_{xc}[\rho]$) accounting for quantum many-body effects. This effective potential (V_{eff}) also includes the ionic potential (V_{ion}) from the nuclei. The Kohn-Sham equations are then solved for the wave functions $\psi_r(\mathbf{r})$ and eigenvalues ε_i , using this V_{eff} . A new electron density is computed as $\rho(\mathbf{r}) = \sum |\psi_i(\mathbf{r})|^2$. This new density is compared to the old one to check for self-consistency. If they do not match within a defined threshold, the cycle repeats with the updated $\rho(\mathbf{r})$. Once self-consistency is achieved (i.e., the electron density no longer changes significantly), the algorithm terminates, and observable quantities like total energy, forces, and stresses are computed. This iterative method ensures that the output reflects the true ground-state properties of the system based on the self-consistent solution of the Kohn-Sham equations.

2.4.3 The Exchange-Correlation Function

The Kohn-Sham formalism presents an exact methodology for the determination of the ground-state electron density and total energy, without the introduction of approximations in its initial formulation. Nevertheless, the precise form of the exchange-correlation functional remains elusive. The Kohn-Sham equations have reformulated the major challenge of solving the full many-body problem, allowing for most of the electron system’s total energy to be computed accurately (Kasim and Vinko, 2021). Only a small portion, the exchange-correlation energy, needs to be approximated. Two primary approaches for deriving these approximations can be identified: empirical and non-empirical. Empirical functions are designed to closely match experimental data, whereas non-empirical functions are based on known physical constraints that the functional must satisfy (Ryabov et al., 2020).

2.4.3.1 Local Density Approximation (LDA)

The primary challenge now is to find an appropriate approximation for the exchange-correlation (XC) functional, $E_{xc}[\rho]$. Historically, the most significant approximation has been derived from the homogeneous electron gas (HEG), where electrons are assumed to move in a uniform positive background charge distribution created by the nuclei. The XC functional can now be expressed in the following simple form (Gritsenko et al., 2016):

$$E_{xc}^{\text{LDA}}[\rho] = \int \rho(\mathbf{r}) e_{xc}^{\text{HEG}}(\rho(\mathbf{r})) d\mathbf{r} \quad (2.49)$$

here, e_{xc}^{HEG} represents the energy density of the HEG. In this case, E_{xc} depends solely on the local value of the density, which is why this approximation is referred to as the LDA. Since the exchange contribution is known analytically, the energy density can be separated into exchange

and correlation components.

$$e_{xc}^{\text{HEG}}(\rho(\mathbf{r})) = e_x^{\text{HEG}}(\rho(\mathbf{r})) + e_c^{\text{HEG}}(\rho(\mathbf{r})). \quad (2.50)$$

The explicit expression for the correlation part remains unknown, so its determination requires an approximation. Initially, approximations based on perturbation theory were developed. More recent expressions are parameterized using data from quantum Monte Carlo simulations of the HEG (Olsen and Thygesen, 2013). Since the HEG resembles a perfect metal, the LDA is particularly suitable for metallic solids. Surprisingly, it also performs well for other systems, such as molecules, due to a systematic error cancellation (Rogers et al., 2016). However, the LDA tends to overestimate binding energies, leading to bond lengths that are too short. Examples of LDA exchange-correlation functionals include the implementations by Vosko, Wilk, and Nusair (VWN), or by Perdew and Wang (PW) (Olsen and Thygesen, 2012).

2.4.3.2 Generalized Gradient Approximation (GGA)

Electron density in real systems is usually inhomogeneous, resulting in non-zero density gradients. The LDA can be viewed as the zeroth-order approximation in a broader expansion involving the density and its derivatives. Consequently, extensions to the LDA have been developed that depend not only on the local value of the density but also on its gradients (He et al., 2014). So-called gradient expansion approximations aimed to include higher-order corrections in terms of $|\nabla\rho(r)|$, $\nabla^2\rho(r)$ etc., but these attempts typically did not improve the results. A significant advancement was made with the introduction of a more general functional involving $\nabla\rho(r)$, known as the GGA, which replaced the previous power series-like expansions. This GGA functional takes the following form (Luo et al., 2018):

$$E_{xc}^{\text{GGA}}[\rho] = \int f(\rho(\mathbf{r}), \nabla\rho(\mathbf{r})) d\mathbf{r}. \quad (2.51)$$

In general, no constraints are imposed on the functional f . GGA functionals are particularly useful for systems with a highly inhomogeneous electron density. In terms of applicability, their behavior can vary significantly depending on the choice of f . One of the most widely used GGA functionals in solid-state physics is the Perdew, Burke and Ernzerhof (PBE) implementation. The PBE functional improves upon LDA by reducing the overestimation of binding energies, but it often slightly overestimates bond lengths (Furness et al., 2020).

Many functionals, such as the PBE functional, are non-empirical, meaning they are not based on any experimentally measured values. This is a key feature of QE calculations, which rely solely on fundamental physics without the need for empirical data. However, there are also

empirical functionals that are designed to closely match experimental data (Peng and Perdew, 2017).

2.4.3.3 GGA+Hubbard potential(U)

GGA+U is a modification of the GGA that includes an on-site Coulomb interaction term (U) to enhance the description of systems with strongly correlated electrons, such as rare-earth compounds, transition metal oxides and actinides (Shokri et al., 2020). Since standard GGA and LDA underestimate electronic band gaps in semiconductors and insulators and unable to accurately represent magnetic properties and electronic configurations in systems with strong electron correlation, the addition of the Hubbard U term in GGA+U imposes a correction on incorrect orbital occupations, enhancing electron localization and providing a more accurate description of these systems (Derkaoui et al., 2024).

The Hubbard model, from which the GGA+U approach is built, has an additional on-site Coulomb interaction component to take into consideration the high repulsion between electrons in the same orbital. The expression for total energy in GGA+U is as follows (Orhan and O'Regan, 2020):

$$E_{GGA+U} = E_{GGA} + E_U - E_{DC} \quad (2.52)$$

where E_{GGA} , E_U and E_{DC} represent energy from the standard GGA functional, on-site Coulomb interaction energy and double-counting correction to avoid overestimating the interaction respectively. The double-counting adjustment eliminates interactions that GGA already takes into account.

In DFT calculations, GGA+U method has several advantages, especially for systems with strongly correlated electrons. Materials containing localized d - or f -electrons, such as transition metal oxides and rare-earth compounds, are better represented by GGA+U. It improves the treatment of these materials' magnetic properties, electronic structures and behavior by taking into account electron-electron interactions within confined orbitals (Sirajuddeen et al., 2020). The band gaps of semiconductors and insulators, particularly those with tightly coupled electrons, are frequently underestimated by standard GGA. This is corrected by GGA+U, which provides more accurate estimates for electronic band gaps. The technique improves the description of magnetism in materials like transition metal oxides and other magnetic materials where the electron spin is important (Jafarova and Orudzhev, 2021). By localizing the electron density within particular orbitals, it is able to forecast magnetic moments and spin states with high accuracy. While offering better precision for correlated materials, GGA+U is still comparatively computationally efficient when compared to other more sophisticated techniques like hybrid functionals or Green's function and Wannier functions for GW interpolation computa-

tions (Timrov et al., 2022). Because of this, it strikes a reasonable balance between computing cost and precision, particularly for big systems. In order to ensure that the occupation of orbitals, particularly d or f , is more realistic, GGA+U aids in accurately characterizing the electronic configurations of systems containing localized electrons. Depending on the system, the value of U can be changed or computed, providing flexibility in adjusting the degree of correlation used in the computations (Mesbahi et al., 2018). By selecting suitable U values that are optimum for the particular system under study, the approach can be modified to work with a variety of materials. With built-in support for GGA+U, many DFT software programs such as Vienna Ab initio Simulation Package (VASP) and QE make it simple to use and employ in a range of simulations (Tesch and Kowalski, 2022).

Despite being an effective technique for enhancing the description of highly coupled systems, GGA+U has a number of drawbacks. For example, the U value selection has a significant impact on GGA+U accuracy. This value is not always the same and frequently needs to be ascertained empirically or by extra computations, which can lead to ambiguity and inconsistent results across various systems. Inaccurate predictions of electronic and magnetic properties may result from selecting the wrong value for U . In addition, even though GGA+U works best with materials like transition metal oxides, rare-earth compounds and actinides that have strongly correlated d - or f -electrons it may yield results comparable to regular GGA for materials with negligible electron correlation, providing no discernible enhancement. Furthermore, because GGA+U relies on equilibrium DFT calculations, it may not be accurate when simulating processes that are out of equilibrium, such as excited-state dynamics, photoemission or non-adiabatic effects. In these situations, alternative techniques, including time-dependent DFT (TDDFT), may be more appropriate (Falletta and Pasquarello, 2022; Kirchner-Hall et al., 2021).

2.4.4 An Instrument for DFT Calculations: Quantum ESPRESSO (QE)

QE is a popular open-source set of algorithms for nanoscale materials modeling and electronic structure computations. Pseudopotentials, plane-wave basis sets and DFT form its foundation, which makes it ideal for researching materials having periodic boundary conditions (Shuaibu et al., 2021). Its abbreviation, "Quantum opEn Source Package for Research in Electronic Structure, Simulation and Optimization," is what it stands for. The very flexible computational software, QE solves the Kohn-Sham equations of DFT by implementing plane-wave basis sets and pseudopotentials. The following properties of QE make it a great option for studying HH compounds from fundamental principles (Marcolongo et al., 2021): The Perdew-Burke-Ernzerhof (PBE), GGA, GGA +U and hybrid functionals are examples of state-of-the-art

exchange-correlation functionals that QE supports, which provide precise predictions of structural, electronic, mechanical, optical, thermal and magnetic properties. QE is parallel computing optimized and therefore it can make effective use of contemporary supercomputers such as High-Performance Computing (HPC) efficiency and drastically cut down on the amount of time needed to compute big systems like HH compounds (Pasanaje et al., 2021). QE provides strong support for spin-polarized DFT calculations for materials such as HH compounds, whose spintronic applications depend on characteristics like magnetic ordering and spin polarization. Additional capabilities including band structure computations, phonon dispersion calculations, DOS analysis, elastic constant evaluation and optical property predictions are made possible by QE. These characteristics are essential for a comprehensive analysis of HH materials (Beck et al., 2022). A sizable scientific community supports and uses QE, which is an open-source program. It has become a popular tool among material scientists worldwide because to the availability of well-documented tutorials and modules (Matsugatani et al., 2021). The structural, mechanical, electronic, optical and magnetic properties of the RhYZ (Y=Zr, Ir, Nb; Z=Li, As, Sb, Si) HH compounds were examined in this work using QE. Because of its strong DFT implementation, excellent precision and demonstrated dependability, QE was chosen for this investigation. Since the code specifically allows the use of a number of exchange-correlation functionals (LDA, GGA and GGA+U), it meets the current study's methodological standards (Çipiloğlu and Özkurt, 2020).

2.4.5 Periodic Boundary Conditions

The primary focus of solid-state physics is the understanding of crystals, which are idealized as periodic systems, at least in theory. In these systems, the nuclei are arranged in a perfectly ordered periodic lattice, making the potential in which the electrons move also periodic. As a result, the entire problem becomes periodic, allowing the use of periodic boundary conditions. This inherent periodicity enables the derivation of macroscopic properties of a crystal based on its primitive unit cell, which comprises a minimal number of atoms. For a periodic potential $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R})$, where $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ ($n_j = 0, 1, 2, \dots$) being an arbitrary translation along the lattice vectors $\mathbf{a}_j$, the Bloch theorem asserts that solutions to the Schrödinger equation take the following general form (Henyš et al., 2019; Tian et al., 2019):

$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{R})u_{\mathbf{k}}(\mathbf{r}). \quad (2.53)$$

The function $u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$ has the same periodicity as the crystal lattice (and hence the potential $V(\mathbf{r})$). Therefore, except for a phase factor, the wavefunctions are also periodic and

given as:

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{k} \cdot \mathbf{R})\psi_{\mathbf{k}}(\mathbf{r}). \quad (2.54)$$

This implies that the probability distribution and consequently the electron density, is also periodic. The Kohn-Sham equations can be solved independently for each $\mathbf{k}$ in the first Brillouin zone of reciprocal space, resulting in a band structure with energy eigenvalues. In theory, we would need to integrate over the entire Brillouin zone. However, in practice, this integration is often approximated by a weighted summation, as the wavefunctions change slowly with $\mathbf{k}$. The electron density is thus computed by (Barclay and Zhang, 2021):

$$\rho(\mathbf{r}) = \frac{1}{N_k} \sum_{\mathbf{k}} \rho_k(\mathbf{k}). \quad (2.55)$$

Here, $\rho_k(\mathbf{r})$ represents the electron density for a specific $\mathbf{k}$ -point, and N_k is the total number of $\mathbf{k}$ -points. The accuracy of the numerical results heavily depends on a proper selection of N_k . Fortunately, the symmetries of the crystal lattice can be utilized to simplify the process. The summation over the Brillouin zone can be reduced to an irreducible wedge and the result can then be extended to the entire Brillouin zone using symmetry operations. However, it is essential to ensure convergence for the chosen $\mathbf{k}$ -point mesh for each system individually in order to obtain reliable results (Colbrook, 2020).

Materials and Methods

Computational Methods

To investigate the structural, electronic, magnetic, mechanical and optical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Sb, Si) HH compounds, which are our model materials, first-principles calculations were performed within the framework of DFT. DFT is a powerful quantum mechanical technique for examining the ground-state properties of many-electron systems like atoms, molecules and solids, by focusing on the system's electron density rather than solving the complex many-body wave function directly. It uses an approximation of the exchange-correlation energy functional to solve the Kohn-Sham equations. The calculations were carried out using the QE package, a widely used suite of programs for electronic structure calculations and materials modeling. It is an open-source software suite for performing quantum mechanical simulations of materials based on DFT, plane-wave basis sets and pseudopotentials. It is widely used in computational materials science for calculating electronic structure, magnetic properties, structural optimization and vibrational properties. QE supports advanced features like DFT+U, spin-polarized calculations and non-collinear magnetism and includes modules for tasks like phonon calculations, charge density analysis and molecular dynamics. Highly parallelized for efficient computation, QE is a powerful and versatile tool for exploring the properties of crystals, surfaces, molecules and nanostructures. It stands for "Quantum open-Source Package for Research in Electronic Structure, Simulation and Optimization."

For the calculation of electronic and magnetic properties, the GGA+U approach was employed in addition to the standard GGA predictions to achieve more realistic and accurate results, because our systems have strongly localized d-electrons elements such as Rh, Nb, Ir and Zr, where U is the Hubbard correction (potential). The GGA method, based on the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, provides a good starting point for a given properties calculations. However, it is well-known that GGA underestimates the effects of electron localization, especially in systems with partially filled d- or f-orbitals. To overcome this limitation, the GGA+U approach introduces the U term, which corrects the on-site Coulomb interactions of localized electrons, improving the description of electronic states and magnetic moments. In this study, the Hubbard U values for the d orbitals of Rh, Zr, Ir and Nb in the RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compound were calculated using the first-principles linear response approach developed by Cococcioni and de Gironcoli (Cococcioni and De Gironcoli, 2005), as implemented in the hp.x module of QE. The process began with SCF calculation

performed using a negligibly small U value ($1 \cdot 10^{-10}$) to obtain the unperturbed ground state. Following this, the `hp.x` code was employed with a $2 \times 2 \times 2$ q-point mesh and a strict convergence threshold ($\text{conv.thr.chi} = 1 \cdot 10^{-6}$) to apply localized perturbations and compute the system's bare and screened response functions. The Hubbard U values were derived from the difference between the inverse of the bare and the fully screened susceptibility matrices. Upon completion, the final U parameters were written to the prefix name `Hubbard.parameters.dat` file, which contains the numerically obtained U values for each relevant atomic species. This methodology ensures that the computed U values are both physically meaningful and specifically adapted to the electronic structure of the compound under investigation.

The calculated U values that were used for the calculation of electronic and magnetic properties are listed in the Table 3.1 below. This systematic approach ensures that the calculated electronic and magnetic properties accurately reflect the materials' intrinsic properties, providing a reliable basis for analyzing their potential applications. The inclusion of U in GGA+ U allowed for an improved description of localized states, the correction of band gap underestimation and more precise predictions of magnetic moment distributions compared to standard GGA. As we observed from Table 3.1 below, the same element, e.g., Rh have different values of U in different compounds. This is due to differences in the local electronic environment and chemical bonding in each compound. The U is not an intrinsic property of an element but is instead environment dependent. The surrounding atoms (Sb or Si) in RhNbSb and RhNbSi , for instance, have different electronegativity and bonding properties, which affect the electronic distribution around Rh and Nb and change the strength of electron-electron interactions. Furthermore, the symmetry and type of nearby atoms have an impact on the crystal field potential that the d-electrons of Rh or Nb experience. The splitting of d orbitals and the intensity of their interactions vary depending on the crystal field environments created by different chemical surroundings, such as those introduced by Sb and Si atoms.

For RhZrZ ($Z = \text{Li, As, Sb}$) HH compounds ultrasoft pseudopotentials (USPP) were employed to describe the electron-ion interactions, but for the other remaining HH compounds the projector augmented wave (PAW) pseudopotentials were used to interpret the interaction of the electron-ionic core. In quantum mechanical simulations, pseudopotentials are a computational tool that makes it easier to handle atoms' core-electrons while concentrating computing resources on valence electrons, which are mostly responsible for regulating chemical bonds and material properties. Because USPPs are flexible in defining valence wave functions, they provide a reduced plane-wave basis set, especially for heavy elements and transition metals where localized d- or f-states require careful handling. For materials where fine resolution of chemical and bonding features is necessary, PAW pseudopotentials, on the other hand, provide an accu-

Table 3.1: Calculated U values of d-block elements in their respective compounds

HH compound	Rh(U)(eV)	Zr(U)(eV)	Ir(U)(eV)	Nb(U)(eV)
RhZrSb	5.2675	2.3144		
RhZrAs	5.2764	2.3464		
RhZrLi	5.2682	2.3143		
RhZrSi	4.8894	2.3137		
RhIrLi	4.8595		3.9104	
RhIrAs	5.2202		4.0239	
RhIrSi	5.2133		4.1434	
RhIrSb	5.1964		4.0386	
RhNbLi	4.4293			2.6348
RhNbAs	4.9996			2.6742
RhNbSi	5.2341			2.8648
RhNbSb	5.0601			2.6945

rate reconstruction of all-electron wave functions by merging pseudopotential and all-electron approaches.

For all HH compounds studied, norm-conserving (NC) pseudopotentials were employed for the optical property calculations, as they are more suitable for accurately capturing these properties. The process began with SCF calculation (scf.in) to obtain the ground-state charge density. Subsequent post-processing steps involved analyzing electronic transitions through the joint density of states (JDOS) using jdost.in, and computing the complex dielectric function via (spectra.in) by applying the epsilon.x module. The outputs included the real (epsr.dat) and imaginary (epsi.dat) components of the dielectric function, as well as the energy loss (eels.dat) and inverse dielectric (ieps.dat) functions. The results of dielectric functions were then used to calculate essential optical parameters such as reflectivity, refractive index, extinction coefficient, absorption coefficient and optical conductivities, offering valuable insights into electronic excitation mechanisms and light-matter interactions in the materials studied.

The crystallographic information file (CIF) of these HH compounds were obtained from the materials project database. The geometry of these HH compounds were optimized by minimizing the total energy and forces. The convergence criteria for total energy 10^{-5} Ry and for forces 10^{-4} Ry/Bohr were used. Convergence tests were done for kinetic energy cutoff, k-points and lattice parameter followed by optimization before structural, mechanical, electronic, optical and magnetic properties calculations. For RhZrZ (Z = Li, As, Sb) compounds, a mesh k-points of 14x14x14 was taken in the first irreducible Brillouin zone but for the calculation of PDOS a more dense k-points of 42x42x42 was used and plane wave basis cutoff energy of 100 Ry was employed. For other remaining HH compounds, a mesh k-point of 12x12x12 was taken

in the first irreducible Brillouin zone but for the calculation of PDOS a more dense k-points of 36x36x36 was used and plane wave basis cutoff energy of 80 Ry was employed. For all HH compounds under our current work different values of lattice parameters were used, where these values were obtained after performing the convergence test. Moreover, using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm, variable cell relaxation was used to structural optimization that involves finding the equilibrium geometry that minimizes the total energy of the system. The optimized structure corresponds to the configuration where the forces acting on all atoms are close to zero, indicating mechanical stability.

To examine the dynamical stability and some vibrational properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds, phonon calculations were carried out using Density Functional Perturbation Theory (DFPT) within the QE suite. The relaxed structures obtained from previous geometry optimizations served as the basis for these simulations. A fine Monkhorst-Pack k-point grid and appropriate energy cutoffs were adopted to ensure reliable convergence of the ground-state calculations. Phonon modes were computed on a regular q-point mesh using the ph.x code, followed by the extraction of interatomic force constants through the q2r.x utility. The phonon dispersion relations were then derived by interpolating these force constants along selected high-symmetry paths using matdyn.x. Furthermore, the phonon density of states (PhDOS) was evaluated by activating the DOS calculation feature in matdyn.x.

For mechanical properties calculations energy-strain method were used. Since all these HH compounds are structurally cubic, only three independent elastic constants (C_{11} , C_{12} and C_{44}) are sufficient for the study of mechanical property of the compound because all other mechanical parameters can be readily obtained from these elastic constants. Each cubic lattice structure was subjected to strains of 0%, $\pm 1\%$, $\pm 2\%$, $\pm 3\%$, and $\pm 4\%$. The resulting minimum total energies, E_0 , were then fitted against these strains using parabolic equations of $\frac{\Delta E}{V_0}$ according to the relation provided below:

$$\frac{\Delta E}{V_0} = \begin{cases} 3(C_{11} - C_{12})\delta^2 \\ \frac{3}{2}(C_{11} + 2C_{12})\delta^2 \\ \frac{1}{2}C_{44}\delta^2 \end{cases} \quad (3.1)$$

with V_0 corresponds to minimum volume of the optimized compound. Finally, we used other supportive packages such as xcrysden, vesta and xmgrace for structural visualization and study, graphical analysis, editing and plotting purposes.

Results and Discussion

4.1 Structural Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Compounds

The structural optimizations of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds in their different atomic arrangements were carried out prior to the calculation and analysis of their electronic, mechanical, optical and magnetic properties. Many theoretical and experimental works show that properties of any HH compounds greatly depend on their atomic configuration (Peng et al., 2025). Thus, for the study of structural properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds, three most common types of their atomic arrangements, namely type I (α phase), type II (β phase) and type III (γ phase) were considered. The positions of atoms in these types of atomic arrangements are illustrated in Table 4.1. These atomic configurations of the compounds are shown in Figure 4.1. The aim of considering these three types of atomic arrangement is to identify structurally the most stable atomic configuration relative to the other.

Table 4.1: Atomic site occupancies in three structural variants of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds.

Phases	Rh	Y	Z
α phase	(1/4, 1/4, 1/4)	(1/2, 1/2, 1/2)	(0, 0, 0)
β phase	(1/2, 1/2, 1/2)	(0, 0, 0)	(1/4, 1/4, 1/4)
γ phase	(0, 0, 0)	(1/4, 1/4, 1/4)	(1/2, 1/2, 1/2)

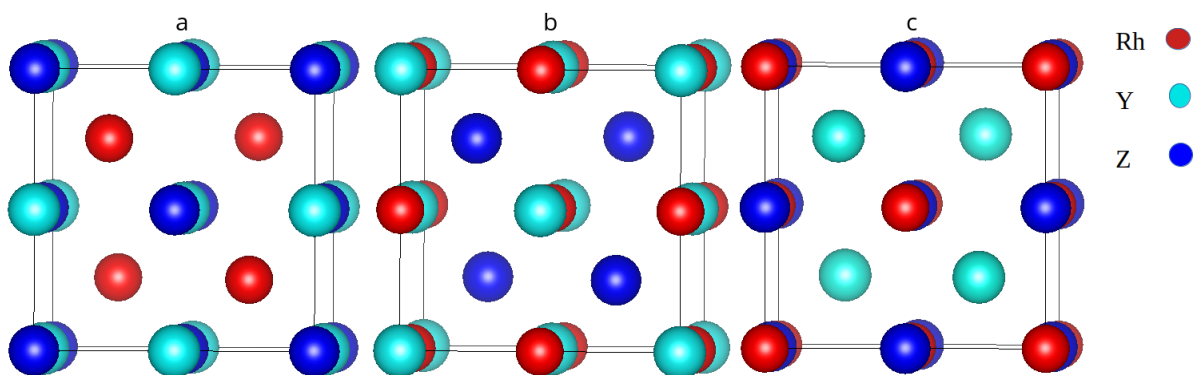


Figure 4.1: Three typical kinds of atomic arrangements for RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds created by VESTA. α phase (a), β phase (b) and γ phase (c).

4.1.1 Lattice Parameters and Structural stability

The calculated equilibrium lattice constants (a_0), minimum volumes (V_0), minimum energies (E_0), bulk modulus (B) and its pressure derivatives (B') for the three types of atomic arrangements of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds by using the most known Birch-Murnaghan equation of state, Equation (2.1) are illustrated in the Table 4.2 below. For the majority of systems, specifically RhZrZ (Z = Li, As, Si, Sb), RhNbZ (Z = Li, As, Si, Sb) and RhIrLi, the α -phase exhibits the lowest total energy (E_0), indicating it as the structurally most stable configuration. In contrast, RhIrZ (Z = As, Si, Sb) prefer the β -phase, reflecting a structural phase dependence on the Ir-site element. Lattice constants (a_0) and unit cell volumes (V_0) generally increase with the atomic size of the Z element, as expected, with Sb-containing compounds showing the largest values. The calculated bulk moduli (B) vary considerably, ranging from approximately 81 GPa to over 221 GPa, indicating significant differences in mechanical stiffness across compounds and phases. Typically, Ir- and Nb-based compounds demonstrate higher bulk moduli compared to Zr-based ones, suggesting greater resistance to compression. Noteworthy examples include RhIrZ (Z = As, Si) in the β -phase and RhNbSi in the α -phase, with the highest B values of 209.9 GPa, 221.1 GPa and 186.3 GPa, respectively, marking them strong candidates for mechanically demanding applications. The pressure derivatives (B') fall within a stable range of ~ 3.7 to 6.3 reported in (Behera et al., 2023), supporting their elastic reliability under pressure. Furthermore, for RhZrZ (Z = As, Si, Sb) and RhNbSi compounds, the calculated lattice parameters show good agreement with existing theoretical and experimental data (Table 4.2), enhancing the validity of these results. Generally, the findings reaffirm the α -phase as the ground state for most compounds and underscore the potential for tailoring mechanical behavior and structural stability through targeted elemental substitution.

Figure 4.2 illustrates the variation of total energy with respect to lattice constant for RhYZ (Y = Zr, Nb, Ir; Z = Li, As, Si, Sb) HH compounds across three structural phases (α , β , γ). In most cases, particularly for RhZrZ (Z = Li, As, Si, Sb), RhNbZ (Z = Li, As, Si, Sb) and RhIrLi in the α -phase (black curve) show the lowest energy minimum, signifying it as the most structurally stable configuration. Conversely, RhIrZ (Z = As, Si, Sb) demonstrate their lowest energy in the β -phase (red curve), indicating a shift in structural stability depending on the specific atomic combination. The curvature and depth of the energy wells also reflect differences in mechanical stiffness, where narrower, deeper wells (e.g., RhIrAs, RhIrSi and RhNbSi) suggest greater incompressibility and higher bulk moduli, consistent with Table 4.2 results. In general, this Figure supports the predominance of the α -phase as the ground state for most compositions while highlighting the phase-dependent stability influenced by Y and Z site substitutions. Figure 4.2 supports the structural stability conclusions drawn from the data in Table 4.2.

Table 4.2: Calculated equilibrium lattice (a_0), minimum volume (V_0), minimum energy (E_0), bulk modulus (B) and its pressure derivatives (B') for three structural types of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds.

HH compound	Phases	$a_0(a.u)$	$V_0(a.u^3)$	$E_0(Ry)$	$B(GPa)$	B'
RhZrLi	α	11.6207	392.32	-340.76564	84	4.30
	β	11.0293	335.42	-340.70793	96.8	4.07
	γ	11.6674	397.07	-340.69158	81.1	3.72
RhZrAs	α	11.5293	383.13	-346.54874	145.9	5.38
		11.5462			153.62	4.52 (Manzoor et al., 2024)
	β	11.5365	383.85	-346.46188	135.8	5.40
RhZrSi	γ	11.8512	416.12	-346.40785	107.4	4.53
	α	11.4812	378.35	-824.28670	142.6	3.87
		11.4139			151.12(Rached et al., 2023)	
RhZrSb	β	11.3965	370.04	-824.23575	137.6	3.78
	γ	11.7323	403.73	-824.13825	111.4	3.67
	α	11.9552	427.18	-345.98118	137.8	4.64
RhIrLi		11.8296 (Tobola et al., 2003), Exp.				
		11.9619 (Benzoudji et al., 2019)				
		11.8316 (Dwight, 1974), Exp.				
RhIrAs	β	12.1538	448.82	-345.82081	110.2	4.42
	γ	12.3246	468.02	-345.80952	97.0	4.08
RhIrSi	α	10.9275	326.21	-1206.68924	134.0	4.35
	β	10.4102	282.05	-1206.62818	135.5	5.23
	γ	10.9546	328.65	-1206.68258	131.1	4.32
RhIrSb	α	11.2456	355.54	-1367.63016	160.0	5.06
	β	10.8882	322.71	-1367.74978	209.9	6.32
	γ	11.2303	354.08	-1367.68306	169.4	5.20
RhNbLi	α	11.0166	334.26	-1238.42732	182.1	4.82
	β	10.6422	301.33	-1238.57796	221.1	5.56
	γ	11.0344	335.88	-1238.46943	186.5	4.76
RhNbAs	α	11.5841	388.62	-1539.34620	150.8	5.35
	β	11.4563	373.90	-1539.39770	168.0	5.57
	γ	11.6238	392.63	-1539.38281	155.5	5.19
RhNbSi	α	11.2772	358.54	-819.45329	107.9	4.95
	β	10.7181	307.82	-819.37449	120.3	4.05
	γ	11.2822	359.02	-819.39770	102.9	4.05
RhNbSb	α	11.3493	365.46	-980.52131	159.5	4.67
	β	11.2886	359.6	-980.48141	162.4	4.72
	γ	11.5151	381.72	-980.46926	142.2	4.72
RhNbSb	α	11.1502	346.56	-851.31002	186.3	4.58
		11.1683 (Ahmed et al., 2024)				5.21
	β	11.1590			193.13	4.57(Gurunani and Gupta, 2024a)
RhNbSb	γ	11.0897	340.96	-851.22902	168.4	3.77
		11.3396	364.53	-851.17688	146.1	5.01
	α	11.7524	405.81	-1152.19053	153.0	4.36
RhNbSb	β	11.8995	421.24	-1152.07581	133.0	5.42
	γ	11.9803	429.87	-1152.10300	126.3	5.45

4.1.2 Formation Energy and Thermodynamic stability

Formation energy represents the energy needed to build a compound from its constituent elements in their most stable states, and therefore it is an important parameter in determining its thermodynamic stability of materials like RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb). A material is said to be thermodynamically stable and amenable to experimental synthesis when its formation energy is negative (Srinivasan et al., 2024). The most stable phase can be identified by analyzing several atomic configurations and comparing formation energies. This aids in the prediction of potential phase transitions under various pressure and temperature ranges.

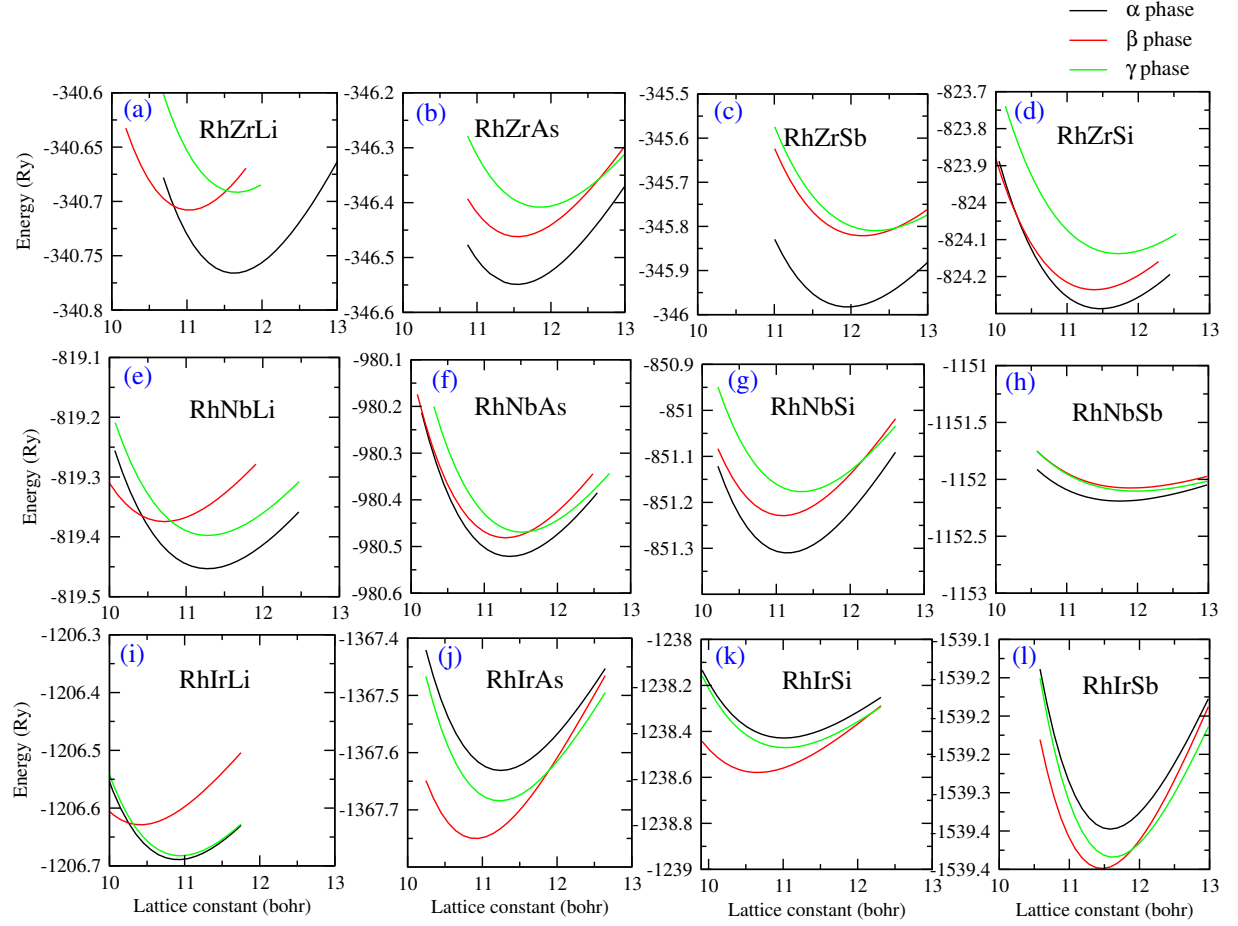


Figure 4.2: Energy vs lattice constant for three atomic configurations of RhYZ (Y = Zr, Nb, Ir; Z = Li, As, Si, Sb) compounds.

Table 4.3: Total energies of individual elements (E_{ind}) calculated using USPP and PAW pseudopotentials.

Element	E_{ind} (eV)	
	PAW	USPP
Rh	-470.17407732	-226.47054679
Zr	-307.21183268	-99.40317987
Ir	-721.54514287	—
Nb	-334.24603482	—
Li	-15.009702113	-14.84947284
As	-175.95287672	-20.41353038
Si	-46.68824353	—
Sb	-347.64254171	-19.86599753

Furthermore, the rivalry between various structural arrangements affects the stability of the material and offers more profound understanding of its phase stability. Since stability is crucial in determining the performance of RhYZ compounds in spintronic and optoelectronic devices, an understanding of these thermodynamic properties is necessary for optimizing these compounds for real-world applications. The total energies of the component elements at their most stable point is indicated in Table 4.3 whereas the total and formation energies of each compound in their three types of atomic arrangements are shown in Table 4.4.

Except RhIrLi, all other HH compounds (Table 4.4) have negative formation energy at least in one of their atomic configuration (phase). Negative value of formation energy indicates that these compounds can not be easily decomposed in to its component elements and can be experimentally synthesized. From structural stability (Table 4.2), RhYZ (Y=Zr, Nb; Z = Li, As, Si, Sb) are all structurally most stable in their α phase. These compounds have low (negative) formation energy in this phase as compared to other phases implying that they are thermodynamically most stable in this α phase. Furthermore, RhIrZ (Z = As, Si, Sb) compounds are structurally most stable in β phase, where they have low (negative) formation energies in this phase as compared to other phases. Structural and thermodynamical stability agreements in the same phase were also reported in (Rached et al., 2022). Thus, from these observations, we conclude that a compound which is structurally most stable in a given phase has lowest (negative) formation energy implying that it is also thermodynamically most stable in this phase compared to other phases. According to our DFT prediction, RhIrLi compound is not thermodynamically stable because its formation energies in its all three phases are positive. This compound can easily decompose into its constituent elements making it difficult to synthesize experimentally. The relatively low E_f values, especially in Zr- and Nb-containing compounds, are consistent with previous works as indicated in the Table 4.4, reinforcing the reliability of the present results. These outcomes highlight both the thermodynamic stability of most Rh-based HH compounds and the tunability of phase stability through targeted elemental substitution.

A structurally stable system, such as HH compounds with a low negative formation energy, has a number of advantages over a structurally unstable system. For example, although stable systems can be developed and grown as bulk or thin films, unstable structures may disintegrate or phase-separate into secondary phases. Consistent material quality during manufacture is ensured via a well defined stability range. Long-term applications can benefit from structurally and thermodynamically stable compounds because they are more resistant to degradation; however, unstable phases may experience structural phase changes, which over time could result in a decline in performance.

Table 4.4: Formation energies of the RhYZ (Y = Zr, Ir, Nb Z = Li, As, Si, Sb) HH compounds.

HH compound	Phases	E_{RhYZ} (Ry)	E_f
RhZrLi	α	-340.76564	-0.0424405
	β	-340.70793	0.0152695
	γ	-340.69158	0.0316195
RhZrAs	α	-346.54874	-0.26148296 -1.007(Manzoor et al., 2024)
	β	-346.46188	-0.17462296
	γ	-346.40785	-0.12059296
RhZrSb	α	-345.98118	-0.24145581 -1.003(Manzoor et al., 2024)
	β	-345.82081	-0.08108581
	γ	-345.80952	-0.06979581
RhZrSi	α	-824.28670	-0.21254647 -0.724 (Manzoor et al., 2024)
	β	-824.23575	-0.16159647
	γ	-824.13825	-0.06409647
RhIrLi	α	-1206.68924	0.039682303
	β	-1206.62818	0.100742303
	γ	-1206.68258	0.046342303
RhIrAs	α	-1367.63016	0.04193691
	β	-1367.74978	-0.07768309
	γ	-1367.68306	-0.01096309
RhIrSi	α	-1238.42732	-0.01985628
	β	-1238.57796	-0.17049628
	γ	-1238.46943	-0.06196628
RhIrSb	α	-1539.34620	0.0155619
	β	-1539.39770	-0.0359381
	γ	-1539.38281	-0.0210481
RhNbLi	α	-819.45329	-0.023475747
	β	-819.37449	0.055324253
	γ	-819.39770	0.032114253
RhNbAs	α	-980.52131	-0.14832114
	β	-980.48141	-0.10842114
	γ	-980.46926	-0.09627114
RhNbSi	α	-851.31002	-0.20166433 -1.4905 (Ahmed et al., 2024)
	β	-851.22902	-0.12066433
	γ	-851.17688	-0.06852433
RhNbSb	α	-1152.19053	-0.12787615
	β	-1152.07581	-0.01315615
	γ	-1152.10300	-0.04034615

For applications in spintronics and optoelectronics, stability guarantees a constant electronic band structure. In contrast, unstable systems may display unexpected electronic states, rendering them unsuitable for device applications. Stable structures exhibit strong elastic and mechanical properties, making them resistant to deformation under stress. However, unstable materials may be brittle or mechanically weak, limiting their practical use. Stability ensures that the material remains functional across a wide temperature and pressure range. Unstable compounds may decompose or react with the environment, reducing efficiency (Krez et al., 2015). Therefore, for the study of mechanical, electronic, optical and magnetic properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds both structurally and thermodynamically most stable phase were considered.

4.1.3 Phonon Dispersion and Dynamical Stability

Phonon dispersion relations, which depict the variation of phonon frequencies as a function of wave vectors throughout the Brillouin zone, are key to evaluating the dynamical stability of crystalline materials since stability is confirmed by the absence of imaginary (negative) frequencies. Additionally, the phonon DOS provides insight into how vibrational modes are distributed across different frequencies, offering valuable information on lattice dynamics and thermodynamic properties such as specific heat. To compute phonon properties from first principles, two widely used methods are DFPT and the finite displacement approach. Both techniques are based on DFT and enable precise calculation of force constants and the dynamical matrix (Mohabbi et al., 2023). In the present work, phonon calculations were carried out to investigate the dynamical stability and vibrational behavior of Rh-based HH compounds, thereby deepening the understanding of their potential for use in advanced functional applications.

Figure 4.3 provides a detailed representation of the phonon dispersion relations and corresponding DOS for the RhZrZ compounds, where Z denotes various elemental substitutions (Li, As, Si, Sb). The phonon dispersion and DOS plots for the compounds collectively confirm their dynamical stability, as evidenced by the absence of imaginary phonon modes across the entire Brillouin zone. This positive-definite phonon spectrum indicates that all four compounds are dynamically stable and free from lattice instabilities. In each case, the dispersion curves display a distinct separation between acoustic and optical branches, a characteristic typically observed in systems composed of atoms with significantly different masses. Notably, phonon band gaps are identified in RhZrLi ($\sim 110\text{--}130\text{ cm}^{-1}$), RhZrAs ($\sim 160\text{--}190\text{ cm}^{-1}$) and RhZrSi ($\sim 125\text{--}165\text{ cm}^{-1}$), arising from mass and bonding mismatches among the constituent atoms. These gaps manifest in the phonon DOS as frequency ranges devoid of vibrational states, reflecting a decoupling between low-frequency acoustic modes and high-frequency optical modes. Such

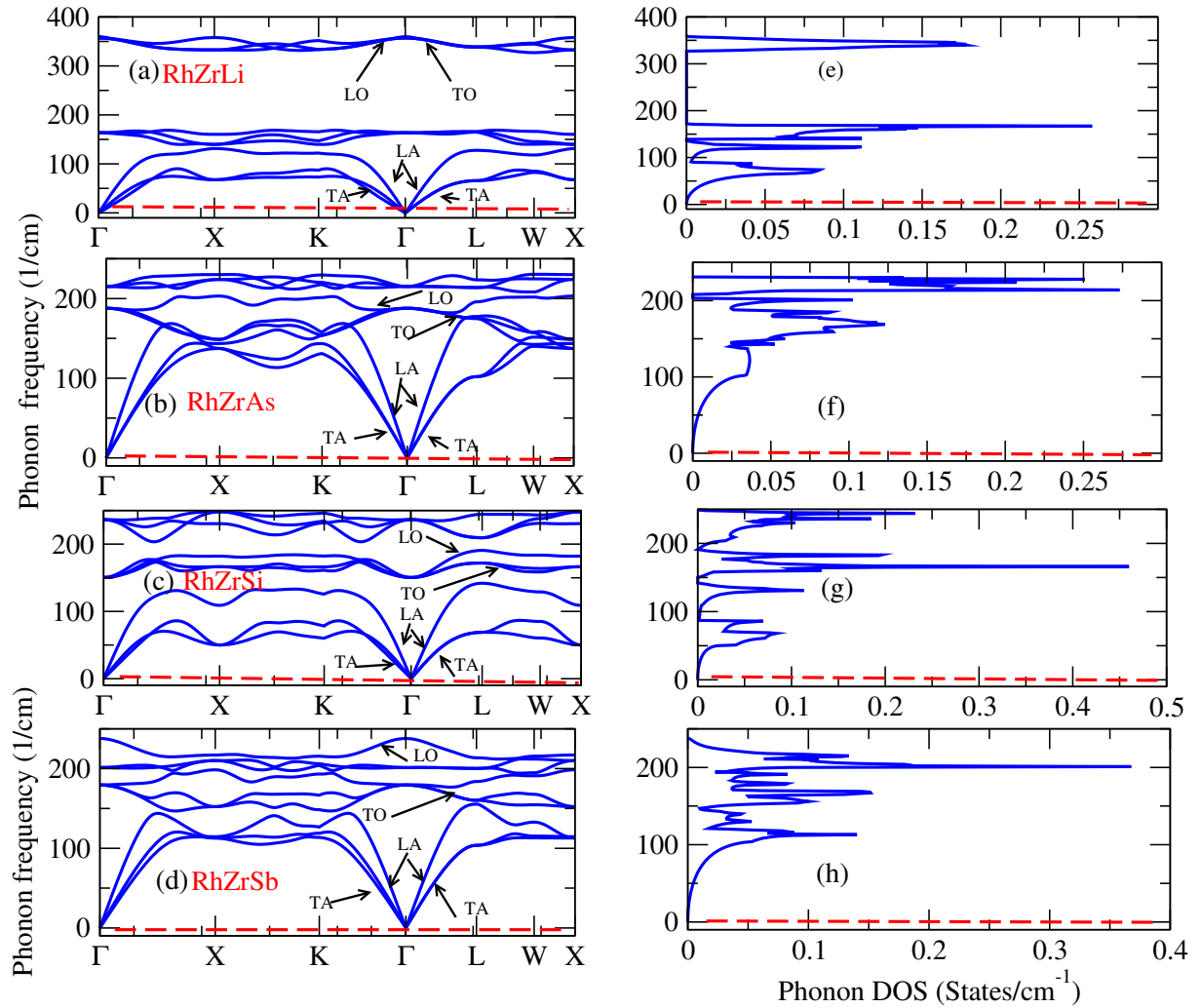


Figure 4.3: Phonon dispersion (a, b, c, d) and DOS (e, f, g, h) for RhZrZ (Z = Li, As, Si, Sb) HH compounds respectively.

decoupling is advantageous for thermoelectric performance, as it can suppress phonon-phonon scattering and thereby reduce lattice thermal conductivity. Although RhZrSb does not exhibit a well-defined phonon gap, its vibrational spectrum remains dynamically stable, characterized by a broad frequency range and prominent high-frequency peaks above 200 cm^{-1} , likely attributable to strong local interactions involving between the atoms. Dynamical stability and phonon dispersion as well as phonon Dos we reported here are in fine agreement with the previous results on some related HH compounds in (Wu et al., 2024).

Figure 4.4 provides an in-depth examination of the phonon dispersion relations and phonon DOS for the RhIrZ series of HH compounds, where Z corresponds to different elemental substitutions: Li, As, Si, and Sb. The sub-figures on the left side (a, b, c, d) illustrate the phonon

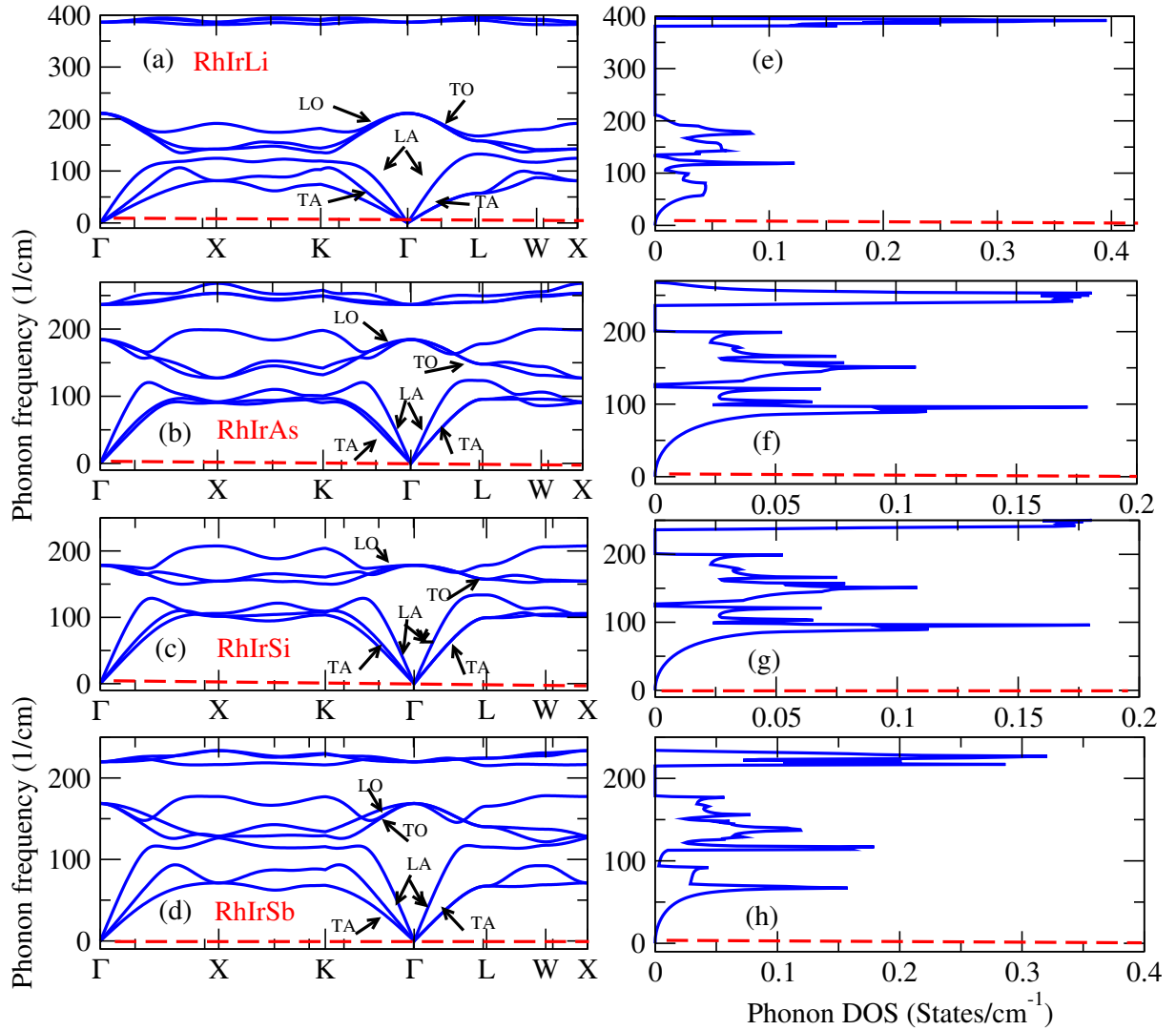


Figure 4.4: Phonon dispersion (a, b, c, d) and DOS (e, f, g, h) for RhIrZ (Z = Li, As, Si, Sb) HH compounds respectively.

dispersion curves calculated along the principal high-symmetry directions in the Brillouin zone, specifically, Γ -X-K- Γ -L-W-X while the corresponding sub-figures on the right (e, f, g, h) present the phonon DOS for each compound. Each row in the Figure represents a specific RhIrZ compound in the sequence: RhIrLi, RhIrAs, RhIrSi, and RhIrSb. In the dispersion plots, the blue lines represent the phonon mode frequencies as a function of the wave vector, with the presence of multiple distinct branches corresponding to various lattice vibration modes, differentiated by their polarization and symmetry. All four compounds exhibit well-defined acoustic branches originating from the Γ point, which gradually increase from zero frequency and represent long-wavelength lattice vibrations. The higher-frequency optical branches arise

from interactions between atoms within the unit cell. Phonon frequencies in all four compounds have positive value in the given range of Brillouin zone confirming the dynamical stability of these compounds. Additionally, certain features in the dispersion curves, such as phonon band gaps or avoided crossings indicate the effect of atomic mass contrasts and bonding differences within the lattice. For example, the dispersion curves for RhIrLi (sub-figure a) are relatively smooth and continuous, suggesting weaker anharmonic interactions and a simpler vibrational landscape. In contrast, the curves for RhIrSb (sub-figure d) show sharper curvatures and more pronounced anomalies, reflecting stronger interatomic interactions and more complex vibrational behavior due to the presence of heavier atoms. The corresponding phonon DOS plots complement the dispersion data by showing the distribution of vibrational states across the frequency range. These DOS graphs quantify the number of phonon modes per frequency interval, with prominent peaks indicating regions of high vibrational state density. RhIrLi (sub-figure e) shows a broad low-frequency peak, consistent with its lighter atomic composition and simpler structure, whereas RhIrSb (sub-figure h) features several distinct high-frequency peaks, implying a more intricate phonon spectrum associated with heavier atomic masses and diverse bonding environments. Altogether, the phonon dispersion and DOS analyses demonstrate how variations in the chemical nature of the Z element significantly influence the vibrational properties of RhIrZ compounds. These differences, in turn, affect key material characteristics such as mechanical strength, thermal conductivity and lattice dynamics, underscoring the importance of phonon studies in evaluating the functional potential of these materials for advanced applications. Results of phonon properties reported in the current work are in consistent with previous reported results on NbIrSn HH compound by Khatri and Adhikar (Khatri and Adhikari, 2023).

Figure 4.5 precisely details the vibrational properties of RhNbZ ($Z = \text{Li, As, Si, Sb}$) compounds through their phonon dispersion relations and phonon DOS. The phonon dispersion curves, depicted in the left column (a, b, c, d) along key symmetry directions of the Brillouin zone ($\Gamma\text{-X-K-}\Gamma\text{-L-W-X}$), illustrate the allowed frequencies of lattice vibrations as a function of wave vector. Each curve represents a distinct phonon mode, characterized by its polarization and symmetry. The presence of acoustic branches, initiating near zero frequency at the Γ point, signifies long-wavelength vibrations inherent to all crystalline structures. Higher-frequency optical branches emerge due to the complex interatomic interactions within the lattice.

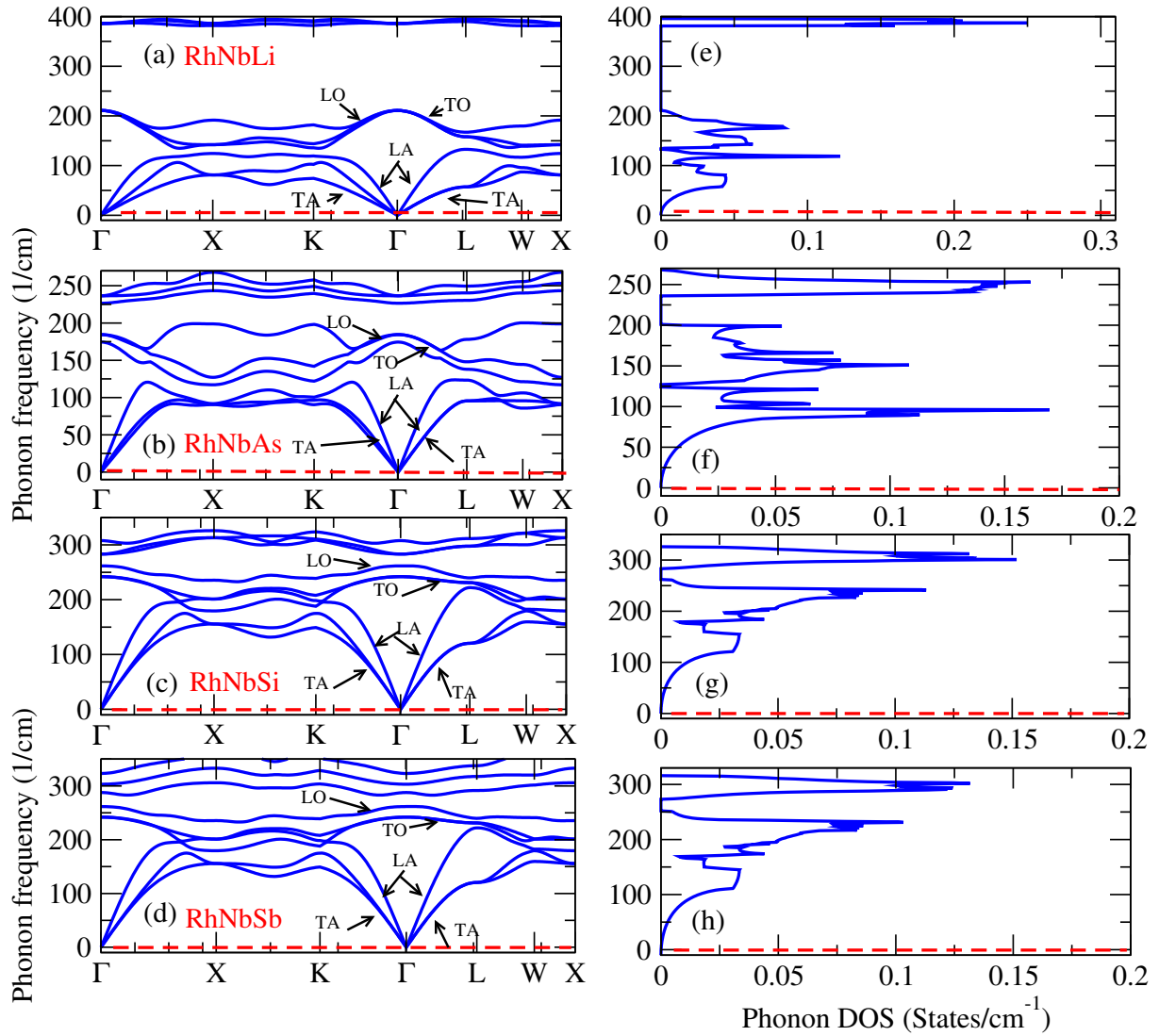


Figure 4.5: Phonon dispersion (a, b, c, d) and DOS (e, f, g, h) for RhNbZ (Z = Li, As, Si, Sb) HH compounds respectively.

The absence of imaginary (negative) frequencies through out the Brillouin zone confirming the dynamical stability of these compounds. Notably, the phonon dispersion of RhNbLi (a) exhibits relatively continuous curves with minimal indications of anharmonicity, likely due to its straightforward lattice arrangement and the presence of lighter atoms. Conversely, RhNbSb (d) displays more significant curvature and irregularities in its dispersion, particularly in the vicinity of the Γ point, suggesting stronger interatomic interactions and the influence of heavier atomic masses. The occurrence of avoided crossings or band gaps within the dispersion curves across all compounds underscores the impact of varying atomic masses and the nature of chemical bonding within their respective lattices. The right column (d, e, f, h) further dis-

plays the phonon DOS, which details the distribution of vibrational modes within the frequency spectrum. Peaks in the DOS plots signify frequency ranges with a higher concentration of vibrational states. RhNbLi (e) shows a broad peak at lower frequencies, consistent with its simpler vibrational dynamics, whereas RhNbSb (h) exhibits multiple sharp peaks at higher frequencies, indicative of a more complex vibrational landscape arising from its heavier constituent atoms and potentially more complex bonding configurations. RhNbAs (f) and RhNbSi (g) demonstrate intermediate behaviors, with DOS features that bridge the gap between the simplicity of RhNbLi and the complexity of RhNbSb. In general, these visual representations emphasize the substantial influence of chemical composition, specifically the choice of the Z element, on both the propagation of lattice vibrations and the distribution of their frequencies. The observed trends suggest that heavier elements like Sb lead to more complex vibrational dynamics, while lighter elements such as Li result in smoother and less complex phonon spectra. This detailed analysis highlights the crucial role of atomic mass and the nature of bonding in determining the phononic properties of these RhNbZ compounds. Results we reported here for RhNbZ (Z = Li, As, Si, Sb) compounds well agree with the previous works reported by Hong and his team workers on NbFeSb HH compounds phonon calculation, which validates results of present work on phonon (Hong et al., 2016).

4.2 Mechanical properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Compounds

Mechanical properties are crucial for evaluating the mechanical stability and practical applicability of materials in diverse technological fields. This section explores the elastic constants, bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and elastic sound velocities of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds through first-principles calculations. These mechanical parameters provide valuable insight into the strength, ductility and anisotropic nature of the materials. The findings are essential for evaluating their potential in real-world applications.

4.2.1 Elastic Properties

A material's elastic properties, which characterize how it reacts to external loads, can be used to evaluate its mechanical stability. The theoretical basis for determining whether a crystal structure is mechanically stable is provided by the Born-Huang stability criterion, Equations (2.3-2.7). In order to ascertain the stability and mechanical behavior of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds, we examined the elastic constants (C_{ij}), bulk modulus (K), shear modulus (G), Young's modulus (E) and Poisson's ratio (ν). From Table 4.5 we observe that

all compounds in this work satisfy Born and Huang mechanical stability criteria and therefore, they are mechanically stable.

Table 4.5: Calculated elastic constants, moduli (bulk, Voigt, Reuss, shear, Young) and related parameters (Poisson's ratio, hardness, anisotropy, Cauchy pressure) for RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds.

Elastic P.	RhZrLi	RhZrAs	RhZrSi	RhZrSb	RhIrLi	RhIrAs	RhIrSi	RhIrSb	RhNbLi	RhNbAs	RhNbSi	RhNbSb
C_{11} (Gpa)	136.33	208.32	202.74	277.62	182.32	378.98	419.25	260.43	144.47	180.61	298.89	205.70
C_{12} (Gpa)	62.56	118.145	119.90	69.40	125.17	130.59	133.78	136.99	93.16	151.89	133.89	128.26
C_{44} (Gpa)	28.44	50.56	78.15	38.59	91.79	108.91	60.34	92.05	86.3	123.38	119.00	83.00
B(Gpa)	87.82	148.21	147.51	138.81	144.22	213.38	228.94	178.14	110.25	161.46	188.89	154.07
G_V (Gpa)	32.22	48.38	32.20	64.80	66.51	115.02	93.30	79.92	62.07	74.03	104.40	65.29
G_R (Gpa)	31.59	48.23	57.67	51.57	48.70	114.55	78.46	76.93	44.36	30.56	101.11	56.95
G(Gpa)	31.91	48.31	44.94	58.19	57.60	114.79	85.88	78.42	53.22	52.30	102.76	61.12
B/G	2.75	3.07	3.28	2.39	2.50	1.86	2.67	2.27	2.07	3.09	1.84	2.52
Y(Gpa)	85.39	130.73	122.40	153.17	152.50	292.00	229.00	205.17	137.53	141.61	260.96	161.95
ν	0.34	0.35	0.36	0.32	0.32	0.27	0.33	0.31	0.29	0.35	0.27	0.32
H(Gpa)	4.64	5.21	4.61	3.90	7.32	15.52	8.59	9.83	8.72	5.41	14.74	7.52
A	0.75	1.12	1.89	0.37	3.21	0.88	0.42	1.49	3.37	8.59	1.44	2.14
CP(Gpa)	34.12	67.57	41.75	30.81	33.38	21.68	73.44	44.94	6.82	28.51	14.89	45.26

The resistance of a material to homogeneous compression is indicated by its bulk modulus (B). Greater incompressibility is indicated by higher values of B. RhIrSi has the largest bulk modulus (228.94 GPa) of all the compounds under this study, indicating exceptional mechanical strength. RhZrLi, on the other hand, has the lowest bulk modulus (87.82 GPa), suggesting a structure that it may be compressible under high stress. RhIrAs (15.52 GPa) and RhZrSb (3.9 GPa) exhibit the highest and lowest hardness, respectively, while the hardness (H) values of the other compounds under this study fall between these two values. These findings imply that compounds based on RhIr and RhNb have higher hardness than those based on RhZr, which is consistent with results reported in the literature (Chen et al., 2025). The resistance to shear deformation of a material is determined by its Voigt shear (G_V), Reuss shear (G_R) and shear (G) moduli. RhIrAs and RhNbSi exhibit the strongest resistance to shear deformation, according to the results, which suggests that they could be used in wear-resistant applications. The anisotropic factor (A) is used to assess elastic anisotropy. When $A = 1$, which is its equilibrium value, isotropy exists; larger deviations signify more anisotropy. RhNbAs (8.59) has the maximum anisotropy, whereas RhZrSb (0.37) has a comparatively lower anisotropic character, indicating isotropic mechanical behavior in the latter. Pugh ratio (B/G) is used to determine brittleness and ductility. The findings show that every compound has B/G ratio higher than its equilibrium value (1.75) (Huang et al., 2024), indicating that they are all ductile. This classification is also supported by the Poisson's ratio (ν), another measure of ductility, as all values are greater than 0.26, indicating that these materials are ductile (Mostari et al., 2020). Materials' stiffness is determined by their Young's modulus (Y). The highest stiffness is shown by RhIrAs

(292.00 GPa), RhNbSi (260.96 GPa) and RhIrSi (229.00 GPa), indicating their applicability for structural applications requiring rigid materials. RhZrLi, on the other hand, has the lowest Young's modulus (85.39 GPa), suggesting that, comparing to the other it is more flexible, results which are in good agreement with the works reported in (Min et al., 2022).

Based on the obtained mechanical properties, the studied RhYZ compounds have potential applications in various fields including spintronic and optoelectronic applications. Due to their ductility nature and mechanical robustness, these compounds are suitable for spintronic and optoelectronic devices where mechanical stability under external stress is crucial. These materials can also be used for applications that require high hardness applications. For instance, when compared to the other RhYZ compounds under this study, RhIrAs, RhNbSi, RhIrSi and RhIrSb show comparatively high bulk modulus (B) and hardness (H). Given that materials with $H > 10$ GPa and $B > 150$ GPa are frequently regarded as appropriate for such applications, these properties make them promising candidates for wear-resistant coatings and mechanical reinforcing materials (Chen et al., 2011). Additionally, the high Poisson's ratio ($\nu > 0.26$) and Pugh's ratio ($B/G > 1.75$) found in a number of RhYZ compounds point to favorable ductility, which is necessary for flexible structural and electronic applications (Pugh, 1954). These results demonstrate RhYZ compounds' mechanical adaptability for both stiff and flexible device components. In this regard RhZrAs, RhZrSi and RhNbAs are the best potential runner for these applications.

4.2.2 Debye Temperature and Sound Velocity

For RhYZ ($Y = \text{Zr, Ir, Nb}$; $Z = \text{Li, As, Si, Sb}$) compounds, the determined density (ρ), elastic sound velocities (v_a , v_l , v_t), Debye temperature (Θ_D) and melting temperature (T_m) are shown in Table 4.6. These parameters are essential for deep understanding of the materials' mechanical and thermal stability as well as possible uses in optoelectronics and spintronics. RhYZ ($Y = \text{Zr, Ir, Nb}$; $Z = \text{Li, As, Si, Sb}$) compounds show notable changes in their estimated ρ , elastic velocities, Θ_D and T_m , which are indicative of variances in atomic bonding and structural stability. While RhZrLi has the lowest density at 5740.44 kg/m^3 , RhIr-based compounds often have the highest, with RhIrAs reaching 12792.03 kg/m^3 . While RhNbSi has the highest average elastic velocity (v_a) at 4189.87 m/s , showing good mechanical stability, RhIrLi has the lowest, indicating a softer structure, at 2453.20 m/s . The transverse and longitudinal velocities show comparable patterns, with compounds that contain Si and As often showing greater values, indicating improved stiffness and stronger atomic connections. The trend of the Θ_D is comparable to that of elastic velocities, with RhNbSi has the greatest Θ_D (484.75 K), indicating high thermal conductivity and intense lattice vibrations. However, RhNbSb has the lowest Θ_D

(234.46 K), suggesting a softer lattice. This could help reduce heat conductivity, which is a desirable feature for thermoelectric applications. RhIrSi (3031.21 K) and RhIrAs (2793.15 K) have the highest T_m values, indicating greater thermal stability, which is also correlated with these trends. RhZrLi (1358.85 K) has the lowest T_m , which denotes a lower level of heat resistance. The calculated values of ρ , Θ_D , Θ_D , elastic sound velocities and T_m for the RhYZ compounds in this study show fair agreement with results reported in (Tavassoli et al., 2017; Kaur et al., 2018; Bamgbose et al., 2023). This alignment reinforces the credibility of our theoretical predictions and highlights the consistency of our results with previously established data. Because of their perhaps lower lattice thermal conductivity, RhNb-based compounds, especially RhNbSb, may be more advantageous for thermoelectric applications, whereas RhIr-based compounds are better suited for high-temperature applications. In general, all these compounds have melting temperature well above 1000 K and can be used in practical heating systems that require high temperatures (Simić et al., 2020).

Table 4.6: Computed density, transverse, longitudinal and average elastic velocities, Debye and melting temperatures for RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds.

HH compounds	$\rho(kg/m^3)$	$v_a(m/s)$	$v_l(m/s)$	$v_t(m/s)$	$\Theta_D(K)$	$T_m \pm 300 K$
RhZrLi	5740.44	2646.53	4765.52	2357.71	293.63	1358.85
RhZrAs	7844.85	2791.19	5206.12	2481.57	311.86	1784.38
RhZrSi	6613.58	2935.58	5600.48	2606.87	330.24	1751.42
RhZrSb	8298.58	2963.89	5106.50	2648.02	319.84	2194.01
RhIrLi	12014.93	2453.20	4289.02	2189.57	303.99	1630.69
RhIrAs	12792.03	3334.54	5352.11	2995.54	394.29	2793.15
RhIrSi	11981.61	3003.36	5353.93	2677.25	363.53	3031.21
RhIrSb	12417.74	2809.92	4771.37	2513.07	316.20	2092.43
RhNbLi	6350.27	3230.38	5341.89	2894.95	369.64	1406.96
RhNbAs	8310.90	2821.88	5274.29	2508.57	320.74	1620.59
RhNbSi	7248.65	4189.87	6705.26	3765.16	484.75	2319.74
RhNbSb	8781.60	2956.50	5179.72	2638.42	234.46	1768.89

The mechanical and thermal properties of these compounds demonstrate how well suited they are for a range of technological uses. RhNbSi is a good choice for mechanical and high-temperature applications due to its high Debye temperature and elastic velocities, whereas RhNbSb's low Θ_D indicates potential for thermoelectric applications where low thermal conductivity is needed. RhIr-based compounds are appropriate for high-performance electronic or structural applications due to their high melting temperatures, which demonstrate their remarkable thermal stability. These results offer important new information about the structure property relationships in Rh-based HH compounds and can be used to help choose materials for optoelectronic and spintronic applications (Bencherif, 2022).

4.3 Electronic Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds

The investigation of electronic properties is crucial for determining the suitability of materials in optoelectronic and spintronics applications. This section presents the electronic band structures and DOS of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds, derived from first-principles calculations. The analysis highlights important features such as band gaps, band dispersion and the properties of states near the E_F . These insights help clarify whether each compound exhibits semiconducting, half-metallic or metallic behavior, guiding their potential applications.

4.3.1 Band Structure and density of states of RhZrZ (Z = Li, As Si, Sb) HH compounds

The electronic properties of RhZrZ (Z = Li, As Si, Sb) compounds have been analyzed using GGA and GGA+U calculations. The band structure plots along the high-symmetry points (Γ -X-K- Γ -L-W-X) provide insight into the nature of their electronic states, while the DOS plots reveal atomic contributions to the electronic structure. The calculated band gaps (E_g) indicate semiconducting behavior for RhZrSb and RhZrAs with respective band gap energies 1.1893 eV (1.2134 eV) and 1.1904 eV (1.3241 eV) as determined from GGA (GGA + U) calculations respectively. The increase in the band gap with GGA+U suggests that electron correlation effects, where in particular Rh and Zr d-orbitals play a vital role in determining the electronic structure. Our calculated results well agree with the previous works by Benzoudji and Manzoor with their co-works as indicated by Table 4.7. Thus, their electronic structures reveal the presence of an energy band gap, making them potential candidates for optoelectronic application (Nazir et al., 2024; Parvin et al., 2021). However, their band dispersion differs, leading to variations in electronic transitions and transport properties. The efficiency of carrier transport and optical absorption are significantly impacted by the band gap type, whether it is direct or indirect. Figure 4.6 (a and b) reveals that RhZrAs exhibits direct band gap as the valence band maximum (VBM) and conduction band minimum (CBM) of the material are found to be at the same k-point (both at the Γ point) in the Brillouin zone.

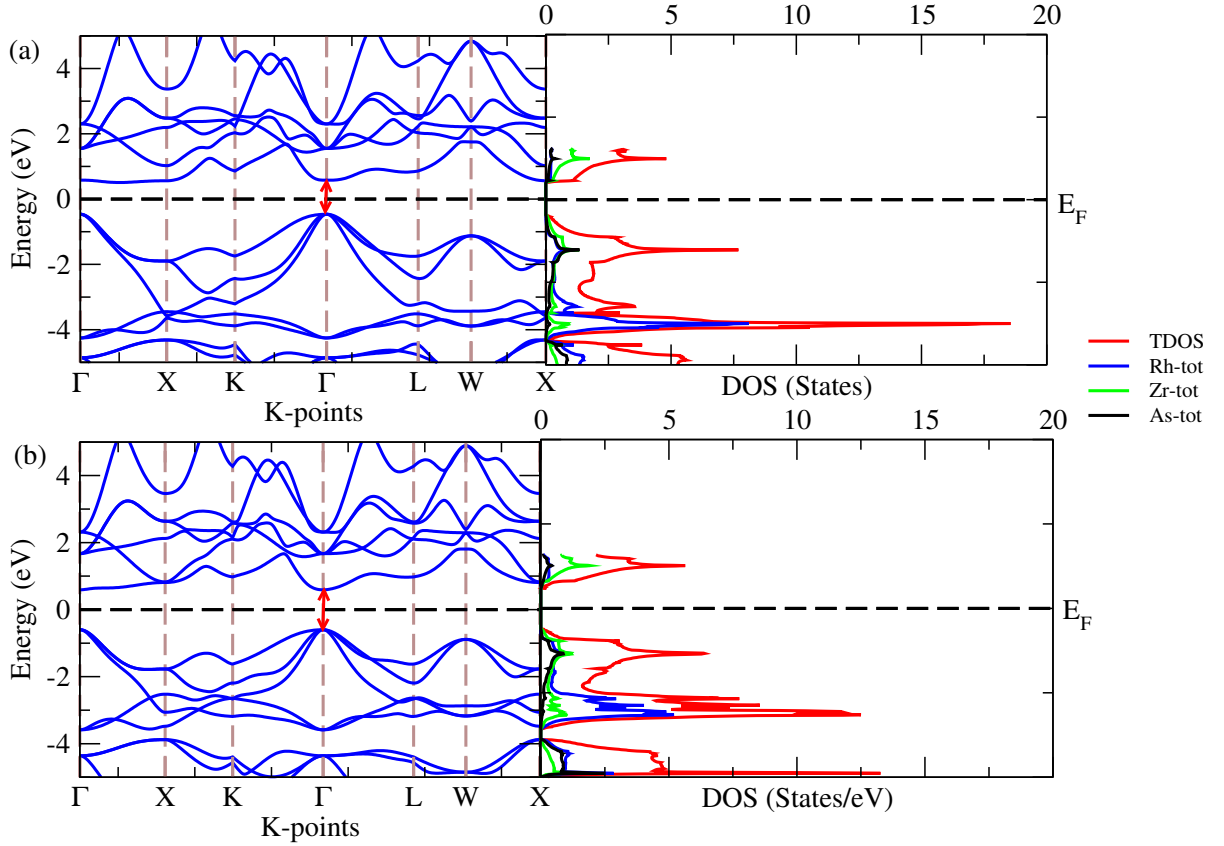


Figure 4.6: Electronic band structure and density of states (total and partial) for RhZrAs compound. (a) for GGA approach whereas (b) is for GGA+U approach. Fermi level at zero eV (black dashed line).

Table 4.7: Calculated band gaps of RhZrZ (Z = As, Sb) HH compounds at equilibrium lattice parameters (GGA and GGA+U).

HH compound	Approach	E_g (eV)
RhZrSb	GGA	1.1893
	Other work	1.17 (Benzoudji et al., 2019)
	Other work	1.14(Manzoor et al., 2024)
	GGA+U	1.2134
	Other work	1.209 (Manzoor et al., 2024)
RhZrAs	GGA	1.1904
	Other work	1.38 (Manzoor et al., 2024)
	GGA+U	1.3975
	Other work	1.426(Manzoor et al., 2024)

On the other hand, from Figure 4.7 of (a) and (b) (RhZrSb) we observe an indirect energy band gap, where VBM and CBM of these compound are situated at different k-points. The

VBM and CBM are occurred at Γ and X in the Brillouin zones respectively, due to its indirect band gap.

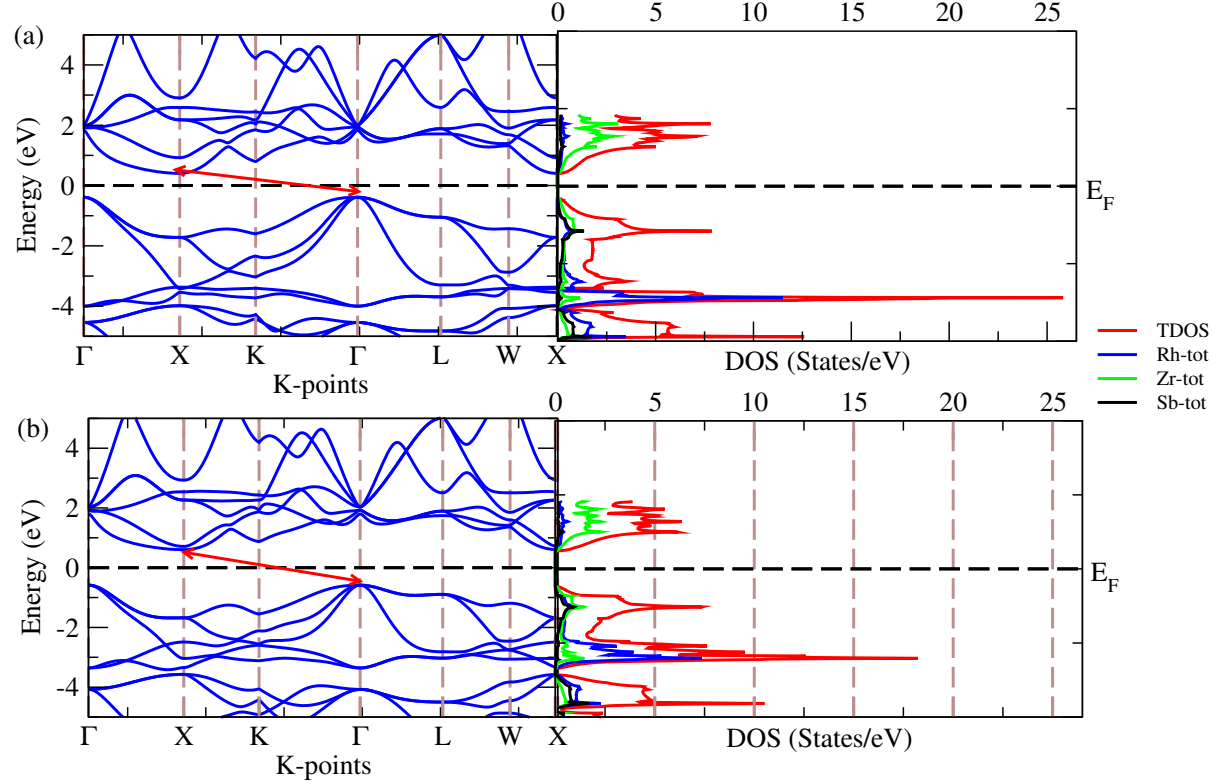


Figure 4.7: Electronic band structure and density of states (total and partial) for RhZrSb compound. (a) for GGA approach whereas (b) is for GGA+U approach. The Fermi level is at zero energy (black dotted line).

Because of its direct band gap, RhZrAs electron-hole recombination proceeds effectively without the need for phonon support, making it advantageous for optoelectronic applications. This implies that optical absorption in RhZrAs is highly efficient, as electrons excited from the valence band to the conduction band can recombine without phonon assistance. Thus, due to its direct band gap, RhZrAs is a strong candidate for applications in optoelectronics, such as photodetectors and solar cells. This finding aligns with previous studies, such as those by Mehtougui and his co-workers, who also highlighted the potential of direct band-gap XZrZ (X = Ni, Cu and Z = C, B) HH semiconductor compounds for similar applications (Mehtougui et al., 2022). The indirect band gap of RhZrSb reflects special electronic properties that make it ideal for a wide range of technological uses. Longer carrier lifetimes allow for efficient photon absorption and emission, making this compound a promising candidate for optoelectronic applications such as light-emitting devices, infrared detectors and photodetectors. Despite being an

indirect band gap semiconductor, this compound shows potential for photovoltaic applications due to its moderate band gap (~ 1.2 eV), which enables absorption of a significant portion of the solar spectrum, and its strong electrical conductivity, which facilitates efficient charge transport and collection. Semiconductor HH compounds, (Ni/Pd/Pt)ScSb that have indirect band gap comparable to RhZrSb compound were reported by Saad and Alsobhi for similar application we mention above for RhZrSb compound (Saad and Alsobhi, 2023).

In general, the electronic band gap (E_g) values for RhZrAs and RhZrSb offer important information about their possible uses, especially in energy harvesting devices and optoelectronics. These materials are appropriate for photovoltaics and light-emitting devices because RhZrAs (1.19–1.32 eV) and RhZrSb (1.17–1.21 eV) have band gaps that are within the ideal range for infrared (IR) and visible-light photodetectors. According to these values, they have the capacity to effectively absorb and emit light in the visible to near-infrared (NIR) spectrum, which is crucial for solar cells and infrared sensing applications as supported by works of Tarekuzzaman research team (Tarekuzzaman et al., 2024).

DOS analysis further supports the semiconducting nature of these compounds, as DOS shows zero states at the E_F , confirming the presence of a band gap in both compounds under both calculations. The distinct contributions of each component are revealed by a thorough analysis of the PDOS. In both compounds and under both calculations, the valence band area is mostly contributed by the rhodium (Rh) d-states. Specifically, the sharp peaks in both cases around -3 eV to -4 eV indicate significant d-orbital interactions. The lower valence band and conduction band are mainly contributed by the states of zirconium (Zr). The lower valence band and occasionally the conduction band are where arsenic (As) and antimony (Sb) elements contribute most while close to the conduction band edge their states seem more confined. One notable drawback of GGA calculation is that the band gap seems to be underestimated in this method. The band gap is widened by applying GGA+U, which increases the precision of the electronic structure predictions. This improvement is especially important for possible uses in optoelectronics, where exact band gap control is required.

Figure 4.8 presents the spin-polarized band structure and DOS of RhZrLi, computed using the GGA approximation. The band structure reveals that both spin-up and spin-down bands cross the E_F , confirming that RhZrLi exhibits a metallic nature. Importantly, the band structure is symmetric for both spin channels, meaning that there is no significant spin polarization within the GGA framework. The TDOS at E_F remains nonzero for both spin-up and spin-down states, reinforcing the metallic character. Examining the PDOS, it is evident that Rh and Zr orbitals dominate near E_F , while Li contribution is relatively minor. This suggests that the conduction mechanism is primarily influenced by the transition metal elements (Rh and Zr),

with Li playing a negligible role. The symmetric nature of the bands and DOS indicates that

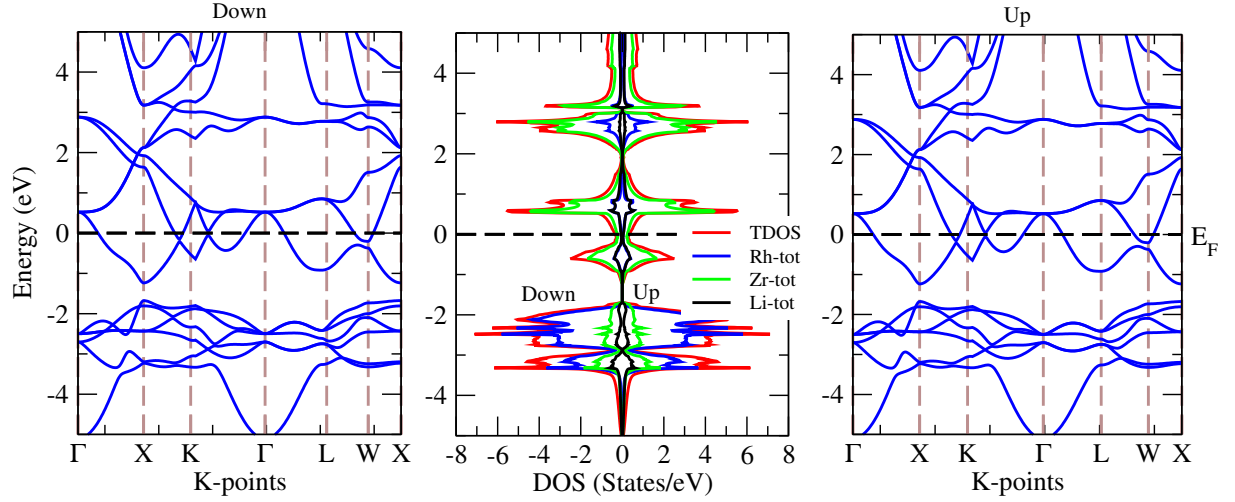


Figure 4.8: GGA calculations of spin-polarized band structures and density of states (for spin-up and spin-down electrons) in RhZrLi compound. Fermi level at zero energy (black dotted line).

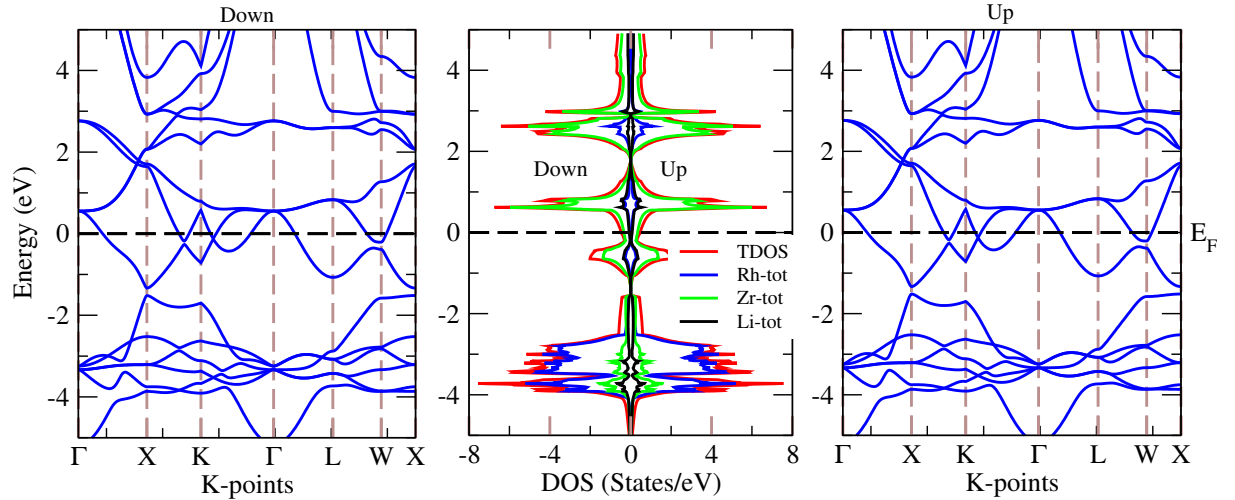


Figure 4.9: GGA+U calculations of spin-polarized band structures and density of states (for spin-up and spin-down electrons) in RhZrLi compound. Fermi level at zero energy (black dotted line).

the material does not exhibit spontaneous spin polarization, making it a non-magnetic metal within the GGA approximation. In Figure 4.9, the GGA+U results for RhZrLi introduce some modifications to the electronic structure while maintaining overall symmetry between spin-up

and spin-down channels. The application of the U correction leads to a redistribution of electronic states, particularly affecting the Rh and Zr orbitals, which become more localized due to enhanced electron-electron interactions. Despite these changes, the band structure remains symmetric between the two spin channels, meaning that no spin polarization is induced by the U correction. The material remains metallic, as bands continue to cross the E_F for both spin-up and spin-down states. The PDOS analysis shows that the primary effect of the U correction is a slight modification in the energy positions of the orbital states, but this does not introduce any significant changes in spin asymmetry. The main observation here is that RhZrLi is non-magnetic (symmetric nature of the bands and DOS) metallic compound under both GGA and GGA+U calculations.

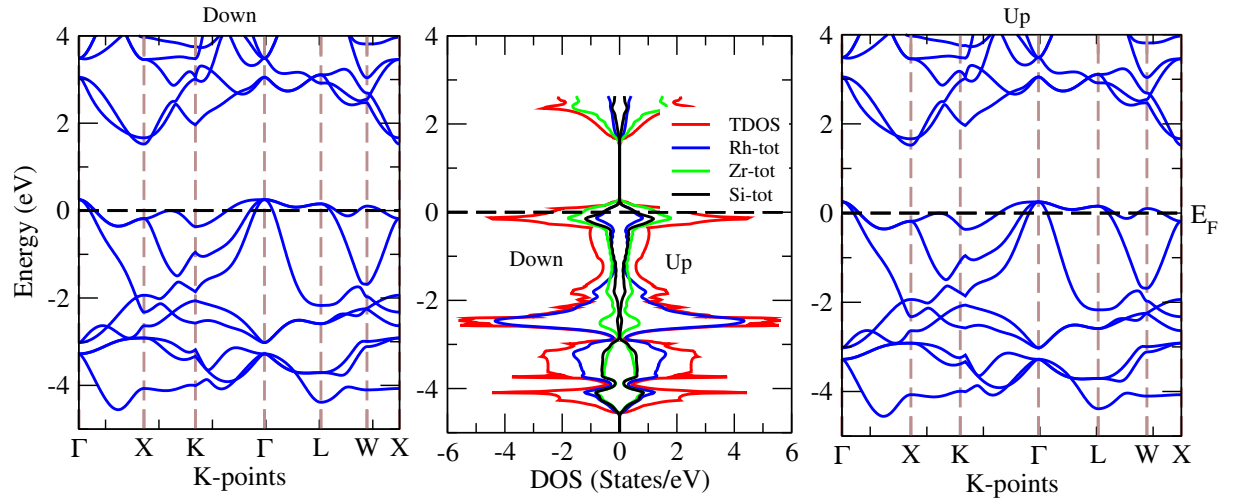


Figure 4.10: GGA calculations of spin-polarized band structures and density of states (for spin-up and spin-down electrons) in RhZrSi compound. Fermi level at zero energy (black dotted line).

Figure 4.10 presents the spin-polarized band structure and DOS of RhZrSi, computed using the GGA approximation. The band structure shows that the bands for both spin-up and spin-down channels cross the E_F , indicating a metallic nature of RhZrSi. Additionally, the band structure remains symmetric for both spin channels, implying an absence of significant spin polarization. The TDOS at E_F is nonzero in both spin channels, further confirming its metallic character. The PDOS reveals that Rh and Zr orbitals contribute dominantly near the E_F , with the Si orbitals playing a minor role. This suggests that the conduction mechanism in RhZrSi is primarily influenced by transition metal elements. The symmetric nature of the spin channels in this Figure indicates that electron correlation effects, which could induce spin polarization, are not prominent under the GGA approximation. Figure 4.11, which presents the GGA+U

results for RhZrSi, shows notable differences compared to Figure 4.10. The inclusion of the U correction enhances electron correlation effects, leading to a redistribution of electronic states and shifts in band positions. However, the band structure and DOS remain symmetric between the spin-up and spin-down channels and they well cross the E_F , similar to the GGA results. Despite this symmetry, the correlation effects modify the band dispersion and influence the density of states, particularly affecting the localization of Rh and Zr states. This suggests that while GGA+U impacts the band structure, it does not induce spin asymmetry in RhZrSi, preserving the non-magnetic metallic nature seen in Figure 4.10. Thus, from both Figures it is observed that RhZrSi remains non-magnetic metallic under both GGA and GGA+U calculations. The electronic properties of RhZrZ (Z = Li, Si) HH compounds reported in this work are reasonably consistent with earlier findings reported by (Li et al., 2025; Behbahani et al., 2016), indicating the reliability of our computational approach.

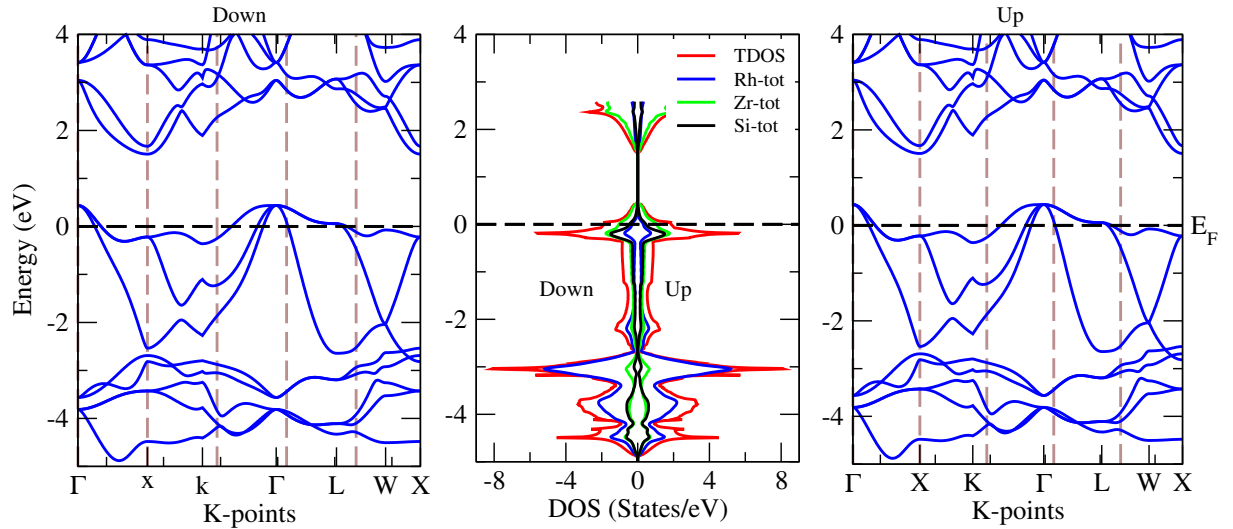


Figure 4.11: GGA+U calculations of spin-polarized band structures and density of states (for spin-up and spin-down electrons) in RhZrSi compound. Fermi level at zero energy (black dotted line).

From the family of RhZrZ compounds under our study, RhZrZ (Z = Li, Si) were determined to be non-magnetic metallic compounds. These compounds, though lacking intrinsic magnetism, have attracted considerable attention for their versatile roles in spintronic, optoelectronic and energy-related applications. In the field of spintronics, these compounds can demonstrate strong SOC, which enables phenomena like the spin Hall effect (SHE), allowing the generation of pure spin currents without relying on magnetic elements, a key advantage for low-power spin-based technologies, a result which is consistent with works in (Sinova et al.,

2015). Their structural compatibility and good electrical conductivity also make them suitable as non-magnetic spacer layers in multilayered spintronic devices such as spin valves and MTJs (Mehmood et al., 2017). Furthermore, certain HH phases are situated near topological phase boundaries and can host non-trivial surface states under specific conditions, highlighting their potential in topological spintronics (Chadov et al., 2010). In optoelectronics, these compounds offer high electrical conductivity and adjustable electronic structures, making them promising candidates for applications such as transparent conductive films, plasmonic components and infrared photodetectors. The broad functional tunability and excellent physical properties of non-magnetic metallic HH compounds, such as RhZrZ ($\text{Z} = \text{Li, Si}$) make them strong candidates for incorporation into a range of next-generation electronic and energy technologies.

4.3.2 Band Structure and density of states of RhNbZ ($\text{Z} = \text{Li, As, Si, Sb}$) HH compounds

Figure 4.12 presents the spin-polarized band structure and DOS of RhNbLi calculated using the GGA approximation. The band structure reveals a symmetric dispersion between the spin-up and spin-down channels, with several bands crossing the E_F in both spin states. This symmetry suggests that the system exhibits a conventional metallic behavior, where both spin-up and spin-down electrons contribute equally to electrical conductivity. The PDOS further supports this observation, as the TDOS remains finite at E_F for both spin channels, confirming the metallic nature of RhNbLi . The PDOS contributions indicate that Rh and Nb orbitals dominate, where near and above E_F PDOS of Nb largely contributes to TDOS but Rh PDOS dominantly contributes to TDOS in the region below and far E_F , which implies that their orbitals are primarily responsible for the material's electronic properties. The symmetric nature of the band structure suggests no apparent spin polarization in this case, meaning the material does not exhibit any half-metallic or magnetic character under the GGA approximation, but have metallic nature.

In contrast, Figure 4.13, which corresponds to the GGA+U calculations, shows a significant deviation from the behavior observed in Figure 4.12. Although the bands still cross the E_F , indicating that the system remains metallic, the spin-up and spin-down bands are no longer symmetric. This asymmetry implies that the material exhibits spin-polarized metallic behavior, meaning that while both spin channels contribute to conduction, they do so in an unequal manner. The inclusion of the U correction enhances electron localization, which leads to a shift in the relative energy positions of spin-up and spin-down states. This shift causes changes in the band dispersion, resulting in different densities of states at E_F for spin-up and spin-down electrons. The DOS analysis further confirms this spin-dependent behavior, as it shows

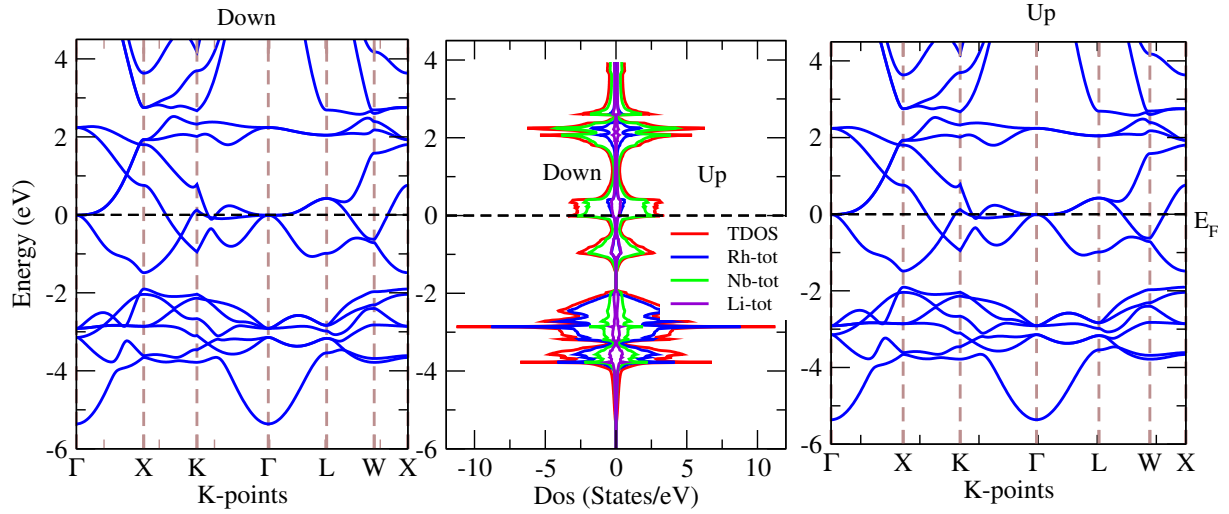


Figure 4.12: Spin-up and spin-down band structures and DOS of RhNbLi compound from GGA. Fermi level at zero (black dotted line).

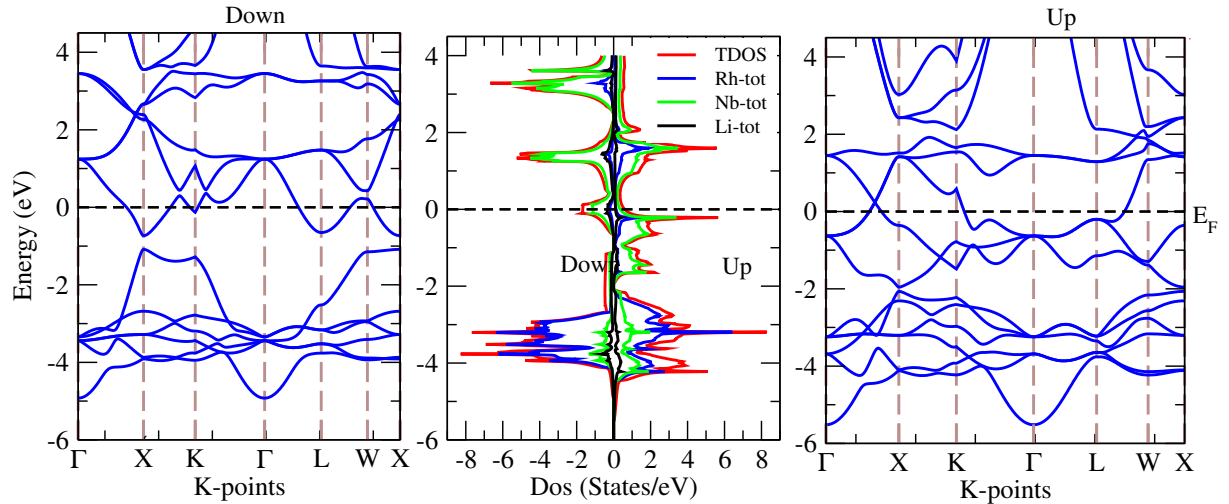


Figure 4.13: Spin-up and spin-down band structures and DOS of RhNbLi compound from GGA+U. Fermi level at zero (black dotted line).

an imbalance between the contributions from different atomic orbitals in each spin channel. The difference between the two approximations lies in the effect of the U correction. While GGA predicts a symmetric metallic system with no spin polarization, GGA+U introduces spin asymmetry, making RhNbLi a spin-polarized metal. This spin-polarization is crucial for potential applications in spintronics, where materials with differing conduction behavior for spin-up and spin-down electrons are desirable for magnetic sensors, spin-filters and spintronic memory

devices. The findings indicate that by applying the U correction, RhNbLi transitions from a non-magnetic metallic state (GGA) to a spin-polarized metallic state (GGA+U), which could be useful for controlling spin-dependent electronic transport. Xiong and his colleagues reported similar properties and technological application of XCoGe (X=V, Nb, Ta) HH compounds that are closely related to the RhNbLi compound (Xiong et al., 2022b).

RhNbLi, Which is identified as magnetic metallic compound, stands out as a potential runner in spintronics and optoelectronics due to its interesting mixture of magnetic order and excellent electrical conductivity. The presence of Rh and Nb imbues it with strong SOC, a vital ingredient for spintronic devices like spin valves and MTJs, where SOC amplifies SHE and spin polarization. Furthermore, Rh-based HH compounds like RhTiP, RhTiAs and RhTiSb which have close similarity with RhNbLi (Pedersen et al., 2020) have showcased impressive optical conductivity and absorption in the visible and ultraviolet spectrum, making them attractive for optoelectronic applications, including transparent conductive electrodes and infrared detectors.

Figures 4.14-4.17 present electronic band structure and DOS of RhNbZ (Z = As, Nb) compounds. From Figures 4.14 and 4.16 respectively, the electronic band structure of RhNbAs and RhNbSb, as obtained using the GGA, reveals metallic behavior in both the majority-spin (up) and minority-spin (down) channels. This is evident from the presence of energy bands crossing the E_F , signifying that there is no band gap at E_F for either of the spin channels. As a result, RhNbAs and RhNbSb are predicted to be metal under GGA. The DOS further supports this observation since its lines remain finite at E_F , confirming the metallic nature of the compounds. The PDOS analysis reveals that the Rh and Nb states contribute dominantly to the electronic states near E_F , while As and Sb states provide some hybridization. The relatively symmetrical distribution of spin-up and spin-down DOS in RhNbAS and RhNbSb under GGA calculation suggests weak spin polarization, indicating that the materials do not exhibit significant spin-dependent electronic properties in its ground state. When compared to RhNbAs, the Sb atom introduces a slightly different hybridization effect, which might influence SOC but does not significantly alter the overall metallic nature of the compound. The lack of half-metallicity or semiconducting in both compounds under GGA calculations suggests that electron correlation effects, which are not well captured by GGA, implying that strong electron correlation effects may be needed for an accurate description of the electronic structure.

When electron correlation effects are considered using the GGA+U approximation, a substantial change in the electronic structure of RhNbAs is observed (Figure 4.15). Notably, a band gap of 1.109 eV opens in the minority-spin (down) channel, while the majority-spin (up) channel retains its metallic character. This results in half-metallic behavior, meaning that only electrons with majority spin contribute to conduction, while the minority-spin electrons en-

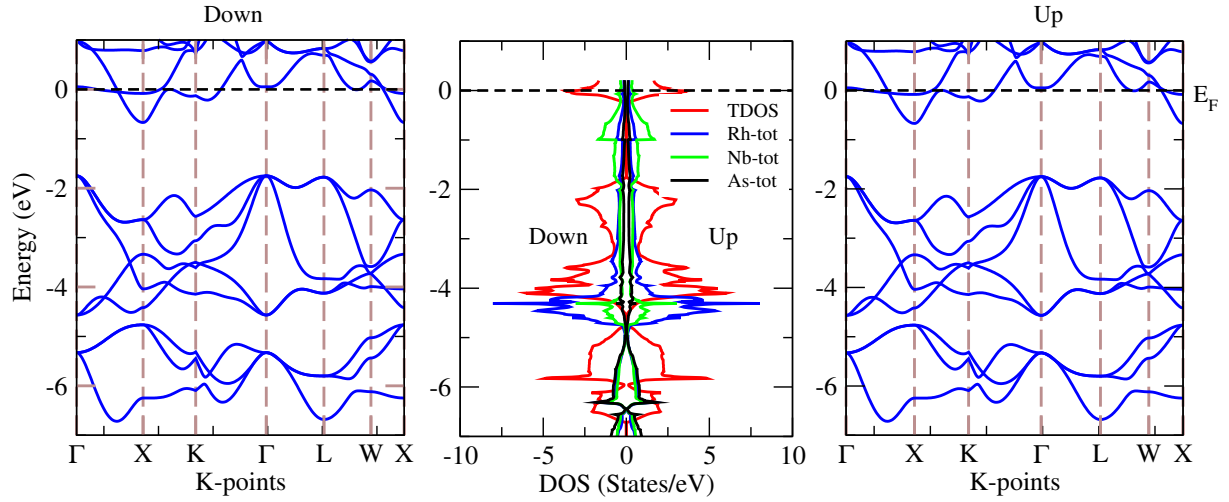


Figure 4.14: Spin-up and spin-down band structures and DOS of RhNbAs compound from GGA. Fermi level at zero (black dotted line).

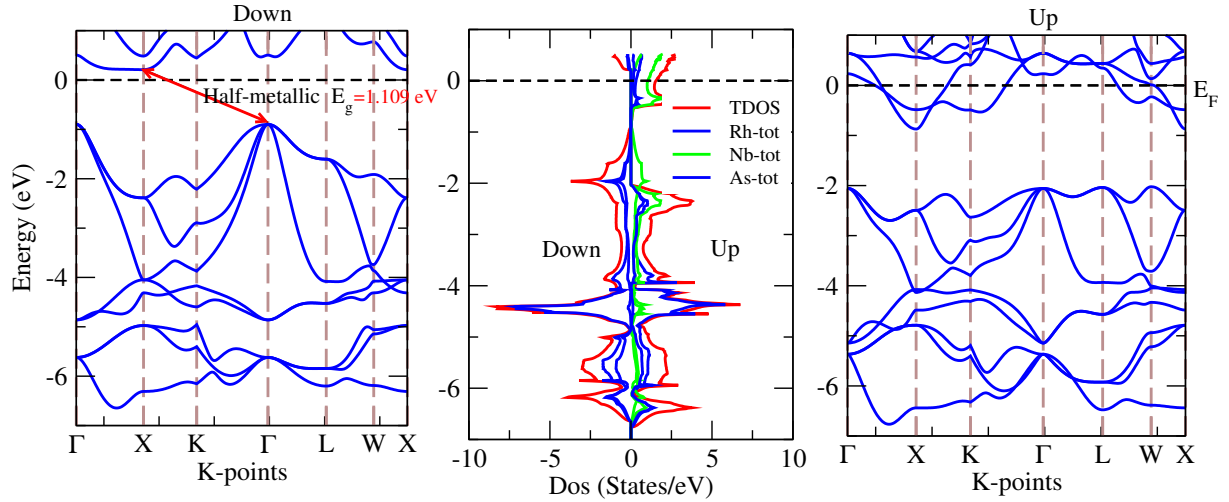


Figure 4.15: Spin-up and spin-down band structures and DOS of RhNbAs compound from GGA+U. Fermi level at zero (black dotted line).

counter energy gap and cannot participate in electrical transport. Similarly, by incorporating on-site Coulomb interactions through the GGA+U approach, a dramatic transformation in the electronic structure of RhNbSb is observed (Figure 4.17). A band gap of 0.83 eV appears in the minority-spin (down) channel, while the majority-spin (up) channel retains its metallic nature. This confirms that RhNbSb, like RhNbAs, is a half-metal under GGA+U. The corresponding DOS plot clearly shows that the DOS at E_F for the minority spin is completely suppressed, indicating that only the majority-spin electrons contribute to electrical conduction reinforcing

the presence of half-metallicity in both compounds. The localization of Rh and Nb electrons is significantly enhanced by the inclusion of U, which leads to stronger electron correlation effects and a redistribution of electronic states. The electronic properties of RhNbZ (Z = As, Sb) HH compounds reported here agree well with previous studies on related HH systems (Dergal et al., 2023), highlighting the accuracy of the employed computational methods.

The half-metallic behavior is particularly important for spintronic applications, as 100% spin polarization at E_F ensures that the material can act as an efficient spin filter or spin injector. Furthermore, the relatively large indirect band gap in the minority-spin channel suggests

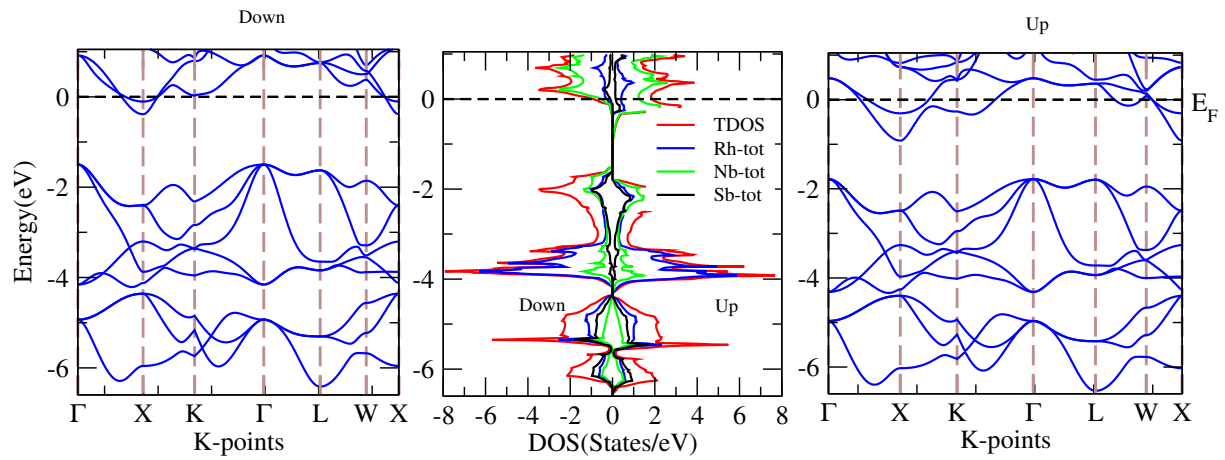


Figure 4.16: Spin-up and spin-down band structures and DOS of RhNbSb compound from GGA. Fermi level at zero (black dotted line).

enhanced thermal stability, which is beneficial for maintaining spin-polarized conduction at elevated temperatures. Compared to RhNbAs, the band gap of RhNbSb in the minority-spin channel is smaller (0.83 eV vs 1.109 eV), suggesting that it may exhibit slightly better carrier mobility while still maintaining strong spin-polarization. This smaller gap in RhNbSb may result from differences in electron localization due to the Sb atom, which influences the d-orbital hybridization differently than As. Despite the smaller band gap, RhNbSb remains an excellent candidate for spintronic applications, as the 100% spin polarization at E_F ensures efficient spin-dependent conduction. The substitution of Sb for As affects orbital hybridization and electron localization, leading to differences in the minority-spin band gap and transport properties. RhNbAs, with As providing stronger localization effects, results in a larger band gap, while RhNbSb, with Sb influencing the d-orbital hybridization differently, has a smaller but still significant band gap. Thus, the results indicate that GGA fails to predict half-metallicity in both RhNbAs and RhNbSb, reinforcing the need to incorporate electron correlation effects through GGA+U. The GGA+U calculations successfully predict half-metallic behavior in both materi-

als, with 100% spin polarization at E_F . This makes both compounds excellent candidates for spintronic applications, where selective spin transport is required. Among the two, RhNbAs exhibits a larger minority-spin band gap (1.109 eV), which enhances its thermal stability, making it suitable for high-temperature spintronics. On the other hand, RhNbSb, with a smaller band gap (0.83 eV), may exhibit better carrier mobility, making it ideal for low-energy spintronic devices. These results suggest that both compounds have strong potential for next-generation spintronics applications, including spin filters, magnetic memory devices and spin-based transistors, where similar results for these such applications were reported in (Gurunani and Gupta, 2024b; Kalita et al., 2022).

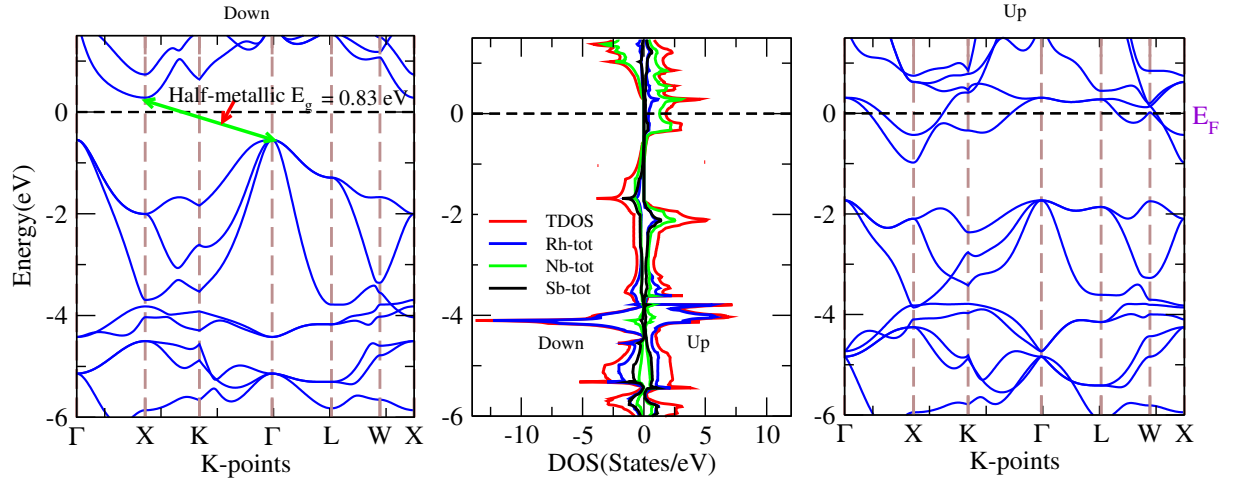


Figure 4.17: Spin-up and spin-down band structures and DOS of RhNbSb compound from GGA+U. Fermi level at zero (black dotted line).

Figures 4.18 and 4.19 present the spin-resolved electronic band structures and DOS for the RhNbSi compound, computed using the GGA and GGA+U approaches, respectively. In both cases, the spin-down and spin-up band structures are displayed on the left and right plots, while the central plot illustrates the TDOS and PDOS. These results provide valuable insight into the compound's electronic structure and magnetic characteristics. In Figure 4.18, which corresponds to the GGA calculation, it is evident that none of the energy bands intersect the E_F , indicating semiconducting behavior. Furthermore, the band structures for both spin channels are essentially identical, demonstrating the absence of spin polarization. This observation is supported by the DOS plot, where the spin-up and spin-down states exhibit a symmetric distribution. The atomic-PDOS for Rh, Nb, and Si also confirms this symmetry, suggesting that RhNbSi is non-magnetic under GGA treatment. Figure 4.19, which includes the on-site Coulomb interaction via the GGA+U method, shows similar behavior. The spin-up and spin-

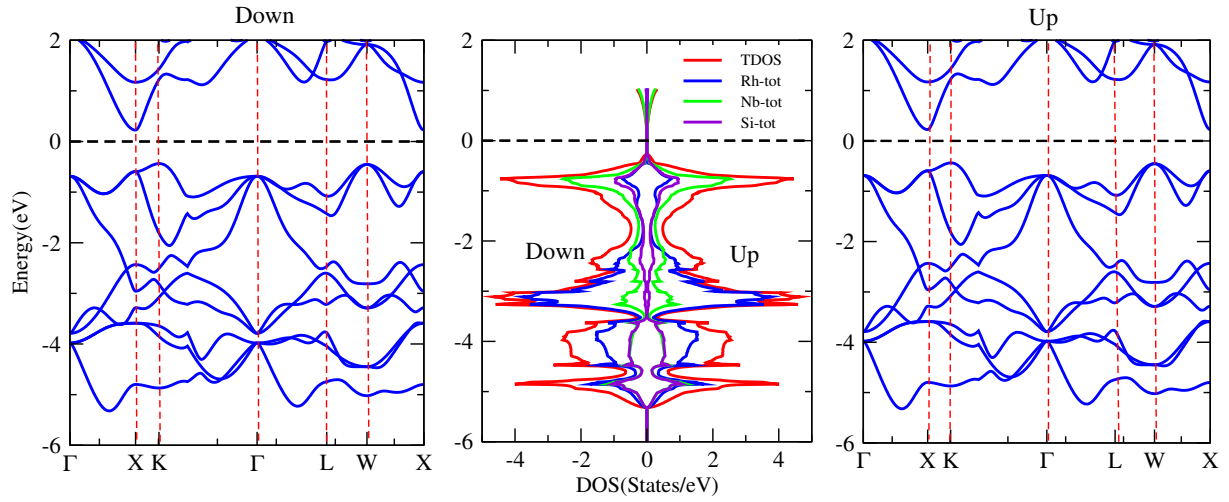


Figure 4.18: Spin-up and spin-down band structures and DOS of RhNbSi compound from GGA. Fermi level at zero (black dotted line).

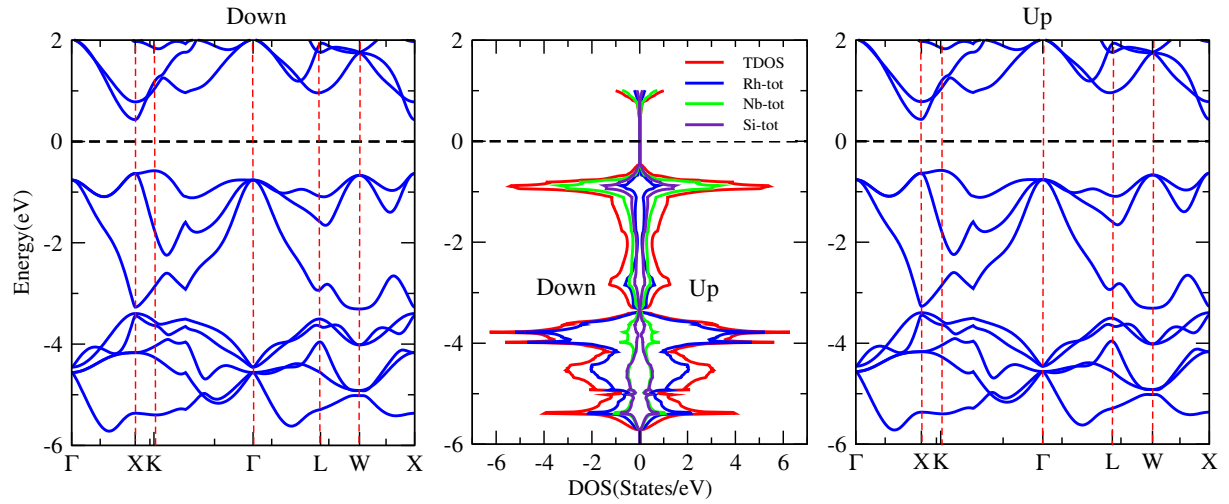


Figure 4.19: Spin-up and spin-down band structures and DOS of RhNbSi compound from GGA+U. Fermi level at zero (black dotted line).

down bands remain nearly identical, and no electronic states appear at the E_F , reaffirming the semiconducting nature of the material. A modest increase in the band gap is observed, consistent with the typical effect of the U correction, which accounts for electron-electron correlation in localized d orbitals. The DOS remains symmetric between the spin channels, and the contributions from individual atoms are balanced, further verifying the compound's non-magnetic character. Therefore, the RhNbSi compound maintains its non-magnetic semiconducting nature under both GGA and GGA+ U frameworks. The lack of spin asymmetry and the absence of

states at the E_F rule out half-metallicity or intrinsic magnetism. As such, while RhNbSi may not be ideal for spintronic applications, its robust semiconducting properties make it a promising material for optoelectronic applications. The calculated values of band gap under both GGA and GGA+U with previous work is illustrated in Table 4.8 showing quite agreement between the two works.

Table 4.8: Electronic band gaps of RhNbSi HH compound at its equilibrium lattice constants, computed with GGA and GGA+U.

HH compound	Approach	E_g (eV)
RhNbSi	GGA	0.662
	Other work	0.68 (Ahmed et al., 2024)
	GGA+U	1.0095
	Other work	-

Because of its unique electronic properties, its indirect band gap is perfect for a variety of technological applications. This compound is a good runner for optoelectronic applications such as LEDs, IR detectors and photodetectors, because longer carrier lifetimes enable effective photon absorption and emission. RhNbSi's moderate indirect band gap and promising electrical properties make it a suitable candidate for photovoltaic solar energy conversion. Our results on RhNbSi compound shows consistent with the previous work on this compound reported by Ahmed with his co-works (Ahmed et al., 2024).

4.3.3 Band Structure and density of states of RhIrZ (Z = Li, As, Si, Sb) HH compounds

The electronic analysis of RhIrLi compound by GGA calculation is presented in Figure 4.20. The band structure indicates that both spin-up and spin-down bands cross the E_F , confirming the metallic nature of RhIrLi. Furthermore, the bands appear symmetric for both spin channels, meaning that no significant spin polarization occurs within the GGA framework. The DOS at E_F remains nonzero for both spin-up and spin-down states, further supporting the metallic character of the material. The PDOS analysis reveals that the Rh and Ir orbitals dominate the electronic states near E_F , while the Li states contribute in small amount. This suggests that the conductivity in RhIrLi is primarily governed by the transition metal elements (Rh and Ir), while Li plays a negligible role. The symmetry between the spin-up and spin-down bands indicates that electron correlation effects are not strong enough under GGA to induce spin polarization in this compound, making RhIrLi a non-magnetic metal within this approximation.

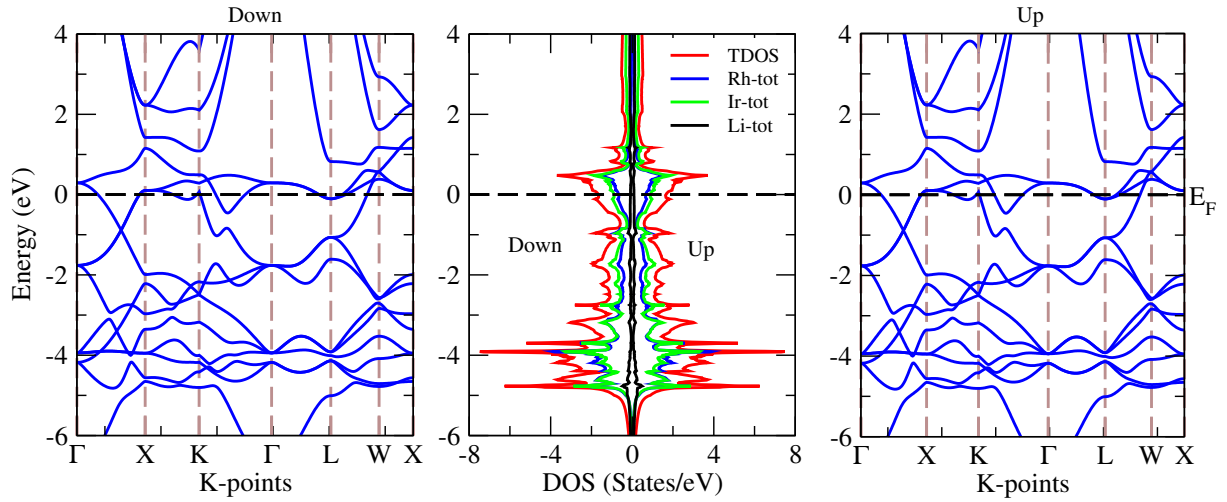


Figure 4.20: Electronic band structure and density of states for spin-up and spin-down states of RhIrLi compound, calculated using GGA. The Fermi level is indicated by the black dotted line at zero energy.

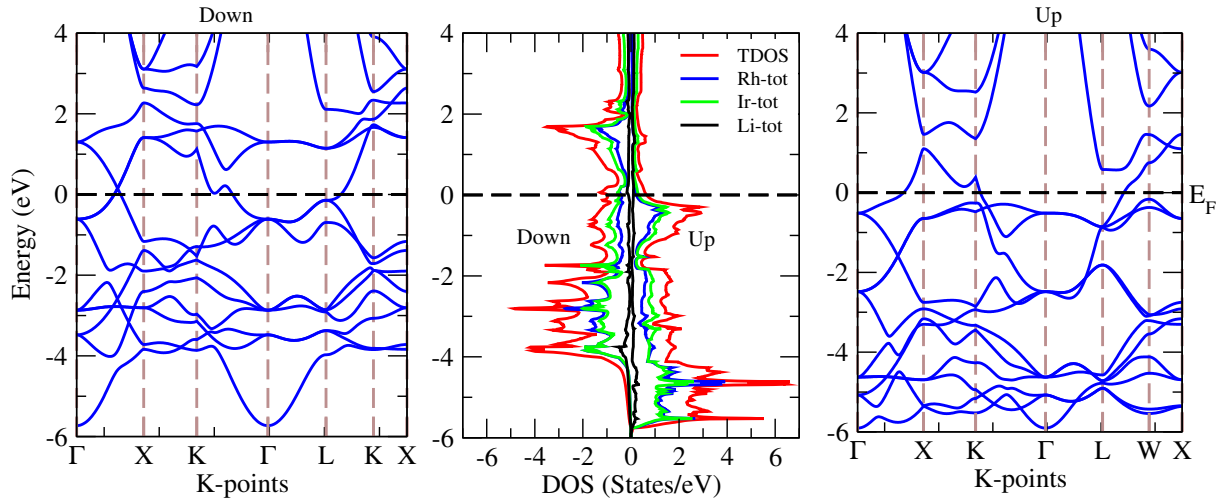


Figure 4.21: Electronic band structure and density of states for spin-up and spin-down states of RhIrLi compound, calculated using GGA+U. The Fermi level is indicated by the black dotted line at zero energy.

In Figure 4.21, the GGA+U results for RhIrLi reveal notable differences compared to the GGA case. The U correction modifies the electronic structure by introducing electron correlation effects, which influence the d-orbitals of Rh and Ir. Unlike in the GGA case, the band structure in Figure 4.21 is no longer symmetric between the spin-up and spin-down channels, indicating that the inclusion of U has broken spin degeneracy and induced a degree of spin po-

larization. Despite this spin asymmetry, the metallic nature persists, as bands continue to cross the E_F in both spin channels. The PDOS analysis shows that Rh and Ir d-states shift due to the correlation effects, leading to differences in the distribution of states between spin-up and spin-down electrons. This suggests that electron-electron interactions are now sufficiently strong to influence the spin channels differently, breaking the symmetry observed in the GGA case. The electronic properties of RhIrLi, as obtained from our calculations, show reasonable agreement with earlier studies on similar HH systems (Babalola and Iyozor, 2022), indicating consistency with established theoretical trends.

Figures 4.22 and 4.23 present the analyzed spin-polarized electronic band structures and DOS of the RhIrAs compound, calculated using two different approaches (GGA and GGA+U). In Figure 4.22, computed using the GGA approach, the band structures exhibit a metallic nature, as several bands cross the E_F in both spin channels. This is further supported by the DOS plot due the presence of DOS lines at E_F , confirming that the material does not exhibit an energy gap. A notable feature of the GGA result is the symmetric nature of both the band structure and DOS between the spin-up and spin-down channels, suggesting that electron correlation effects are weakly pronounced in this approximation. The atomic-resolved DOS reveals that Ir and Rh contribute the most to the TDOS near the E_F , indicating that their orbitals play a dominant role in defining the electronic states around E_F . On the other hand, the contribution from As is relatively low compared to these atoms, suggesting that it has the least impact on the TDOS in this energy region. The strong hybridization among these atoms is evident from their overlapping DOS features, reinforcing the delocalized nature of the electronic states.

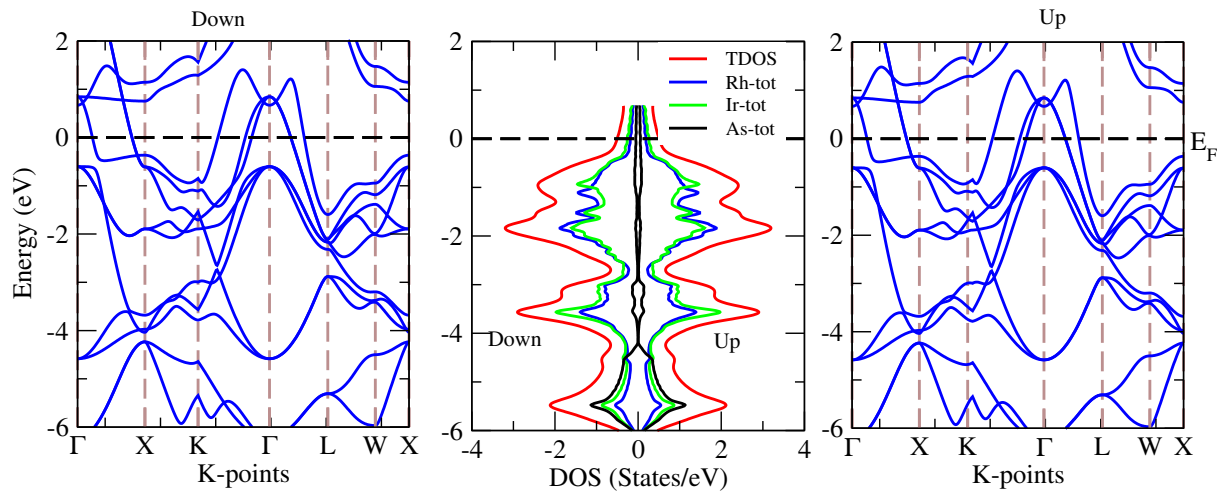


Figure 4.22: Electronic band structure and density of states for spin-up and spin-down states of RhIrAs compound, calculated using GGA. The Fermi level is indicated by the black dotted line at zero energy.

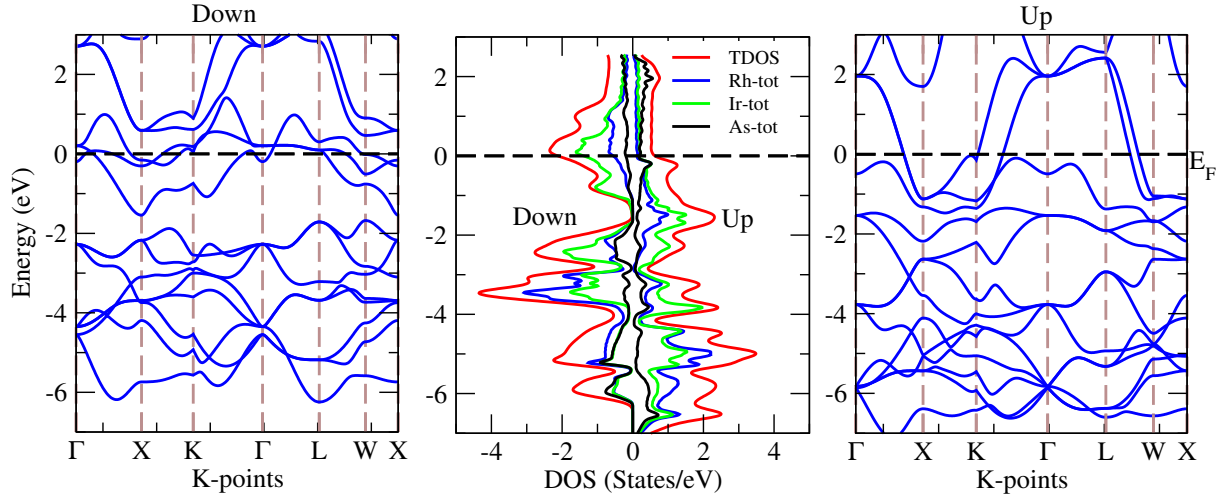


Figure 4.23: Electronic band structure and density of states for spin-up and spin-down states of RhIrAs compound, calculated using GGA+U. The Fermi level is indicated by the black dotted line at zero energy.

In Figure 4.23, where the GGA+U approach is employed, noticeable changes in the electronic structure are observed due to the inclusion of the U potential. The band dispersion is modified and the electronic states become more localized compared to the GGA results. However, despite these differences, the E_F is still crossed by band lines in both spin channels, indicating that the compound retains its metallic behavior. This observation is also reflected in the DOS plot, where a finite DOS remains at E_F . Unlike the GGA result, the GGA+U approach introduces an asymmetry between the spin-up and spin-down electronic structures, suggesting that electron correlation effects induce spin-dependent localization and redistribution of electronic states. Similar to the GGA case, Ir and Rh remain the dominant contributor to the TDOS, while As continues to be the least contributor. The U correction enhances spin splitting and orbital localization, yet it does not introduce a full band gap, which would be required for a transition to a semiconducting or insulating state. The atomic contributions to the TDOS remain significant, confirming the persistent hybridization effects in the compound. The electronic properties of RhIrAs as obtained from our calculations, show commonsense agreement with previous studies on related HH compounds (Paul et al., 2024), reflecting consistency with established theoretical expectations.

Figures 4.24 and 4.25 illustrate the spin-polarized electronic band structures and DOS of the RhIrSi compound, calculated using two different approaches: GGA and GGA+U. In Figure 4.24, obtained using the GGA approach, the band structures indicate a metallic nature, as multiple bands cross the E_F in both spin-up and spin-down channels. This metallic character

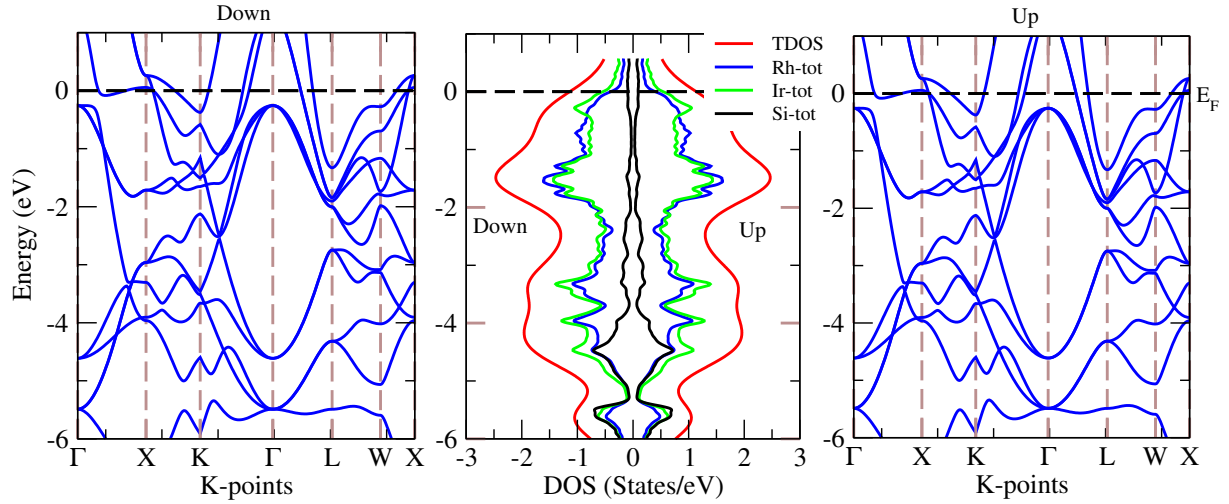


Figure 4.24: Electronic band structure and density of states for spin-up and spin-down states of RhIrSi compound, calculated using GGA. The Fermi level is indicated by the black dotted line at zero energy.

is further supported by the DOS plot, where a finite TDOS is present at E_F . There is a nearly symmetric distribution of the band structures and DOS between the spin channels, suggesting a relatively weak spin polarization in the GGA approach. The atomic-resolved DOS indicates that Ir and Rh contribute the most to the TDOS near the E_F , signifying that their orbitals play a dominant role in shaping the electronic properties of the compound. In contrast, the contribution from Si is the least significant, indicating that it has a minimal influence on the total electronic states at E_F . The presence of hybridization between Rh, Ir and Si atoms is evident from the overlapping DOS curves, reinforcing the delocalized nature of the electronic states.

In Figure 4.25, where the GGA+U approach is applied, notable modifications in the electronic structure are observed due to the inclusion of the U correction. The band structures exhibit significant changes, with some bands shifting away from the E_F , leading to increased localization of electronic states. However, despite these modifications, bands still cross the E_F , confirming that the compound retains its metallic behavior. The DOS plot also shows a finite TDOS at E_F , consistent with the metallic nature of RhIrSi.

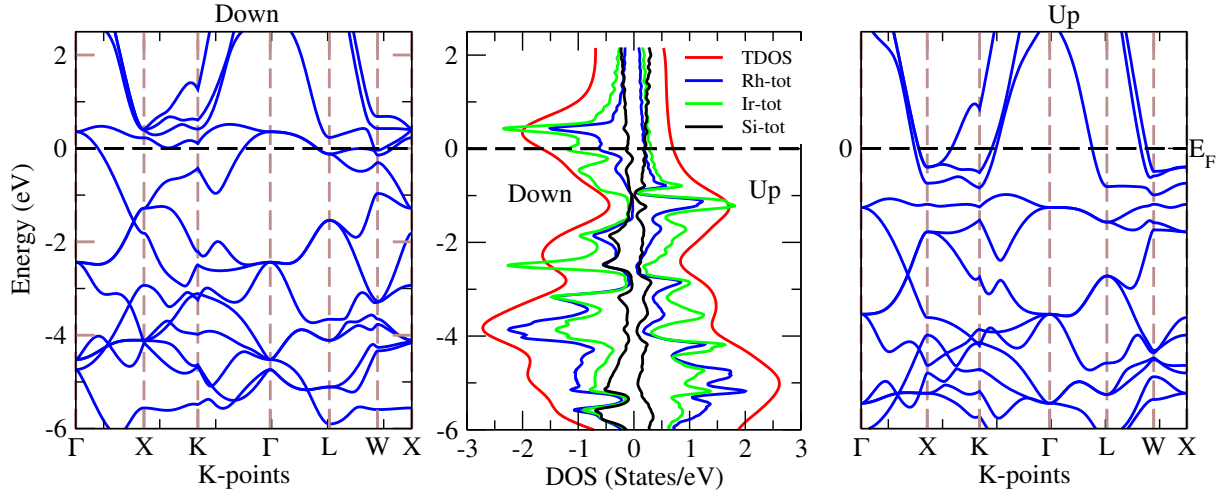


Figure 4.25: Electronic band structure and density of states for spin-up and spin-down states of RhIrSi compound, calculated using GGA+U. The Fermi level is indicated by the black dotted line at zero energy.

One striking difference between GGA and GGA+U results is the introduction of asymmetry in both the band structures and DOS in Figure 4.25 between the spin-up and spin-down channels. This asymmetry implies that the U correction enhances spin polarization by modifying the exchange splitting between the spin states. Similar to the GGA case, Ir remains the dominant contributor to the TDOS followed by Rh, while Si continues to contribute the least. The U correction increases the localization of d-electrons, particularly in Ir and Rh atoms, which leads to the observed changes in band dispersion and DOS. The electronic properties of RhIrSi, as determined from our calculations, are in acceptable agreement with earlier reports on related HH compounds (Shi et al., 2021), demonstrating consistency with established theoretical findings.

Figures 4.26 and 4.27 illustrate the spin-polarized electronic band structures and DOS of the RhIrSb compound which were computed using the GGA and GGA+U approaches. In Figure 4.26, the GGA-based band structure reveals a metallic nature of the RhIrSb compound, as multiple band lines cross the E_F in both spin-up and spin-down channels. The corresponding DOS plot also confirms the metallic behavior, with a finite DOS at E_F . The main observation in the GGA approach is the symmetry in the electronic structure between the spin channels, suggesting weak spin polarization effects. The atomic-PDOS indicates that Ir and Rh contribute the most to the TDOS near the E_F , implying that their orbitals dominate the electronic states governing the transport properties of the compound. Conversely, Sb contributes the least, suggesting its minimal role in the conduction mechanism. The hybridization among Rh, Ir and Sb atoms is evident from the overlapping DOS features, signifying strong electronic interactions

within the compound.

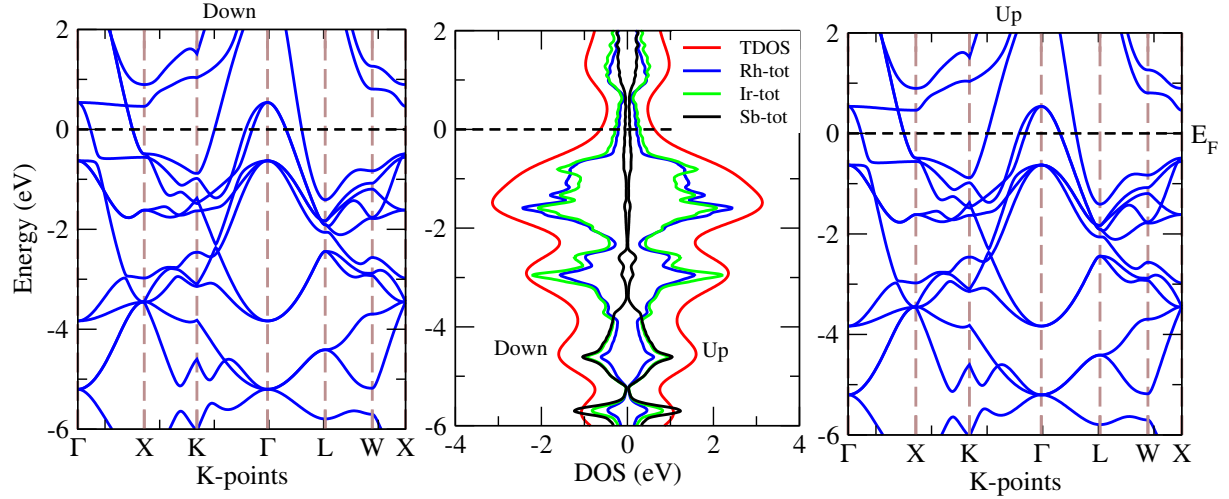


Figure 4.26: Electronic band structure and density of states for spin-up and spin-down states of RhIrSb compound, calculated using GGA. The Fermi level is indicated by the black dotted line at zero energy.

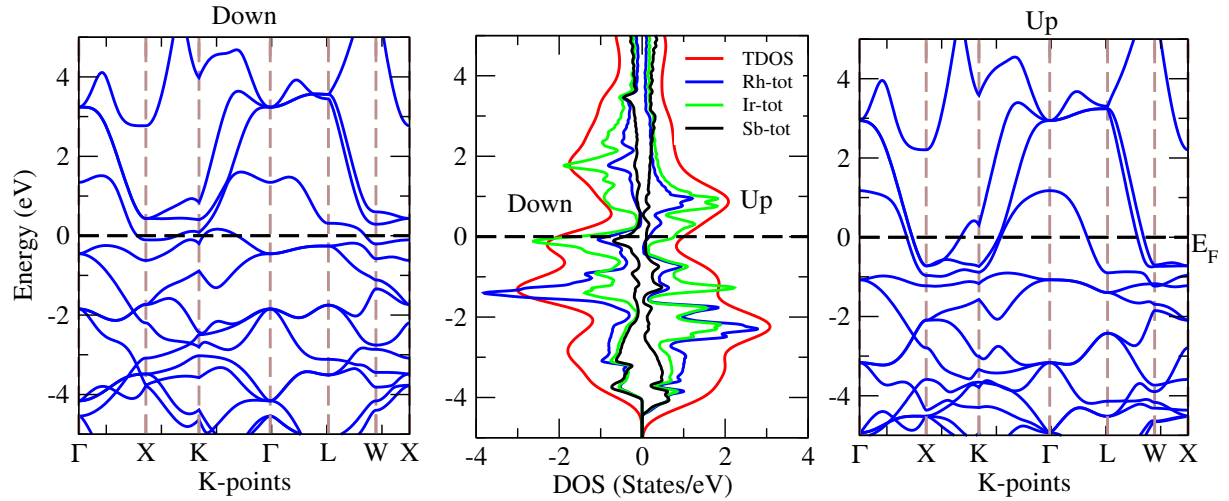


Figure 4.27: Electronic band structure and density of states for spin-up and spin-down states of RhIrSb compound, calculated using GGA+U. The Fermi level is indicated by the black dotted line at zero energy.

In Figure 4.27, the GGA+U calculation introduces noticeable modifications to the electronic structure due to the inclusion of electron correlation effects. Compared to the GGA results, the band structure in the GGA+U case shows a significant shift in band positions, leading to increased localization of electronic states. However, despite these changes, bands still cross

the E_F , indicating that the metallic character of RhIrSb is preserved. The DOS plot further supports this observation, as a finite DOS lines remain at E_F . One of the most notable differences between the two approaches is the introduction of asymmetry in the band structures and DOS under GGA+U, particularly between the spin-up and spin-down channels. This asymmetry suggests that the U correction enhances spin polarization by modifying the exchange splitting between spin states. Similar to the GGA case, Ir and Rh remain the most significant contributor to the TDOS, while Sb exhibits the lowest contribution. The application of U increases the localization of Ir and Rh d-electrons, which alters the electronic dispersion and DOS profile. The electronic properties of RhIrSb obtained from our calculations exhibit consistent agreement with previous studies on comparable HH compounds (Paul et al., 2024), affirming the reliability of the theoretical approach used.

As magnetic metallic materials, the RhIrZ (Z = Li, As, Si, Sb) compounds combine metallic conductivity and magnetic ordering, making them attractive options for cutting-edge spintronics, optoelectronics and energy-related technologies. Strong SOC, which is beneficial for spintronic devices like spin valves and MTJs, where SOC boosts SHEs and spin polarization, is facilitated by the presence of heavy elements like Rh and Ir. Ir-based HH compounds have shown advantageous electronic structures and optical characteristics in the field of optoelectronics, which makes them appropriate for uses such as infrared detectors and transparent conductive electrodes (Erkisi and Candan, 2023; Wei and Wang, 2017).

4.4 Optical Properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds

The exploration of optical properties in RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) compounds is pivotal for evaluating their potential in optoelectronic applications. Key parameters such as the dielectric function, refractive index, extinction coefficient, absorption coefficient, electron energy loss, reflectivity and optical conductivity offer vital insights into electronic transitions and light-matter interactions within these materials. A thorough understanding of their optical response is essential for advancing technologies such as photovoltaics, photodetectors and infrared devices. We employed first-principles DFT calculations to systematically investigate the frequency dependent behavior of these optical properties. Our results were compared with previously reported studies and found to be in good agreement, indicating the reliability and accuracy of the present computational approach.

4.4.1 Optical Properties Analysis of RhZrZ (Z = As, Li, Si, Sb) HH Compounds

Figure 4.28 illustrates some optical parameters against photon energy for RhZrAs compound. The real part of the dielectric function (ϵ_1) starts with a high positive value at low photon energy, indicating strong polarization effects. As photon energy increases, ϵ_1 gradually decreases and crosses the zero axis at a certain energy threshold, which corresponds to the plasma frequency, indicating a transition from dielectric to metallic behavior. The imaginary part, ϵ_2 , represents the material's absorption response. It exhibits a peak in the lower photon energy region, suggesting strong interband transitions due to electron excitations. The decrease in ϵ_2 at higher energies indicates a reduction in absorption as photon energy increases. The refractive index (n) follows a trend similar to ϵ_1 , initially showing a high value at low photon energies and gradually decreasing. This suggests that RhZrAs has strong optical refraction in the low-energy region with $n(0) = 4.99$, which is almost consistent with the findings of Manzoor with his colleagues (Manzoor et al., 2024), but it is higher than the refractive index of common semiconductors such as silicon. This high value may be due to very strong interband electronic transitions near the band edge. The extinction coefficient (k), which describes the material's absorption of light, exhibits a peak at lower photon energies, corresponding to the peak in ϵ_2 . This confirms that the material has strong optical absorption in this region, making it a candidate for optoelectronic applications requiring efficient light absorption.

The reflectivity (R) curve indicates moderate reflectance at low photon energies ($R(0) = 0.49$), which decreases as energy increases. Moderate R value at low energy ranges indicate that part of the light is reflected but a significant amount of light is either absorbed (by interband transitions or free carriers) or transmitted (if the band gap allows it). The reduction in reflectivity at higher energies suggests that RhZrAs allows more light transmission in these high photon energy ranges. The absorption coefficient (α), which quantifies the penetration depth of light in the material, exhibits a rapid increase at certain low photon energy ranges. This sharp rise corresponds to strong optical transitions and suggests that RhZrAs is highly absorbing in these certain energy ranges. The electron energy loss function (L), which measures the energy dissipated by fast electrons moving through the material, shows a prominent peak at the plasma frequency. This peak marks the point where the dielectric function crosses zero, indicating collective oscillations of free carriers (plasmons). The optical conductivity components (σ_1 and σ_2) show strong responses at low to mid-photon energy ranges, suggesting that RhZrAs exhibits good optical conductivity. In conclusion, the results of the studied optical properties of the RhZrAs compound are in fair agreement with other previous optical analysis

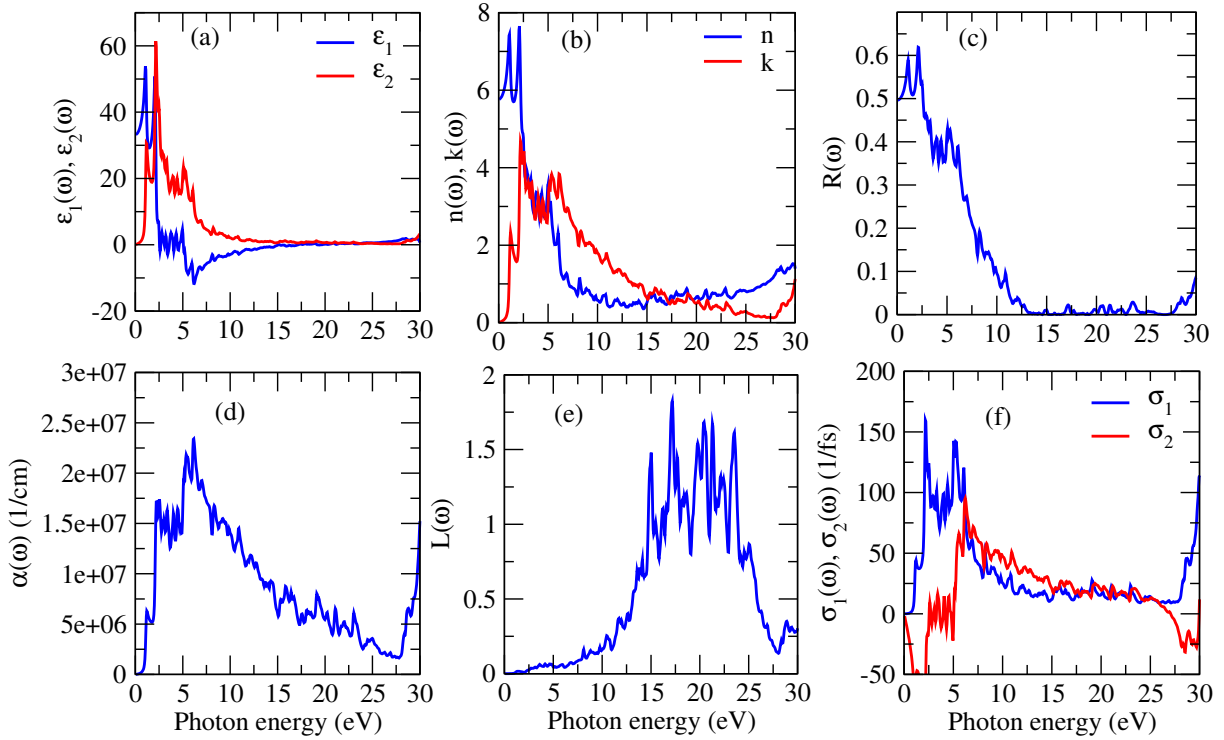


Figure 4.28: Optical properties of RhZrAs as a function of photon energy (GGA calculation): (a) Dielectric function (ϵ_1 , ϵ_2), (b) Refractive index (n) and extinction coefficient (k), (c) Reflectivity (R), (d) Absorption coefficient (α), (e) Electron energy loss (L), (f) Optical conductivity (σ_1 and σ_2).

and reveal that the compound exhibits strong optical absorption, moderate reflectivity, low electron energy loss and good optical conductivity (Manzoor et al., 2024). The presence of plasma frequency suggests metallic behavior at higher energies, while the strong peaks in the absorption coefficient and extinction coefficient indicate potential applications in optoelectronics and photovoltaics (Hosseinzadeh et al., 2022; Wafula, 2023). These results highlight RhZrAs as a promising material for advanced optical applications, since it is semiconductor HH compound.

The optical properties of RhZrSb compound have been systematically investigated using the GGA approach. Figure 4.29 illustrates various optical parameters as functions of photon energy, providing insights into the compound's interaction with electromagnetic radiation. The real part, $\epsilon_1(\omega)$, which represents the material's ability to store electric energy, exhibits a sharp peak at low photon energy, indicating strong polarization effects. It then gradually decreases and stabilizes at higher energies. The imaginary part, $\epsilon_2(\omega)$, corresponds to the material's absorption of incident photons due to interband transitions. A prominent peak in $\epsilon_2(\omega)$ at low energy suggests strong optical absorption in the visible range, implying that RhZrSb has a considerable

optical response in this region. The refractive index ($n(\omega)$) follows a trend similar to $\varepsilon_1(\omega)$, with

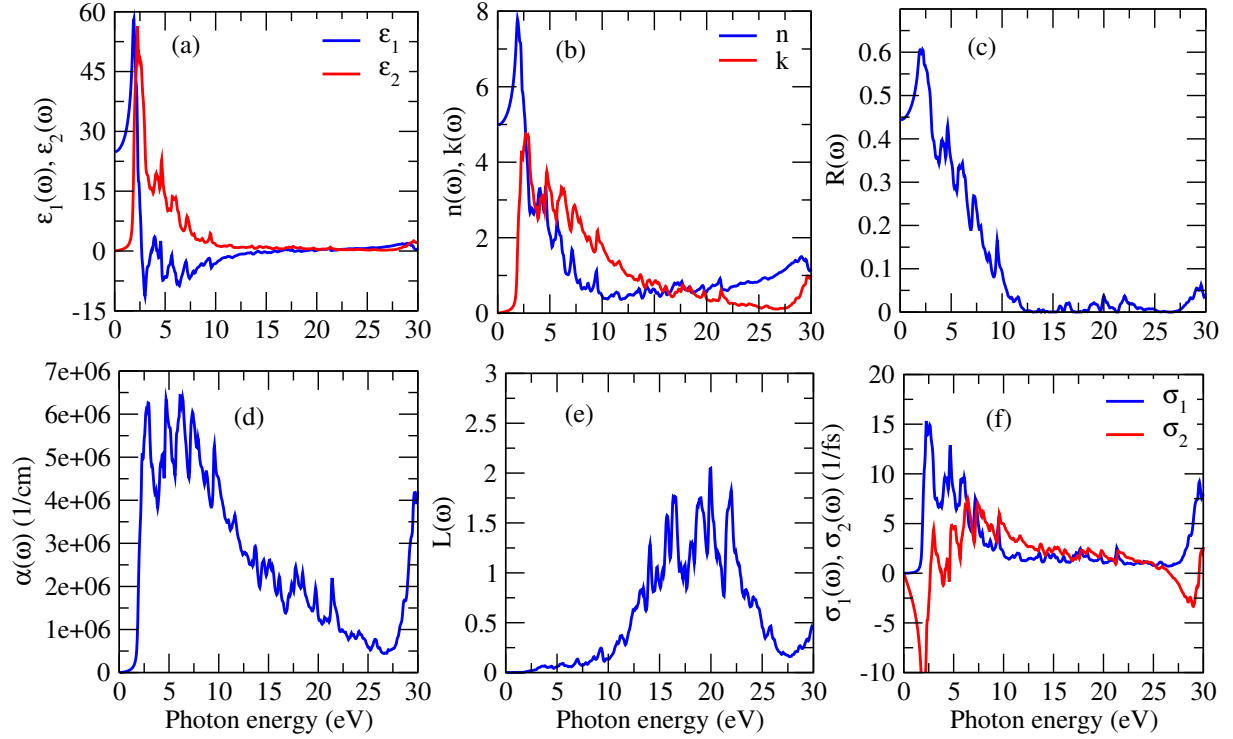


Figure 4.29: Optical properties of RhZrSb as a function of photon energy (GGA calculation): (a) Dielectric function (ε_1 , ε_2), (b) Refractive index (n) and extinction coefficient (k), (c) Reflectivity (R), (d) Absorption coefficient (α), (e) Electron energy loss (L), (f) Optical conductivity (σ_1 and σ_2).

$n(0) = 4.60$, a value which nearly in consistent with the previous works by benzoudjis' research team (Benzoudji et al., 2019), reaching its maximum value in the visible energy region before decreasing sharply. This behavior suggests a high initial refractive response, which diminishes at higher energies. The extinction coefficient, $k(\omega)$, which is directly related to the material's absorption capability, follows the pattern of $\varepsilon_2(\omega)$, confirming that RhZrSb exhibits significant absorption in the visible to low UV photon energy ranges.

Reflectivity, $R(\omega)$ decreases steadily as photon energy increases. This indicates that RhZrSb has moderate reflectivity in the low-energy region, which diminishes at higher photon energies. The absorption coefficient, $\alpha(\omega)$ characterizes the material's ability to absorb light at different photon energies. The significant absorption observed at lower energies aligns with the peaks in $\varepsilon_2(\omega)$ and $k(\omega)$, confirming strong optical transitions. The electron energy loss function, $L(\omega)$ provides insights into plasmonic behavior. Peaks in this function correspond to plasmon excitation energies, where collective oscillations of electrons occur. The presence of a distinct

peak suggests that RhZrSb may exhibit plasmonic behavior at specific photon energies. The real part of optical conductivity, $\sigma_1(\omega)$ corresponds to absorptive optical conductivity and exhibits prominent peaks in regions of strong absorption. The imaginary part of optical conductivity, $\sigma_2(\omega)$ which is related to the material's inductive response, follows a trend similar to $\varepsilon_1(\omega)$. The observed behavior suggests that RhZrSb has significant optical conductivity in the low-energy region, making it a potential candidate for applications in transparent conductive materials. The results of optical properties obtained for RhZrSb compound are in good agreement with previous works reported in (Knyazev et al., 2024; Mehta and Saini, 2024). In general, the optical properties of RhZrSb indicate strong absorption, high refractive index and low electron energy loss in the low photon energy range, making it a promising material for optoelectronic application such as solar cells, photodetectors and optical switches..

Figure 4.30 illustrates the variation of different optical parameters of RhZrLi with photon energy, providing valuable insights into the material's interaction with electromagnetic radiation. In the low photon energy range (0-1.35 eV), this compound exhibit strong metallic behavior, as indicated by a negative real part (ε_1) and a large imaginary part (ε_2) of the dielectric function. This leads to a high extinction coefficient (k), showing strong absorption, while the refractive index (n) is typically low with $n(0) = 0.39$. These optical constants contribute to high reflectivity with $R(0) = 0.94$, making this material ideal for infrared mirrors and thermal coatings. The large k also translates into a high absorption coefficient, indicating significant weakness of light within a short penetration depth, key for applications in optical limiters, broadband absorbers and plasmonic devices. The electron energy loss function (L) remains low at very low photon energies but shows a characteristic peak near the plasma frequency, where $\varepsilon_1 = 0$, signaling strong plasmon excitation which is useful in plasmonics and energy loss spectroscopy. Additionally, the real part of optical conductivity, σ_1 is high in the low photon ranges, denoting strong free-carrier absorption typical of metals, while the imaginary part, σ_2 often appears negative due to the negative ε_1 . The results of optical properties we obtained here below 10 eV well agree with previous works on related Zr_2XBiNi_2 ($X = Al, Ga$) double HH compounds reported in (Douinat et al., 2023). This complex conductivity profile reflects the dominance of Drude-like intraband transitions and supports applications in infrared sensors, plasmonic electronics, and electromagnetic shielding.

Above 10 eV photon energy, both ε_1 and ε_2 flatten out and approach zero, leading to a corresponding drop in both n and k . The refractive index becomes very low and stable and the extinction coefficient approaches zero, indicating negligible interaction with high energy photons. As a result, reflectivity and absorption coefficient drop sharply, and the material behaves almost like a transparent medium with minimal optical response. On the other hand, the L

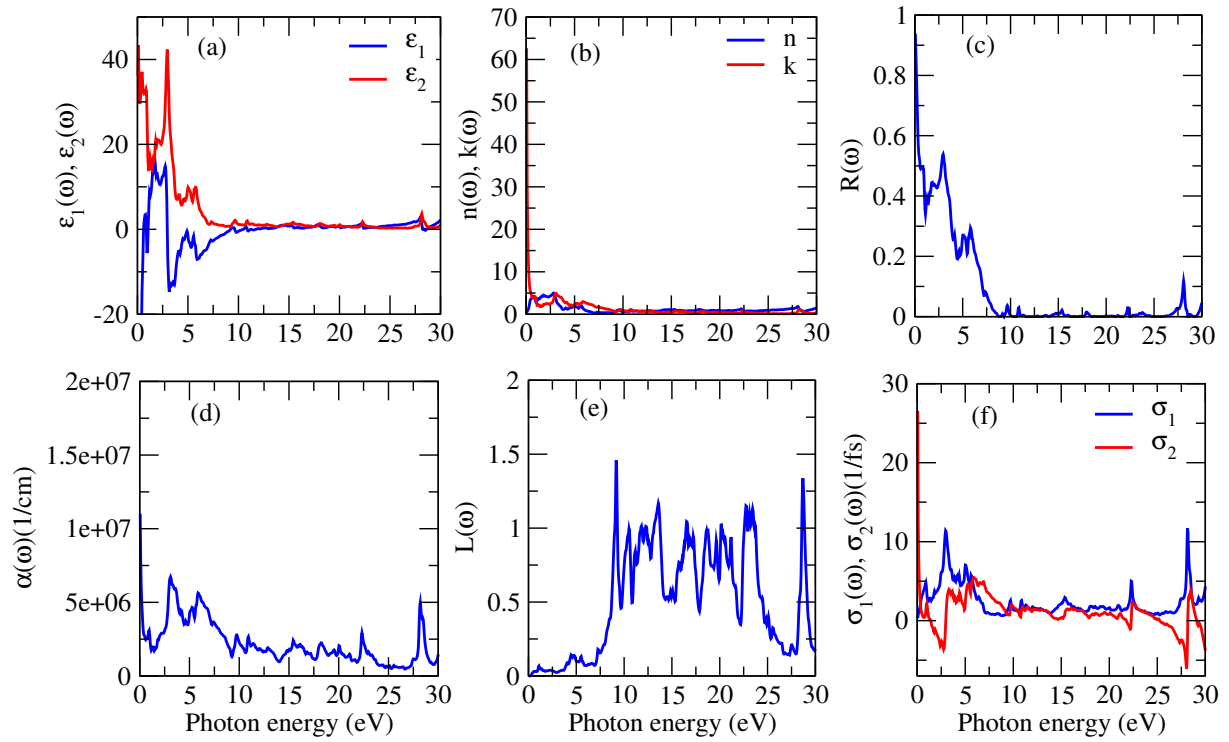


Figure 4.30: Optical properties of RhZrLi as a function of photon energy (GGA calculation): (a) Dielectric function (ϵ_1 , ϵ_2), (b) Refractive index (n) and extinction coefficient (k), (c) Reflectivity (R), (d) Absorption coefficient (α), (e) Electron energy loss (L), (f) Optical conductivity (σ_1 and σ_2).

sharply raises to have high peak at around 9 eV, with many peaks between energy ranges of 9-28 eV signifying the presence of significant inelastic electron interactions or collective excitations. Finally, both the real and imaginary parts of the optical conductivity tend to have small values from 10 eV to 25 eV, indicating that the material lacks free-carrier or interband transition contributions at these high energy ranges. This defines a boundary beyond which the material is no longer useful for active optoelectronic functions. Thus, the optical response of RhZrLi compound is predominantly confined to the very low energy range, where its strong metallic and plasmonic properties can be effectively utilized in infrared optics, plasmonic circuits, thermoelectric modules and protective coatings for energy management and device efficiency, as supported by the findings in (Idrissi et al., 2024; Amudhavalli et al., 2018).

Figure 4.31 presents various optical parameters of the RhZrSi compound as a function of photon energy, providing insights into its electronic transitions, optical response and potential applications in optoelectronic and plasmonic devices. In the low photon energy range of 0–0.6 eV, RhZrSi displays clear metallic properties, as indicated by the negative real part of the di-

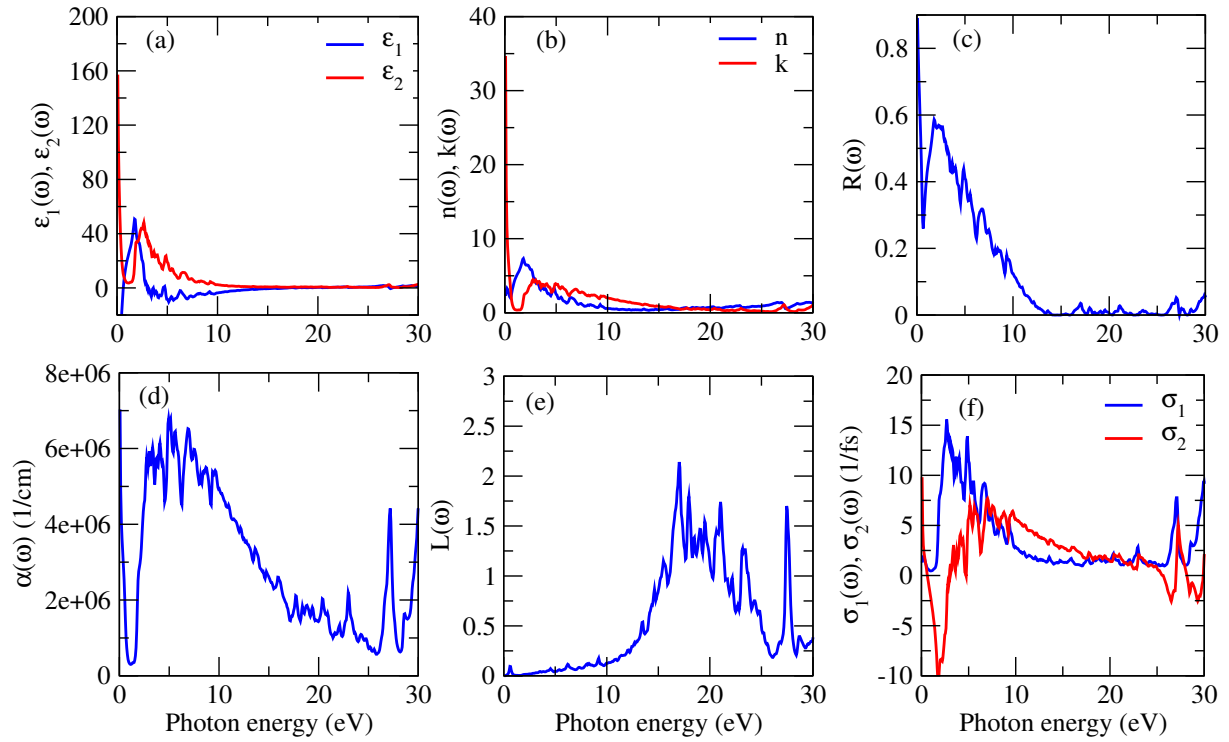


Figure 4.31: Optical properties of RhZrSi as a function of photon energy (GGA calculation): (a) Dielectric function (ϵ_1 , ϵ_2), (b) Refractive index (n) and extinction coefficient (k), (c) Reflectivity (R), (d) Absorption coefficient (α), (e) Electron energy loss (L), (f) Optical conductivity (σ_1 and σ_2).

electric function (ϵ_1) and the large values of imaginary part (ϵ_2). The negative ϵ_1 reflects the material's ability to support free-electron oscillations, a key feature of metals and plasmonic materials, while the large ϵ_2 suggests significant energy dissipation arising from free-carrier absorption and possible low-energy interband transitions. In this region, the refractive index, n is relatively low, starting from $n(0)=2.27$, while the extinction coefficient, k is high, confirming strong absorption (α) of electromagnetic waves. As a result, the reflectivity, R is also remarkably high, particularly at zero photon energy where $R(0)=0.89$, indicating efficient reflection of incident infrared light, typical of metallic surfaces. The electron energy loss function (L) is minimal across 0–10 eV, implying negligible energy loss due to small inelastic electron scattering, further supporting the idea of limited electron excitation in this energy window. Interestingly, the imaginary part of the optical conductivity (σ_2) appears negative in this region, consistent with the negative ϵ_1 , which reinforcing the metallic behavior of the compound. Meanwhile, the real part of the conductivity (σ_1) is positive, indicating that the material absorbs electromagnetic energy effectively. The optical response of RhZrSi within the 0–10 eV range aligns well with

earlier studies on related HH systems in (Bouhadjer et al., 2024), supporting the reliability of our findings in these energy ranges. These combined features make RhZrSi a strong candidate for use in infrared optical technologies, such as thermal barrier coatings, low-emissivity mirrors and plasmonic waveguides.

In contrast, above 13 eV, both ε_1 and ε_2 diminish significantly and remain nearly constant with increasing photon energy, signifying a shift to a regime of optical inactivity. In this high-energy range, the electrons are no longer responsive to incident photons via interband transitions or collective excitations, resulting in minimal interaction with light. Consequently, the refractive index and extinction coefficient both decrease to very small values and remain flat, indicating near-transparency of the material. The absorption coefficient, which depends on k , also becomes very low, suggesting that RhZrSi does not absorb much radiation at these energies. Reflectivity drops significantly as well, since the dielectric response weakens, allowing most photons to pass through the material. Notably, the electron energy loss function (L) rises sharply starting around 10 eV, peaking at 17 eV, where $\varepsilon_1 = 0$, a condition that marks strong plasmon excitation, a useful property for plasmonic applications and electron energy loss spectroscopy. Between 17 and 27 eV, multiple peaks in the loss function indicate significant inelastic electron interactions and collective excitations, despite the material's low optical activity in terms of dielectric and conductivity responses. During this range, both the real and imaginary parts of the optical conductivity remain small, confirming limited electronic transitions or conduction processes. The optical properties obtained here for RhZrSi HH compound above 13 eV are consistent with the optical properties of the LiSrX (X = P, As) compounds to HH studied in (Azouaoui et al., 2023). Although these properties above 13 eV limit the use of RhZrSi in high-energy optoelectronics, its UV-range transparency may be beneficial for UV-pass filters, protective optical coatings, or transparent support layers in complex multilayer device architectures where selective spectral filtering is required (Rezazadeh, 2022).

4.4.2 Optical Properties Analysis of RhNbZ (Z = As, Li, Si, Sb) HH Compounds

The optical properties of RhNbSi compound have been analyzed using the GGA approach. Figure 4.32 presents various optical parameters as functions of photon energy, revealing key insights into the material's response to electromagnetic radiation. The real part of the dielectric function ($\varepsilon_1(\omega)$), which describes the polarization capability of the material, shows a high peak at low photon energy, followed by a gradual decrease as energy increases. This indicates strong optical response in the infrared and visible regions. The imaginary part of the dielectric function ($\varepsilon_2(\omega)$) related to the absorption of incident photons due to interband transitions,

exhibits a sharp peak in the low-energy region, suggesting strong optical absorption from mid IR to ultraviolet ranges. The refractive index, $n(\omega)$ follows a similar trend to $\varepsilon_1(\omega)$, showing a peak at low photon energy, with $n(0) = 4.71$ and then decreasing as energy increases, implying high refractive response in the infrared region. The extinction coefficient, $k(\omega)$ which describes the material's absorption, follows the trend of $\varepsilon_2(\omega)$ and confirms significant absorption in the low-energy range.

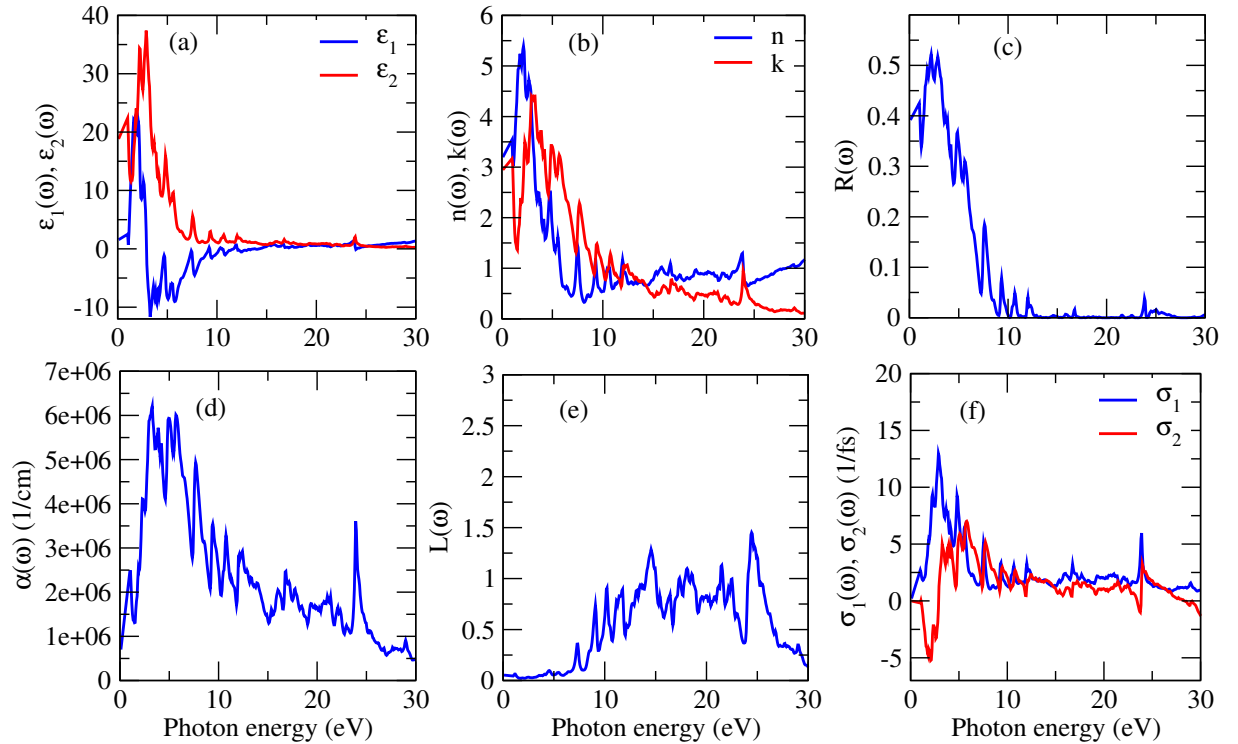


Figure 4.32: GGA-calculated optical properties of RhNbSi as a function of photon energy: (a) dielectric function (ε_1 and ε_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

The reflectivity, $R(\omega)$ has relatively moderate value in the low-energy region, where $R(0) = 0.42$ and decreases as energy increases, suggesting that RhNbSi exhibits good reflectivity at lower photon energies but becomes more transparent at higher energies. The absorption coefficient, $\alpha(\omega)$ describes the material's ability to absorb incident photons. A high absorption coefficient in the visible range indicates strong interband transitions. The absorption decreases at higher energies, suggesting limited absorption in the deep ultraviolet region. The electron energy loss function, $L(\omega)$ provides insights into plasmonic behavior. Peaks in this function correspond to plasmon excitation energies, where collective oscillations of electrons occur. A

distinct peak in $L(\omega)$ at higher photon energies suggests that RhNbSi exhibits plasmonic behavior in the ultraviolet region. The real part of conductivity, $\sigma_1(\omega)$ indicates strong absorption with prominent peaks in the low-photon energy ranges, indicating high electronic transitions. The imaginary part of optical conductivity, $\sigma_2(\omega)$ which describes the material's inductive response, follows a similar trend to $\varepsilon_1(\omega)$. The obtained result for optical properties of RhNbSi compound is in good agreement with the previous report by Ahmed and his co-works (Ahmed et al., 2024), indicating the reliability of the present calculation. These observations suggest that RhNbSi has significant optical conductivity in the infrared, visible and ultraviolet regions, making it a promising material for transparent conductive applications. Generally, the optical properties of RhNbSi reveal strong absorption, high initial refractive index and low electron energy loss in the low photon energy ranges, indicating that it can be considered as a potential candidate for wide range of optoelectronic and energy-related applications, in agreement with the reports of Mesbah and Alrashdi research team (Mesbah et al., 2021; Alrashdi et al., 2022).

The optical response of the RhNbAs compound has been investigated using the GGA. The various optical parameters presented in Figure 4.33 provide insights into the material's interaction with electromagnetic radiation, including absorption, reflection and conductivity. The real part of the dielectric function represents the material's ability to store electric energy, with a high peak at low photon energies, followed by a gradual decrease. This suggests strong polarization effects in the infrared and visible regions. The imaginary part of the dielectric function is associated with optical absorption due to interband transitions. It exhibits a strong peak in the low-energy region, indicating that RhNbAs absorbs photons effectively in the visible and ultraviolet ranges. The refractive index, $n(\omega)$ follows a trend similar to $\varepsilon_1(\omega)$, displaying a peak at low photon energies, with $n(0) = 2.75$ and gradually decreasing with increasing energy. This indicates medium optical refractivity at lower photon energies. The extinction coefficient ($k(\omega)$) follows the pattern of $\varepsilon_2(\omega)$, reinforcing the observation of strong absorption in the ultraviolet region. The reflectivity, $R(\omega)$ indicates the material's ability to reflect incident light. RhNbAs exhibits fair reflectivity in the lower-energy region with $R(0) = 0.22$, which diminishes with increasing photon energy. This suggests that RhNbAs is noticeably reflective in the infrared and visible regions but becomes more transparent at higher energies. The absorption coefficient, $\alpha(\omega)$ measures how effectively the material absorbs photons. The compound has high absorption coefficient in the visible and ultraviolet ranges suggests strong interband transitions. The absorption decreases at higher photon energies, indicating limited absorption in the deep ultraviolet region. The electron energy loss function, $L(\omega)$ provides insights into the plasmonic behavior of RhNbAs. It has small values in low energy ranges and show incremental until it reaches its highest peak at 24 eV. The presence of peaks at higher photon energies

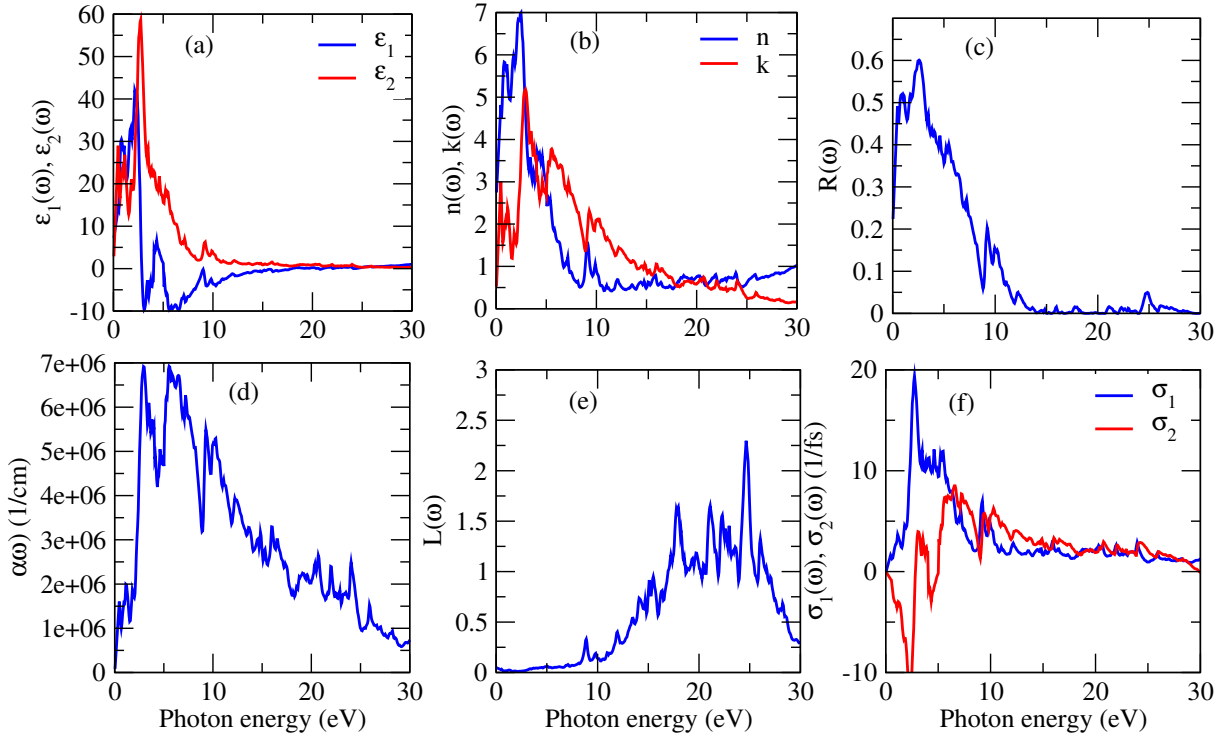


Figure 4.33: GGA-calculated optical properties of RhNbAs as a function of photon energy: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

indicates the occurrence of plasmon excitations, which are collective oscillations of electrons. The real part of optical conductivity, $\sigma_1(\omega)$, which corresponds to absorption conductivity, exhibits strong peaks in regions of high absorption, confirming significant electronic transitions between bands. The imaginary part of the optical conductivity, $\sigma_2(\omega)$ follows a trend similar to $\epsilon_1(\omega)$, reinforcing the dielectric behavior of the material. The nature of optical properties of RhNbAs compound obtained here is in fair agreement with the previous works on the optical properties that were reported in (Zerrouki et al., 2021) and the optical properties of RhMnZ (Z= Si, Ge) HH compounds studied by Gurunani and Gupta (Gurunani and Gupta, 2024b). The presence of high optical conductivity in the visible, infrared and ultraviolet regions suggests that RhNbAs could be utilized in transparent conductive coatings and optoelectronic applications. In conclusion, RhNbAs exhibits strong optical absorption in the ultraviolet range, high initial refractive index and potential plasmonic behavior, making it a promising material for optoelectronic, spintronic and energy-related applications, as claimed by the findings and applications in the literature reported by Osafile and Nenuwe (Osafile and Nenuwe, 2021).

The optical properties of the RhNbSb compound have been investigated using the GGA calculation and illustrated in Figure 4.34. The real part of the dielectric function (ϵ_1) represents the polarization response of the material to an external electric field. It exhibits a peak at low photon energy, indicating strong optical response in the visible region, followed by a steady decline as photon energy increases. The imaginary part of the dielectric function (ϵ_2), which corresponds to the material's absorption due to interband electronic transitions, shows a high peak at lower photon energies, suggesting significant absorption in the visible and ultraviolet (UV) regions. The decline of ϵ_2 at higher energies indicates reduced optical absorption. The refractive index (n) follows a trend similar to ϵ_1 , which have a maximum at low photon energy with $n(0) = 2.74$, suggesting that RhNbSb exhibits strong refractive behavior in the infrared and visible regions. The extinction coefficient (k), which represents the loss of light due to absorption, follows the trend of ϵ_2 , confirming strong absorption in the visible range. RhNbSb exhibits moderate reflectivity in the low-energy region with $R(0) = 0.28$, indicating that it can fairly reflect infrared radiation. However, reflectivity decreases with increasing photon energy, suggesting that the material becomes more transparent in the higher energy (UV) region.

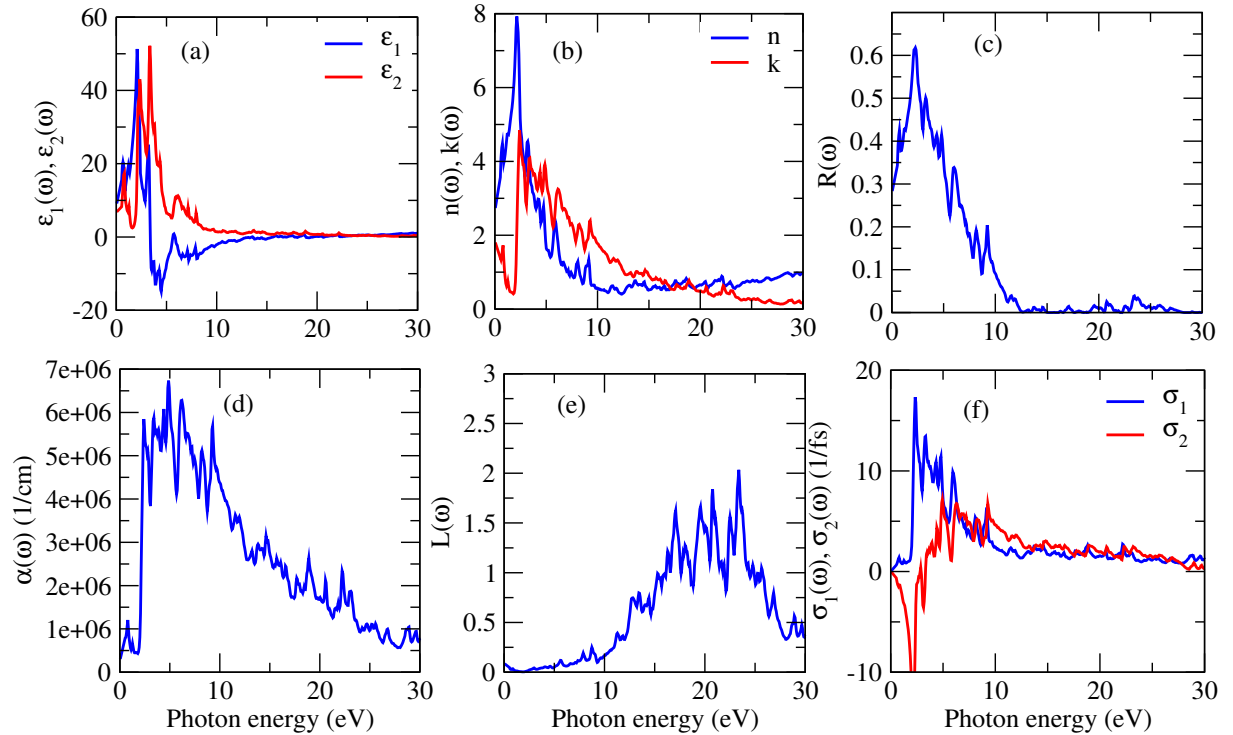


Figure 4.34: GGA-calculated optical properties of RhNbSb as a function of photon energy: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

The absorption coefficient (α), indicates how effectively the material absorbs incident photons. RhNbSb shows a high absorption coefficient in the visible and UV regions, confirming strong interband transitions. The absorption decreases at higher photon energies, indicating lower absorption in the deep UV region. The electron energy loss function provides information about plasmon excitations in the material. Peaks in L indicate the characteristic plasma resonance frequency, where collective oscillations of electrons occur. The presence of peaks at higher photon energies suggests that RhNbSb exhibits plasmonic behavior. The real part of the optical conductivity (σ_1), which corresponds to absorption conductivity, exhibits strong peaks in the lower photon energy region, indicating high optical absorption and electronic transitions. The imaginary part of the optical conductivity (σ_2) follows a similar trend to ε_1 , confirming the dielectric nature of the material.

Optical properties of RhNbSb obtained under current study are in good agreement with reports on optical properties of NbAgSi HH compound investigated by Kalita with his colleagues (Kalita et al., 2022). In general, RhNbSb exhibits strong optical absorption in the visible region, high refractive index at low energies and plasmonic behavior at higher photon energies. These properties make it a promising material for optoelectronic applications, including UV photodetectors, solar cells and transparent conductive coatings. Its high reflectivity in the infrared region also suggests potential applications in optical coatings and mirrors (Pavluhina et al., 2024).

The optical response of the RhNbLi compound has been investigated using the GGA which is presented in Figure 4.35. The analysis of these optical parameters provide a comprehensive understanding of the material's interaction with electromagnetic radiation. The real part of the dielectric function (ε_1) represents the material's ability to store electrical energy, while the imaginary part of the dielectric function (ε_2) corresponds to the absorption of photons due to electronic transitions. The peak in ε_1 at lower photon energies indicates strong polarization in the visible region. The imaginary part shows a significant peak at low photon energy, implying strong interband transitions in the visible and in lower UV ranges, followed by a gradual decrease as photon energy increases. The refractive index, $n(\omega)$ follows the trend of $\varepsilon_1(\omega)$, with a peak at lower photon energies, where $n(0) = 3.20$ suggesting strong optical dispersion in the visible and infrared regions. The extinction coefficient, $k(\omega)$ which is linked to absorption losses, follows the pattern of $\varepsilon_2(\omega)$, indicating significant optical absorption in the visible and UV regions. The reflectivity, $R(\omega)$ indicates how much of the incident light is reflected by the material. The medium reflectivity ($R(0) = 0.39$) in the lower energy region suggests that RhNbLi is fairly reflective in the infrared, visible and in lower UV spectrum. As photon energy increases, reflectivity declines, indicating increased transparency in the UV region.

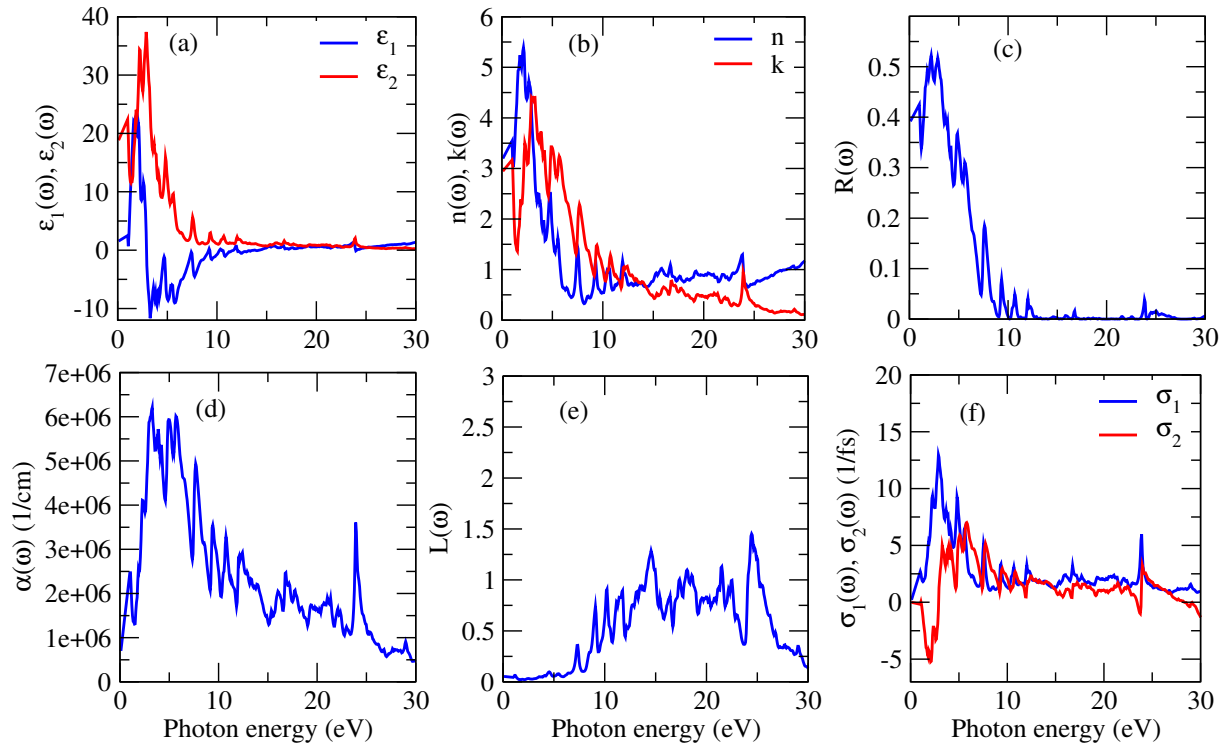


Figure 4.35: GGA-calculated optical properties of RhNbLi as a function of photon energy: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

The absorption coefficient, $\alpha(\omega)$ describes the ability of the material to absorb light at different photon energies. The strong absorption peaks at low photon energy signifies efficient absorption in the visible and in the lower UV region. The absorption decreases with increasing photon energy, suggesting reduced optical absorption in the deep UV range. The electron energy loss function, $L(\omega)$ provides insights into the plasmonic excitations of the material. Peaks in $L(\omega)$ correspond to plasma resonance frequencies, where collective oscillations of free electrons occur. The presence of sharp peaks at higher photon energies indicates that RhNbLi has strong plasmonic activity. The real part of the optical conductivity, $\sigma_1(\omega)$, which represents dissipative conductivity, shows strong peaks at lower photon energies, indicating significant electronic transitions and high optical absorption. The imaginary part of the optical conductivity, $\sigma_2(\omega)$ follows a similar trend to $\epsilon_1(\omega)$, reinforcing the dielectric nature of the material. The optical response of RhNbLi, as investigated in this study, shows good agreement with earlier studies on related HH materials reported in (Radouan et al., 2022). Generally, the optical properties of RhNbLi suggest strong absorption in the visible and lower UV regions, moderate refractive index

at lower photon energies and prominent plasmonic behavior at higher energies. These characteristics make it a promising material for UV-based optoelectronic applications, including solar cells, photodetectors, and transparent conductive films. Additionally, its high reflectivity in the infrared region suggests potential applications in optical mirrors and coatings (Shakil et al., 2021).

4.4.3 Optical Properties Analysis of RhIrZ (Z = As, Li, Si, Sb) HH Compounds

The optical properties of RhIrZ (Z = Li, As, Si, Sb) compounds have been analyzed using the GGA and are depicted in Figures 4.36-4.39. The real part (ϵ_1) describes the dispersion of the electric field within the material, while the imaginary part (ϵ_2) is associated with absorption due to interband transitions. A critical observation is that ϵ_1 exhibits negative values at lower photon energies for all four compounds. This behavior suggests that these materials exhibit metallic-like or plasmonic characteristics in the corresponding energy range, leading to strong reflection of incident light. The imaginary part (ϵ_2) for all four compounds has high value at very low photon energy corresponding to electronic transitions from occupied to unoccupied states, highlighting the optical absorption behavior. For all four compounds both parts of dielectric function have small values after 2 eV that have insignificant variation with photon energy. The dielectric functions (ϵ_1 and ϵ_2) of RhIrSi have many peaks from IR to small UV energy ranges which indicates that both optical dispersion and absorption can take place in the material in these energy spectrum. The refractive index (n) and extinction coefficient (k) are crucial in describing the propagation of light within the materials. For all RhIrZ (Z = Li, As, Si, Sb) compounds, the refractive index is observed to have relatively small values across all energy ranges with almost no variation, including the low-energy region. This suggests that the materials do not significantly slow down the propagation of light. The values of n at zero frequency, i.e., $n(0) = 2.12, 1.37, 0.07$ and 0.85 for the compounds respectively. Meanwhile, the extinction coefficient starts with high values in the small energy regions, indicating strong absorption due to electronic transitions and sharply drops to very small value at around 1 eV and continuous to show very small variation with photon energy as n from 1 eV up to 30 eV. The reflectivity (R) describes the fraction of incident light reflected by the material. All four compounds exhibit high reflectivity at lower photon energies, particularly in the range where ϵ_1 is negative. This further confirms the metallic nature of the compounds in this energy region, as negative $\epsilon_1(\omega)$ typically leads to high reflection. The values of R for the compounds at zero frequency are respectively 0.88, 0.86, 0.86 and 0.81. At higher photon energies, the reflectivity decreases, indicating that the materials become more transparent as interband transitions dominate, results which are in consistent with

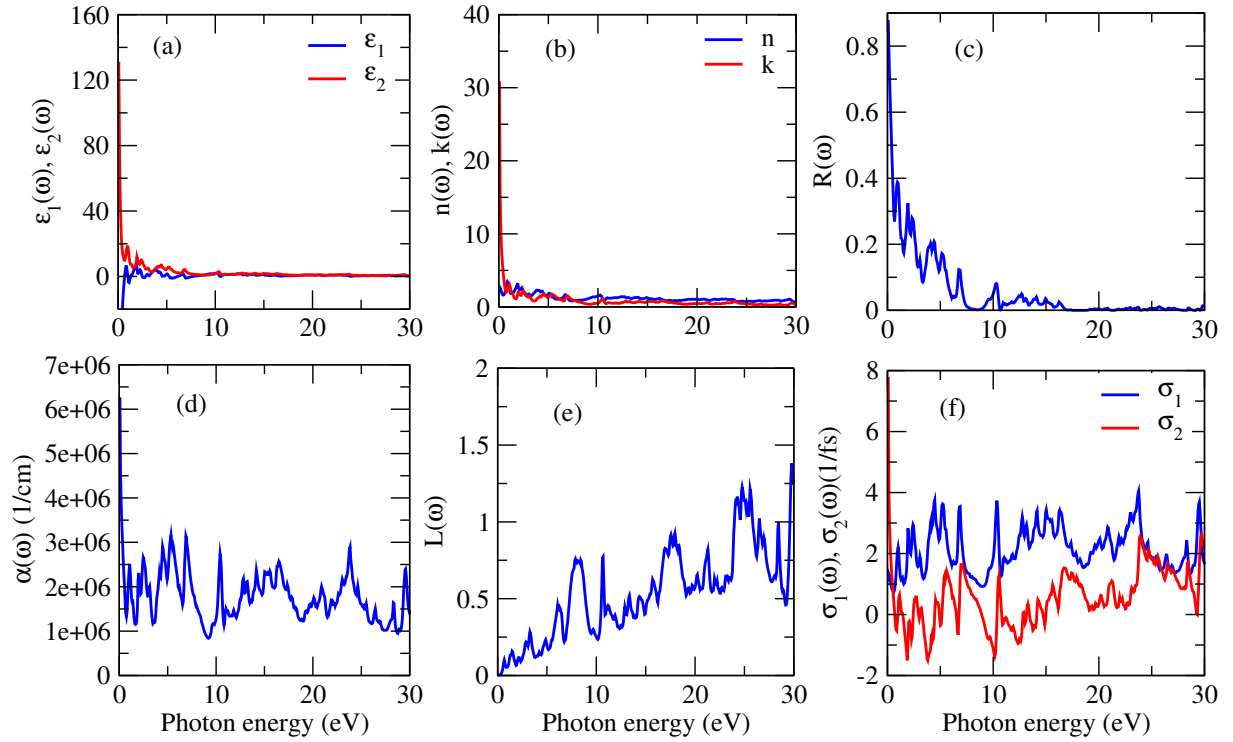


Figure 4.36: Photon energy dependence of the optical functions of RhIrLi calculated with GGA: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

the works on NbIrSn by Khatri and Adhikari (Khatri and Adhikari, 2023).

The absorption coefficient (α) is a measure of how strongly a material absorbs light. For all four compounds, the absorption coefficient is observed to have very high values in the very low energy region close to 0 eV, followed by a sharp decrease before increasing again in the low UV range, implying strong absorption at higher photon energies. This is consistent with electronic transitions between occupied and unoccupied states. A high value of the absorption coefficient in the low-energy range indicates that the material strongly absorbs photons in that region. Since these materials have metallic properties in low photon energy ranges, free carriers (electrons) of these compounds can absorb low energy photons efficiently, leading to a high absorption coefficient in the low energy region, a result which is similar to previous results reported by Koushik and Mukherjee (Koushik and Mukherjee, 2024). The electron energy loss function, $L(\omega)$, provides information about plasma oscillations and energy dissipation within the material. Peaks in $L(\omega)$ correspond to plasmonic resonances, which occur at high energies where $\epsilon_1(\omega)$ changes sign from negative to positive. The presence of peaks in $L(\omega)$ at high pho-

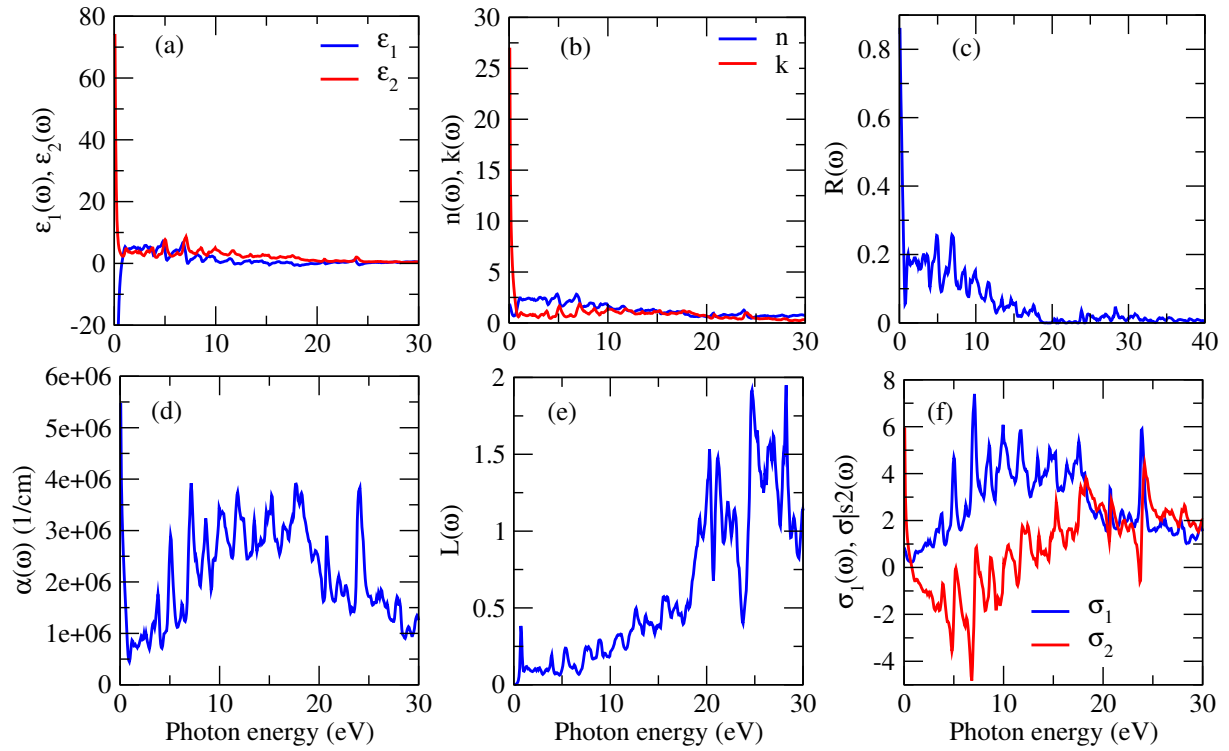


Figure 4.37: Photon energy dependence of the optical functions of RhIrAs calculated with GGA: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

ton energy suggests significant energy dissipation due to collective electronic excitations which could be attributed to intraband transitions within the conduction band for metals. It can also indicate a resonance condition where incoming photons excite electrons with minimal energy loss. For all four compounds, distinct peaks are observed at higher photon energies, indicating the presence of collective electron oscillations. Some of these compounds (except RhIrLi) also show peak in the near IR region indicating the presence of plasmonic resonance in this energy region. The negative $\epsilon_1(\omega)$ values at low energy further support the possibility of plasmonic behavior. The optical conductivity (σ_1 and σ_2) characterizes the response of the material to an external electromagnetic field. The imaginary part of the optical conductivity, σ_2 is associated with energy storage in the medium, while the real part, σ_1 is linked to direct electronic transitions. The real part of the optical conductivity represents the dissipative (absorptive) response of the material, meaning how much energy is absorbed by the system from the incident electromagnetic waves. A negative σ_2 in certain energy ranges, especially at low photon energies, suggests that the materials exhibit gain instead of loss, meaning it could behave as an

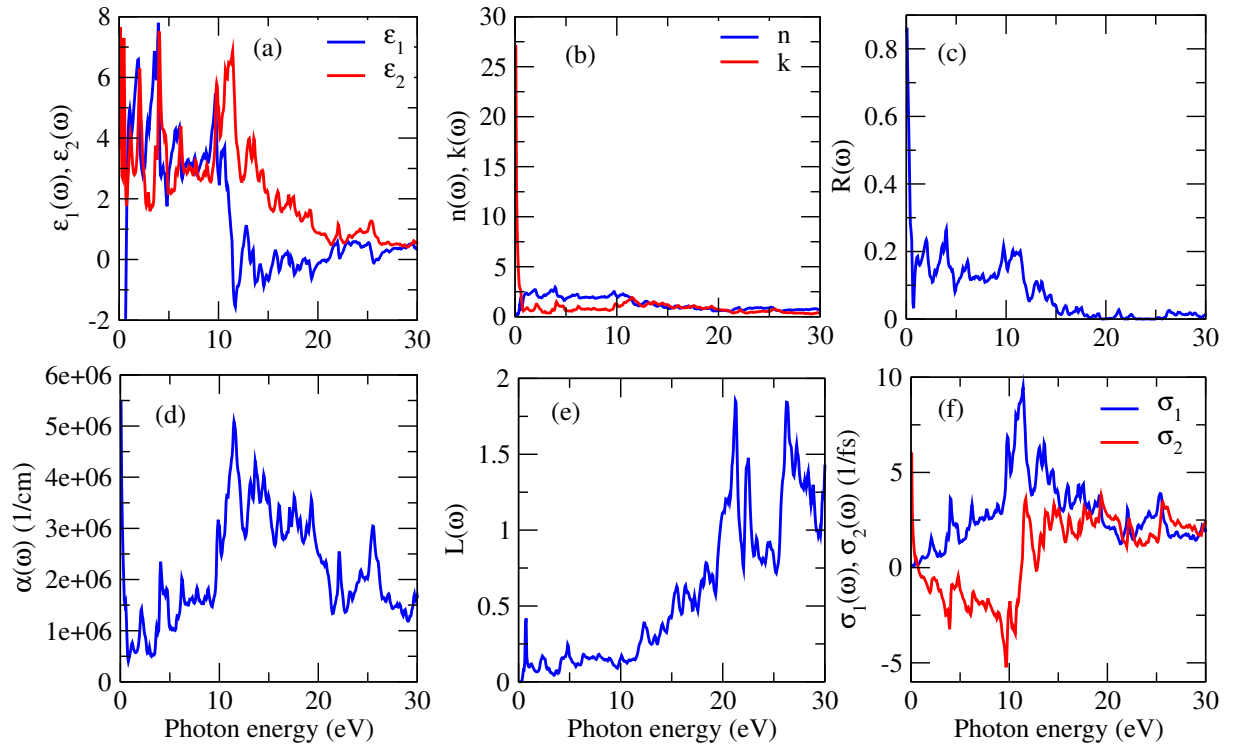


Figure 4.38: Photon energy dependence of the optical functions of RhIrSi calculated with GGA: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

active medium rather than a passive absorber and have metallic behavior in this region. The always positive σ_1 implies that the material does not exhibit extreme loss mechanisms such as strong damping from free carriers and the response is dominated by bound electron excitations, supporting optical transitions rather than just free-carrier absorption. The results of optical properties of RhIrZ ($Z = \text{Li, As, Si, Sb}$) compounds reported under current work well agree with the previous work on XYZ ($X = \text{Ir, Pt, Au}$; $Y = \text{Mn}$; $Z = \text{Sn, Sb}$) related HH compounds reported by Amudhavalli with his co-workers (Amudhavalli et al., 2017). In general, the optical response of these RhIr-based HH compounds suggests their potential utility in plasmonic applications, optoelectronic devices and UV-protective coatings. Their strong absorption characteristics and plasmonic behavior are consistent with previous findings (Goswami et al., 2017; Nakatsuji et al., 2017), further indicating their potential as promising candidates for spintronic and photonic applications.

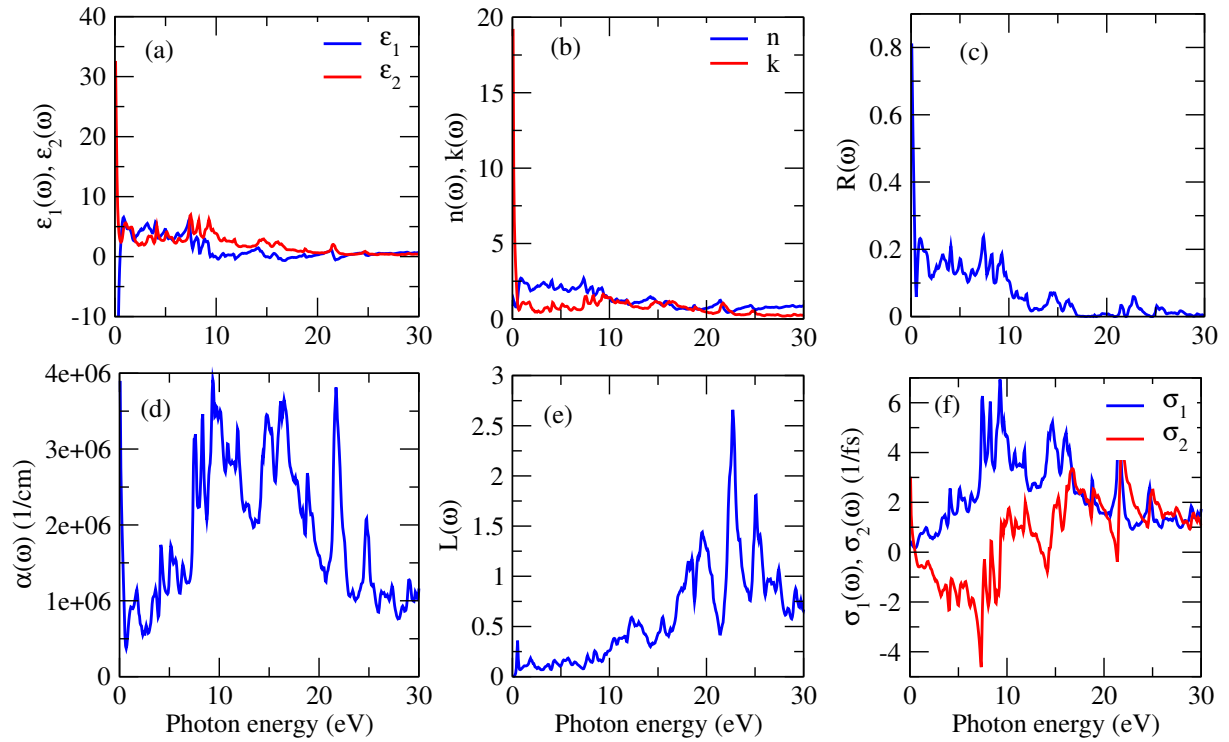


Figure 4.39: Photon energy dependence of the optical functions of RhIrSb calculated with GGA: (a) dielectric function (ϵ_1 and ϵ_2), (b) refractive index (n) and extinction coefficient (k), (c) reflectivity (R), (d) absorption coefficient (α), (e) electron energy loss (L), and (f) optical conductivity (σ_1 and σ_2).

4.5 Magnetic Properties of RhYZ (Y =Zr, Ir, Nb; Z = Li, As, Si, Sb) HH Compounds

Table 4.9 presents the calculated magnetic moments (in μ_B) for RhYZ compounds using both GGA and GGA+U methods. The total magnetic moments (M_T) are compared with the SP predicted values, providing insight into the effect of electron correlation on the magnetic properties. The individual atomic contributions of Rh (M_{Rh}), Y (M_Y) and Z (M_Z) are also examined. For all RhZr-based compounds, both GGA and GGA+U calculations predict zero magnetic moments for all atoms, resulting in a total magnetic moment (M_T) of $0.00 \mu_B$. This indicates a non-magnetic ground state. The SP rule predicts a total moment of $0.00 \mu_B$, for RhZrAs and RhZrSb Compounds confirming that these compounds follow the expected behavior for HH structures where the valence electron count does not support spin polarization. Since these compounds have 18 valence electrons, their M_T must be zero (Equation (2.33)) indicating that they are semiconductor HH compounds. Their semiconductor nature were also proved by their

electronic property calculations. The addition of U does not introduce any significant electron localization effects in these materials. For RhZrLi and RhZrSi, the SP rule predicts M_T of 4.00 μ_B and 1.00 μ_B , respectively. However, both the GGA and GGA+U calculations give a total magnetic moment of 0.00 μ_B for these compounds. This indicates a significant deviation from the SP rule. Possible reasons for deviation may include electronic structure and hybridization, delocalization of electrons and correlation effects and exchange splitting. Regard to electronic structure and hybridization, the SP rule is based on the assumption of an idealized band filling and a rigid band model. However, in real materials, hybridization between different atomic orbitals can redistribute the electron states, leading to a suppression of magnetism. In RhZrLi and RhZrSi, strong hybridization between Rh, Zr and Li/Si states might lead to complete spin compensation, preventing the expected magnetic moment from emerging. In view of delocalization of electrons, magnetic moments typically arise from localized electrons (such as in transition metals with partially filled d-orbitals). If the electrons in RhZrLi and RhZrSi are more delocalized (as in metallic or covalent-like bonding), the net spin polarization can become zero, leading to a non-magnetic ground state despite the SP prediction. In terms of exchange splitting, the failure of GGA and GGA+U to capture a finite moment suggests that electron correlation effects might not be strong enough in these compounds to induce a spin-polarized state. If the exchange splitting (the energy difference between spin-up and spin-down states) is small, thermal fluctuations or quantum effects could further suppress magnetism. The result of non-magnetic nature for RhZrLi and RhZrSi compounds from both GGA and GGA+U were also observed in spin polarized band structure and DOS calculation for these compounds by GGA and GGA+U. Figures 4.8-4.11 for these compounds support the non-magnetic nature of these compounds since their band structures and DOS are symmetric (both spin up and spin down channels have equal contributions) under both calculations.

Table 4.9: Calculated and Slater-Pauling predicted magnetic moments (μ_B) of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds.

compound	M_{Rh}^{GGA}	M_Y^{GGA}	M_Z^{GGA}	M_{Tcalc}^{GGA}	M_{Rh}^{GGA+U}	M_Y^{GGA+U}	M_Z^{GGA+U}	M_{Tcalc}^{GGA+U}	M_{SP}
RhZrLi	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	4.0000
RhZrAs	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
RhZrSi	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
RhZrSb	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
RhNbLi	0.0000	0.0000	0.0000	0.0000	-0.2812	1.3459	0.0627	2.9007	3.0000
RhNbAs	-0.0001	-0.0001	-0.0001	0.0000	-0.1427	0.8173	-0.0554	0.9800	1.0000
RhNbSi	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
RhNbSb	0.0444	0.4944	0.0032	0.7500	-0.1684	0.9369	-0.0655	1.0000	1.0000
RhIrLi	-0.0001	0.0000	0.0000	0.0000	1.0362	1.1730	-0.0072	2.4900	1.0000
RhIrAs	0.0002	0.0002	-0.0000	0.0000	0.9687	1.1697	-0.0157	2.4600	5.0000
RhIrSi	0.0000	-0.0000	0.0000	0.0000	0.6293	0.9517	-0.0560	1.8700	4.0000
RhIrSb	-0.0000	-0.0001	0.0000	0.0000	0.4621	0.7436	-0.0326	1.4300	5.0000

In the GGA approach, all RhNb-based compounds exhibit very small or negligible magnetic moments, indicating a nearly non-magnetic state. However, with GGA+U, significant changes are observed. RhNbLi shows a strong enhancement in magnetization when U is included, with Rh carrying a moment of $-0.2812 \mu_B$, Nb contributing $1.3459 \mu_B$ and Sb showing a small value of $0.0627 \mu_B$, leading to a total moment of $2.9007 \mu_B$. This is close to the SP predicted moment of $3.00 \mu_B$, indicating that the inclusion of U restores the expected spin alignment. RhNbAs also shows an increase in magnetization under GGA+U, with a total moment of $0.98 \mu_B$, which is in good agreement with the SP prediction of $1.00 \mu_B$. This suggests that electron correlation effects play a crucial role in stabilizing the magnetic state in these compounds. RhNbSi remains non-magnetic under both approaches, with a total moment of $0.00 \mu_B$, matching the SP prediction because it is a non-magnetic semiconductor HH compound. RhNbSb exhibits better magnetization in the GGA approach ($M_T = 0.7500 \mu_B$), and the inclusion of U further increases the total moment to $1.00 \mu_B$, aligning well with the SP rule. Generally, for RhNb-based compounds, GGA+U significantly enhances magnetic moments and brings them closer to the SP rule, indicating the importance of correlation effects in these systems.

Unlike RhZr and RhNb compounds, RhIr-based materials show relatively high magnetization under GGA+U compared to GGA. RhIrLi displays a significant increase in magnetization with U, with Rh carrying $1.0362 \mu_B$, Ir having $1.1730 \mu_B$ and a small contribution from Li, resulting in a total moment of $2.4900 \mu_B$. This deviates from the SP prediction of $1.00 \mu_B$, suggesting that electron correlations alone are not sufficient to fully align the spins as per the rule. RhIrAs exhibits similar behavior, with a total moment of $2.4600 \mu_B$ in GGA+U, significantly higher than the nearly zero value in GGA. The predicted SP value is $5.00 \mu_B$, indicating partial agreement. RhIrSi shows moderate magnetization in GGA+U, with a total moment of $1.8700 \mu_B$, while GGA predicts a non-magnetic state. The SP prediction of $4.00 \mu_B$ suggests that the correlation effects enhance magnetization but do not fully recover the expected spin configuration. RhIrSb follows a similar trend, where the GGA+U total moment ($1.4300 \mu_B$) is significantly larger than the negligible value in GGA. However, this is still lower than the SP prediction of $5.00 \mu_B$, indicating that while U improves spin localization, additional interactions might be required to fully stabilize the expected spin polarization.

The SP rule provides a theoretical prediction of the total magnetic moment based on the valence electron count. A direct comparison with the calculated values from both GGA and GGA+U reveals several insights: due to its limited handling of on-site electron-electron interactions, the GGA is known to occasionally underestimate the magnetic moment or fails to forecast magnetism in specific correlated systems. Strong electronic correlations, which GGA alone might not be able to adequately capture, can be essential in stabilizing magnetism in HH

compounds, especially those with partially filled d or f orbitals. Therefore, in order to obtain more precise magnetic behavior, adjustments such as GGA+U are frequently required (Anisimov et al., 1991). On the other hand, GGA+U significantly improves the agreement with the SP rule, particularly for RhNb-based compounds, where the moments align well with the predicted values. However, RhIr-based compounds exhibit only partial agreement with the SP rule under GGA+U, suggesting that additional effects, such as SOC, may be influencing the magnetic properties. In general, the calculated magnetic moments of RhYZ compounds show a strong dependence on the exchange-correlation functional used. While GGA predicts mostly non-magnetic behavior, the inclusion of U enhances magnetic moments, bringing them closer to the expected SP values. This effect is particularly evident in RhNb-based compounds, where the total moment under GGA+U matches well with the predicted values. RhIr-based compounds, however, show only partial agreement, suggesting that additional interactions might play a role in determining their magnetism. These findings highlight the necessity of including electron correlation effects when studying the magnetic properties of HH compounds, especially for accurate predictions of their potential applications in spintronics.

Conclusions and Recommendations

5.1 Conclusions

In conclusion, this work has provided a comprehensive investigation to the structural, mechanical, electronic, optical and magnetic properties of RhYZ (Y = Zr, Ir, Nb; Z = Li, As, Si, Sb) HH compounds by employing GGA and GGA+U calculations. The analysis of structural properties reveal that except RhIrZ (z = As, Si, Sb) compounds which are most stable in their β phase, all other compounds are structurally most stable in their α phase. RhIrLi has positive formation energy in all of its three atomic configurations (phases) and therefore it is thermodynamically unstable and can be easily decomposed in to its component elements. On the other hand, all other remaining compounds have negative formation energy at least in their structurally most stable phase and are thermodynamically stable which implies that they can not be easily decomposed in to their constituent elements and can be synthesized experimentally. The obtained values of thermodynamic parameters such as Debye temperatures, sound velocities and melting temperatures are in good range for these materials functionality in spintronic and optoelectronic applications. The absence of imaginary phonon modes across the entire Brillouin zone in these all compounds confirms their dynamical stability, further supporting their structural robustness and suitability for functional applications. From mechanical point of view, the three elastic constants (C_{11} , C_{12} and C_{44}) for all the compounds satisfy Born and Huang mechanical stability criteria and therefore all the compounds are mechanically stable.

From the electronic property calculations, RhZrZ (Z = As, Sb) and RhNbSi compounds are semiconductors under both GGA and GGA+U predictions, which is very curial property for optoelectronic applications. In particular, RhZrAs can be considered as a potential runner in this field due to its direct band gap. The obtained band gaps under GGA+ U are greater than that calculated by standard GGA approach, due to its better accounts for electron correlation in localized d-states. RhNbAs and RhNbSb are both half-metallic compounds with 100% spin polarization at the F_E , making them strong candidates for spintronic applications. Based on the SP rule, both are expected to exhibit a total magnetic moment of $1\mu_B$. This is confirmed for RhNbSb, while RhNbAs shows a slight deviation, with a calculated moment of $0.98\mu_B$, likely due to minor hybridization effects or numerical factors in the DFT calculations. Notably, RhNbAs features a larger indirect band gap in its semiconducting spin channel (1.09 eV) compared to RhNbSb (0.83 eV). This wider gap enhances its thermal stability and reduces the risk of spin depolarization at higher temperatures. As a result, despite the small deviation in magnetic mo-

ment, RhNbAs is the more favorable material for spintronic device applications than RhNbSb. From the Rh-based compounds studied here, RhZrZ ($Z = \text{Li, Si}$) show non-magnetic metallic property which could be useful in plasmonic applications, including nanophotonic devices and surface plasmon resonance applications, whereas RhNbLi and RhIrZ ($Z = \text{Li, As, Si, Sb}$) reflect magnetic metallic property without half-metallic nature. As magnetic metallic compounds, they combine metallic conductivity and magnetic ordering, making them attractive options for cutting-edge spintronics, optoelectronics and energy-related technologies.

From optical property calculations, the semiconductor HH compounds, RhZrZ ($Z = \text{As, Sb}$) and RhNbSi have substantial real part of dielectric function, refractive index and absorption coefficient but low electron energy loss at low photon energy ranges indicating that they are ideal for optoelectronic applications. While the half-metallic HH compounds, RhNbZ ($Z = \text{As, Sb}$) are ideal for spintronic applications, they can also have potentials in optoelectronic applications, especially where spin and electromagnetic wave interacts due to their moderate dielectric function, refractive index and absorption coefficient and low electron energy loss at small photon energy ranges. RhZrZ ($Z = \text{Li, Si}$) have negative value of real part of dielectric function in the low photon energy ranges indicating that they have metallic nature in these energy ranges. Since these compounds are non-magnetic metallic materials they have high reflectivity, metallic conductivity and capacity to sustain surface plasmon resonance and therefore, they can be employed in plasmonic and photonic applications. Similarly, RhIrZ ($z = \text{Li, As, Si, Sb}$) compounds have negative real parts of dielectric function and optical conductivity in low photon energy ranges showing that they are metallic as well as have magnetic property and thus they can be used in controlling spin-polarized currents and light-matter interactions under magnetic fields, hence can be utilized in spin-optoelectronic and magneto-optical systems. With the exception of RhNbSb, RhIrAs, RhIrSi and RhIrSb, which display finite magnetic moments, the majority of compounds display non-magnetic behavior, according to the calculated total magnetic moments under the GGA technique. In certain instances, such as with RhNbSb, RhNbAs and RhIr-based compounds, the addition of U potentials improves the magnetic response. When the results are compared to the SP rule, some systems show deviations, whereas other compounds that were predicted to be half-metallic showed good agreement with SP rule.

5.2 Recommendations

In the context of spintronic and optoelectronic applications, the investigation of RhYZ ($Y = \text{Zr, Ir, Nb; } Z = \text{Li, As, Si, Sb}$) HH compounds has demonstrated encouraging mechanical, electronic, magnetic and optical properties. The following suggestions are put out for further study in order to increase the materials' usefulness and comprehension:

- **Examining thermoelectric properties:** Future research should concentrate on investigating the thermoelectric performance of RhYZ compounds due to their structural and electronic plasticity. Their effectiveness in transforming waste heat into electrical energy will be ascertained by specifically looking at factors including the Seebeck coefficient, electrical conductivity and thermal conductivity. This can greatly increase the value of these materials in thermal management and power generating systems and is essential for sustainable energy solutions.
- **Experimental synthesis and validation:** Structural, thermodynamic and mechanical stability are predicted theoretically, but experimental synthesis is necessary to validate these results. Their practicality will be confirmed by synthesis under various pressure and temperature circumstances, followed by structural and transport investigations.
- **Doping strategies:** Additional research could examine the impacts of doping inside the Rh, Y, or Z sites to customize electronic, magnetic or thermoelectric performance. These changes can improve spin polarization, decrease lattice heat conductivity or fine-tune band topologies.

List of Publications

During my PhD work the published articles are:

A. Published articles

1. **Adem Beriso Bejo**, Megersa Wodajo Shura, Mesfin Asfaw Afrassa, Kumneger Tadele, Fekadu Tolessa Marem and Kunsu Haho Habura: Structural, Electronic, Mechanical and Optical Properties of RhZrZ (Z = As, Sb) Half-Heusler Compounds: First-Principles Calculations, **Advances in Condensed Matter Physics**, (2024) 2024, <https://doi.org/10.1155/2024/5772579>.
2. **Adem Beriso Bejo**, Megersa Wodajo Shura, Kumneger Tadele, Mesfin Asfaw Afrassa and Fekadu Tolessa Maremi, Structural, electronic, mechanical, optical and magnetic properties of RhNbZ (Z = Li, Si, As) Half-Heusler compounds: a first-principles study, **Mater. Res. Express** 12 (2025) 016510, <https://doi.org/10.1088/2053-1591/ada5b1>.
3. **Adem Beriso Bejo**, Megersa Wodajo Shura, Mesfin Asfaw Afrassa, Kumneger Tadele, Fekadu Tolessa Marem and Kunsu Haho Habura: First-principles calculations to investigate Structural, Electronic, Mechanical, Optical and Magnetic Properties of RhNbSb Half-Heusler Compound, **Advances in Condensed Matter Physics**, (2025) 2025, <https://doi.org/10.1155/acmp/6686777>.

B. Manuscripts ready for submission

1. **Adem Beriso Bejo**, Megersa Wodajo Shura, Kumneger Tadele, Mesfin Asfaw Afrassa and Fekadu Tolessa Maremi, DFT Study of Mechanical and Thermoelectric Properties of RhZrZ (Z = Li, Si) Half-Heusler compounds.
2. **Adem Beriso Bejo**, Megersa Wodajo Shura, Kumneger Tadele, Mesfin Asfaw Afrassa and Fekadu Tolessa Maremi, Investigation of Mechanical, Electronic and Thermoelectric Properties of RhIrZ (Z = Li, As, Si, Sb) Half-Heusler compounds: First-Principles Calculations.

C. Manuscript under preparation

1. **Adem Beriso Bejo**, Megersa Wodajo Shura, Kumneger Tadele, Mesfin Asfaw Afrassa and Fekadu Tolessa Maremi, Investigation of Mechanical, Electronic and Thermoelectric Properties of RhIrZ (Z = Si, Sb) Half-Heusler compounds: First-Principles Calculations.

List of Conference Participation and Paper Presentation

1. Certificates of participation on 16th Annual Conference of the Ethiopian Physical Society, held at Madda Walabu University, held from February 18-19, 2022.
2. Certificates of research paper Presentation February 21-22, 2025 on 19th Annual Conference of the Ethiopian Physical Society, held at Haramaya University.
3. Certificates of participation on 19th Annual Conference of the Ethiopian Physical Society, held at Haramaya University, held from February 21-22, 2025.

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