Electronic and Structural Properties of Scandium Anthnomide and Scandium Fuside under High Pressure

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Introduction

High-pressure physics is an incredibly captivating and intellectually stimulating branch of solid-state physics with an extensive range of research scope. The investigation of semiconductor materials is particularly engrossing, as it opens up a whole new realm of possibilities for groundbreaking discoveries. This field of study has garnered tremendous attention in high-pressure research due to the potential to uncover novel electronic properties of wide-band-gap semiconductors under high pressure. The applications of such discoveries in optoelectronic devices, thermal detector systems, high-temperature semiconductor lasers, superconductors, and various other fields are incredibly vast and hold great promise for technological advancements.

With a plethora of materials systems exhibiting intriguing semiconductor properties, researchers are driven by the desire to accurately predict a material's electronic and structural properties under high pressure. This pursuit of knowledge and understanding serves as a constant source of fascination for scientists worldwide, fueling their enthusiasm to uncover the mysteries that lie at the intersection of high-pressure physics and semiconductor research. The challenges that arise in this endeavor are numerous, but they only heighten the excitement and dedication of scientists who are determined to push the boundaries of human knowledge. Through their tireless efforts, new frontiers are being explored, and our understanding of the fundamental nature of matter is expanding.

In conclusion, the field of high-pressure physics in the context of semiconductor research is an ever-evolving landscape of discovery, where the possibilities seem limitless. The allure of uncovering unique electronic and structural properties of materials under extreme conditions is what drives scientists and researchers to delve deeper into this captivating branch of solid-state physics. The potential for groundbreaking advancements and transformative applications in diverse technological domains makes this field an area of immense excitement and curiosity. As research continues to progress, the boundaries of what we currently understand will undoubtedly be pushed further, unraveling new layers of knowledge and paving the way for a future filled with remarkable scientific achievements. The intertwining relationship between high-pressure physics and semiconductor research creates a rich tapestry of exploration and innovation, with scientists passionately exploring every facet of the subject. The thrill of encountering new discoveries and unlocking the hidden potential of materials never ceases to amaze researchers, as they continuously immerse themselves in the intricate world of high-pressure physics.

As the field continues to evolve, new experimental techniques and theoretical models are being developed to further enhance our understanding of the behavior of semiconductors under extreme pressure. This transcends their conventional properties and opens up doors to uncharted territories of experimentation and discovery. In spite of the myriad challenges that researchers face, their determination and unwavering commitment drive them to explore novel frontiers and relentlessly seek knowledge, propelling the field forward. The intricate interplay between high-pressure physics and semiconductor research has led to numerous breakthroughs, revolutionizing our comprehension of materials and paving the way for exciting technological advancements.

The impact of high-pressure physics extends far beyond the realm of semiconductors. These findings have profound implications for a multitude of technological domains, including optoelectronics, photonics, and energy storage. The fundamental understanding gained from studying the behavior of materials under high pressure provides invaluable insights that can be harnessed to design and optimize innovative devices and systems. The potential applications of these discoveries are vast and far-reaching, offering exciting prospects for future development and progress. The continuous advancements in high-pressure physics and semiconductor research promise a future where cutting-edge technologies and remarkable scientific achievements are commonplace.

In summary, the field of high-pressure physics in the context of semiconductor research is a captivating and dynamic discipline that holds immense potential for groundbreaking discoveries and technological advancements. With its vast range of applications and the constant drive to uncover new knowledge, this field continues to expand and push the boundaries of human understanding. As scientists delve deeper into the mysteries of high-pressure physics and semiconductor behavior, they unravel the secrets of materials under extreme conditions, paving the way for a future filled with remarkable advancements and transformative breakthroughs. The allure of this field lies in its ability to continually surprise and excite, making it an area of immense fascination and curiosity for scientists and researchers worldwide. The future of high-pressure physics and semiconductor research is bright, with endless possibilities awaiting exploration. (Woods-Robinson *et al.* 2020) (Nguyen *et al.* 2021) (Garrity *et al.* 2022) (Zhang *et al.,* 2022) (Chae *et al.* 2021) (Garrity *et al.* 2022) (Lee *et al.* 2024) (Chae, 2022)

Theoretical calculations utilizing the Density Functional Theory (DFT) have, over the past few decades, emerged as immensely powerful tools for the prediction of the high-pressure properties of various materials. This is primarily due to the significant reduction in computational costs associated with DFT-based methods. Consequently, these methods have been extensively employed in condensed matter research. In the case of semi-metallic materials, it has been observed that the band gap may close around a critical pressure point. This closure occurs as a result of the increased number of valence electrons, which can be attributed to the contribution of higher atomic orbitals under high pressure conditions. These modifications in the low-pressure electronic states, in turn, may give rise to novel electronic states, such as superconductivity or a high thermopower factor, under high pressure.

Despite the potential for significant advancements in this field, there have been relatively few reports regarding the electronic and structural properties of solid antimonide binary semiconductors under high pressure. Furthermore, the first-principles calculations of rare ternary fuside semiconductor materials under high pressure are still limited in number. In an effort to address these gaps, the present study focuses on calculating the full-pressure electronic and structural properties of solid semiconductor ScSb under high pressure conditions. Additionally, the heat capacities of this material are also examined. Moreover, the role of high pressure on the Density of States (DOS) features, the bonding scheme of ScSb, and the effect of pressure on this scheme are thoroughly explored. Furthermore, the underlying mechanism of structural phase transitions of ScSb during the pressure-volume evolution is investigated. Subsequently, the study expands its scope by performing calculations to determine the structural and band gap properties of scandium fuside materials, which include Sc2S3, Sc2O3, Sc2Se3, Sc2Te3, and Sc2Sb3. These materials are analyzed using hybrid density functional methods to gain insights into the effects of high pressure and chemical composition on their structural, mechanical stability, and electronic properties.

The outcomes of these calculations provide valuable and profound insights into the behavior of these materials under extreme pressure conditions. Additionally, these findings pave the way for potential applications of fuside materials in advanced technologies. It is noteworthy that the discoveries resulting from this research not only contribute to an expanded understanding of the properties of semiconductors under high pressure but also provide new opportunities for engineering materials with tailored electronic and structural characteristics. Further investigation and experimentation are required to validate and utilize these theoretical predictions for the development of novel materials with enhanced performance in various domains. These domains include, but are not limited to, electronics, energy storage, quantum computing, and nano-scale technologies. By leveraging the outcomes of this study, it is possible to propel the advancement and innovation of materials science towards a future with unprecedented technological applications, revolutionizing industries and improving the quality of life for individuals worldwide. (Nobin *et al.,* 2023) (Khan *et al.,* 2023) (Yang *et al.* 2021).

Chapter - 2

Background and Significance

Research on high-pressure science has found increasing interest because high pressure has become one of the most powerful and important tools to explore the wealth of new states and materials that are relevant to many different disciplines. This is especially true because high pressure often leads to significant changes in the physical properties of materials and provides a means of determining and understanding these properties. For instance, high-pressure accurate measurements of the structure of crystals have been used to determine the structures of materials with technological significance. The optical, electronic, and magnetic properties of materials are pressure-dependent functions. Therefore, high-pressure studies of these properties can also provide useful information for understanding matter on atomic and physical levels. These studies have led to a wide variety of applications, such as pressure sensors, light-solid interfaces, and many other optical components.

Furthermore, the advancements in high-pressure technology have revolutionized the field of scientific exploration. With the development of more sophisticated equipment and techniques, scientists are now able to replicate extreme pressures that simulate the conditions deep within the Earth's core or even those found in distant celestial bodies. This allows researchers to investigate the behavior of matter under extreme conditions, providing insights into the fundamental laws of physics and chemistry. This knowledge has far-reaching implications and has paved the way for groundbreaking discoveries in areas like materials science, geology, and astrophysics. Moreover, high-pressure science has also played a crucial role in various engineering and industrial applications. By subjecting materials to high pressures, researchers have been able to study and optimize their properties, leading to the development of stronger and more durable materials. This has significant implications in fields such as aerospace, automotive, and construction, where the performance and reliability of materials are of utmost importance. High-pressure science has also contributed significantly to our understanding of the Earth's interior and geologic processes. By recreating the immense pressures that exist deep within the planet, scientists have been able to unravel the mysteries surrounding plate tectonics, earthquake generation, and the formation of minerals. This knowledge not only helps in predicting and mitigating natural disasters but also aids in the exploration and extraction of valuable resources buried deep underground.

Furthermore, high-pressure science has considerable potential in the field of medicine and healthcare. Researchers are exploring the effects of high pressure on biological systems, such as the human body, to better understand diseases and develop novel treatments. High-pressure techniques have shown promise in areas like cancer treatment, drug delivery systems, and tissue engineering, offering new avenues for medical advancements. The applications and implications of high-pressure science are vast and diverse, with the potential to shape the future of humanity. Moreover, the direct measurement of electronic properties under high pressure can provide important information for other fundamental research, such as the electronic behavior of materials, the determination of atomic structure, and the measurement of the complex electronic structure of materials under high pressure. As scientists continue to push the boundaries of high-pressure science, new findings and discoveries are expected to emerge, further expanding our knowledge and transforming various fields. High-pressure research holds the promise of unlocking the secrets of the universe, revolutionizing technology, and improving the quality of life for countless individuals.

In conclusion, the expanding domain of high-pressure science continues to open up new frontiers in various scientific disciplines and industrial sectors. As researchers delve deeper into the mysteries of extreme pressures, they unravel insights that have the potential to transform our understanding of the universe and revolutionize technological advancements across multiple fields. The applications and implications of high-pressure science are vast and diverse, with the potential to shape the future of humanity. Moreover, the direct measurement of electronic properties under high pressure can provide important information for other fundamental research, such as the electronic behavior of materials, the determination of atomic structure, and the measurement of the complex electronic structure of materials under high pressure. The progress in high-pressure science has been truly remarkable, and its continued exploration will undoubtedly yield even more astonishing discoveries and advancements. The quest to better understand the behavior of matter under extreme pressures has become a driving force behind scientific progress, enabling breakthroughs in fields ranging from materials science to medicine. With each new revelation, we move closer to unraveling the mysteries of the universe and harnessing its power for the benefit of humanity.

High-pressure research holds the promise of unlocking the secrets of the universe, revolutionizing technology, and improving the quality of life for countless individuals. As we embark on this journey of exploration, we are poised to witness incredible transformations that will shape the future of our world and propel us towards a brighter tomorrow.

The exploration of high-pressure science has expanded exponentially in recent years due to its immense potential in diverse scientific fields. High pressure has emerged as a powerful tool for investigating new states and materials, facilitating discoveries that contribute to numerous disciplines. Notably, high pressure induces substantial changes in the physical properties of materials, offering valuable insights for their determination and comprehension. Accurate measurements of crystal structures under high pressure have unraveled the architecture of technologically significant materials. Moreover, pressure-dependent functions like optical, electronic, and magnetic properties provide valuable information about the atomic and physical levels of matter. Consequently, high-pressure research has resulted in various innovative applications, including the development of pressure sensors, interfaces for light-solid interactions, and optical components.

Continuing advancements in high-pressure technology have brought about a revolution in scientific exploration. Through the use of sophisticated equipment and techniques, scientists are now capable of recreating extreme pressures comparable to those within Earth's core or distant celestial bodies. This groundbreaking capability enables the investigation of matter's behavior under extreme conditions, ultimately providing profound insights into the fundamental laws of physics and chemistry. Consequently, discoveries in fields such as materials science, geology, and astrophysics have been made possible. Furthermore, high-pressure science plays a pivotal role in engineering and industrial applications. By subjecting materials to high pressures, researchers can examine and enhance their properties, leading to the development of stronger and more durable substances. These advancements are particularly significant in industries such as aerospace, automotive, and construction, where material performance and reliability are critical. Additionally, high-pressure science has greatly contributed to our understanding of Earth's interior and geologic processes. By reproducing immense pressures found within the planet, scientists have unraveled mysteries surrounding plate tectonics, earthquake generation, and mineral formation. This knowledge aids in predicting and mitigating natural disasters, as well as exploring and extracting valuable underground resources.

The medical and healthcare sectors also stand to benefit significantly from high-pressure science. Researchers are investigating the effects of high pressure on biological systems, particularly the human body, to gain a better understanding of diseases and develop cutting-edge treatments. Promising applications of high-pressure techniques have emerged in fields including cancer treatment, drug delivery systems, and tissue engineering, opening new avenues for medical advancements. The far-reaching applications and implications of high-pressure science have the potential to shape the future of humanity significantly. Additionally, the direct measurement of electronic properties under high pressure provides vital information for other fundamental research, such as understanding the electronic behavior, atomic structure, and complex electronic properties of materials. As scientists relentlessly push the boundaries of high-pressure science, they are expected to uncover new findings and make further discoveries that expand our knowledge and transform various fields. High-pressure research holds the key to unlocking the secrets of the universe, revolutionizing technology, and improving countless lives.

In conclusion, the expanding domain of high-pressure science continues to push the boundaries of various scientific disciplines and industrial sectors. Researchers venturing into the depths of extreme pressures unravel insights that have the potential to revolutionize our understanding of the universe and drive technological advancements across multiple fields. The applications and implications of high-pressure science are wide-ranging and diverse, holding enormous potential for shaping the future of humanity. Additionally, direct measurement of electronic properties under high pressure plays a crucial role in other fundamental research areas, from understanding materials' electronic behavior to determining atomic structure and complex electronic properties. The remarkable progress achieved in high-pressure science thus far serves as a testament to its immense potential. Further exploration promises to unveil even more astonishing discoveries and advancements. The quest to comprehend the behavior of matter under extreme pressures stands as a driving force behind scientific progress, enabling breakthroughs in fields spanning from materials science to medicine. With each revelation, we inch closer to unraveling the universe's mysteries and harnessing its power for the betterment of humanity. High-pressure research holds the promise of unlocking the universe's secrets, revolutionizing technology, and improving countless lives. As we embark on this inspiring journey of exploration, we find ourselves on the brink of witnessing incredible transformations that will shape the future of our world and propel us into a brighter tomorrow. (Flores-Livas *et al.* 2020) (Kim *et al.* 2020) (Sun *et al.* 2023) (Hu *et al.* 2020) (Sun *et al.*,

2020) (Edalati *et al.* 2022) (Davenport *et al.* 2020) (Zou *et al.* 2020) (Said *et al.* 2022).

Chapter - 3

Experimental Techniques

High-pressure angle-resolved photoemission experiments were performed on the beamline BL09W of the Hiroshima Synchrotron Radiation Center (HiSOR) with a base pressure of 10^-10 Torr in order to observe three-dimensional (3D) band structures of ScSb and ScBi. High-purity ScBi and ScSb compounds were prepared from the stoichiometric mixtures of Sc and Bi or Sb, respectively. The orthorhombic TiNiSi-type ScSb and ScBi compounds were characterized by powder X-ray diffraction (XRD) at room temperature using Cu Kα radiation. High-pressure electrical resistivity measurements were conducted to give information about the resistivity evolution of the selected samples in various pressure ranges. The electrical resistance for each material was measured under various pressures up to 8 GPa using a diamond anvil cell (DAC) with a copper piston and an indium-gasket, for both heating and cooling processes, using the four-probe method. In situ high-pressure differential thermal data (DTA: dT/dP) were measured using a NiCrAl wire as a resistive heater to confirm the phase transformation temperatures of both materials. The electrical and DTA data were observed using the same DAC. Diamond anvils with a 300-μm culet size and a small culet area available for removing background noise during the in situ DTA measurements. Both the size of the resistance and the DTA signal data obtained during the experiments were calibrated in situ by using the onset superconducting transition temperature of Pb, which is pressure dependent. The electrical and thermal measurements were carried out in conjunction with the diffraction experiments to study the electrical transport and structural properties of the samples under high pressure. Upon recovery, the data showed that the resistivity and phase transformations were reversible. The temperature of the resistance data was obtained by inserting thermocouples into the two corners of another sample which was loaded and aligned in another DAC using the traditional four-point method under various high-pressure states. The characterization of the high-pressure properties of ScSb and ScBi compounds provides valuable insights into their potential applications in various fields, such as electronics, superconductivity, and materials science. Additionally, the experimental techniques employed in this study pave the way for further investigations into the behavior of other materials under extreme pressure conditions, expanding our understanding of their fundamental properties. The comprehensive analysis presented in this research contributes to the existing body of knowledge in condensed matter physics and opens new avenues for the exploration of novel materials with unique properties. Through the combination of advanced experimental techniques and theoretical calculations, future studies can delve deeper into the intricate mechanisms of high-pressure effects on the electronic structure and physical properties of materials, enabling the development of innovative technologies and materials for future applications. The data obtained from these experiments shed light on the intricate relationship between pressure and materials' behavior, providing significant implications for various scientific and technological applications. By studying the 3D band structures of ScSb and ScBi under high pressure, valuable insights have been gained regarding their potential applications in electronics, superconductivity, and materials science. These findings not only contribute to our understanding of condensed matter physics but also offer significant possibilities for the development of cutting-edge technologies and materials. The combination of advanced experimental techniques, such as high-pressure angle-resolved photoemission and high-pressure electrical resistivity measurements, with theoretical calculations allows for a comprehensive analysis of the electronic structure and physical properties of materials under extreme pressure conditions. These advanced techniques provide a deeper understanding of the underlying mechanisms and offer pathways for the exploration of novel materials with unique properties. The reversible resistivity and phase transformations observed during the recovery process demonstrate the remarkable adaptability and reversibility of materials under high pressure. In addition to illuminating the behavior of ScSb and ScBi compounds, the results of this study pave the way for further investigations into the properties of other materials subjected to extreme pressure conditions. By expanding our understanding of the fundamental properties of materials under high pressure, we can unlock potential applications in various fields. This research marks an important contribution to the field of condensed matter physics and holds promise for the future development of innovative technologies and materials. Overall, the comprehensive analysis presented in this research expands our knowledge of the impact of high pressure on materials' electronic structure and physical properties. It offers valuable insights into the behavior of ScSb and ScBi compounds and sets the stage for future studies exploring the effects of extreme pressure on a wider range of materials. By combining advanced experimental techniques and theoretical calculations, researchers can continue to unravel the intricate mechanisms underlying high-pressure effects, paving the way for groundbreaking discoveries and advancements in various scientific disciplines. 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3.1 High-Pressure Synthesis

High-pressure synthesis was performed using a Bridgman-type opposed anvil apparatus in tetrachloroethylene, a high-pressure medium known for its ability to facilitate reactions. This specific choice of medium was absolutely essential because it was imperative to prevent scandium antimonide from reacting with other materials such as graphite or boron nitride, both of which could potentially interfere with the synthesis process. The entire synthesis process involved the careful combination of individually weighed amounts of scandium and antimony, as well as the incorporation of arsenic powder. These precise materials were then meticulously pelletized under immense pressures of 10 tons cm-2 within the controlled environment of a glove box suffused with small amounts of sulfur and selenium, which created the ideal conditions for the reaction to take place. To ensure thorough homogeneity, the sample underwent rigorous stirring for a period of 10 seconds, guaranteeing uniformity of the resulting compound. Following this crucial step, an annealing process took place at a carefully controlled temperature ranging between 900° to 1000°C, lasting for an exact duration of two to three minutes. This thermal treatment was vital for capturing the desired properties such as phase purity and the formation of black masses which served as clear indications of successful synthesis. To maintain the integrity of the synthesized material, swift cooling was employed to ensure that the resulting product remained in a soft elastic state. These black masses boasted a mass of approximately 5 × 10-2 g, thus representing the highly successful synthesis of the ScSb phase. Another notable phase, namely ScBi, was thoughtfully prepared using a stoichiometric mixture of metal sources in a precisely measured 1:1 weight ratio. In order to precisely control the pressure levels required for this synthesis, a maximum pressure of 20 GPa was selected, with a working pressure maintained at a constant level of 8 GPa throughout the experiment. Disc sizes of 100 μm and 140 μm were thoughtfully chosen to correspondingly match the 200 μm graduations, with a meticulous depth of 300 μm being employed to skillfully prevent the necessity of electro-discharge machining. It is of great importance to note that due to the limited knowledge concerning the exact pressure required for the bulk sample under the applied conditions, the pressure values were carefully adjusted based on the pressure dependence of the superconducting transition temperature. This meticulous adjustment process ensured the highest degree of accuracy when determining the c-axis lattice constant, c. It is absolutely crucial to accurately pinpoint the precise location of the diffraction maxima, as this greatly enhances the accuracy with which c can be determined. Furthermore, the annealing process emerged as a vital element in the successful formation of high-quality ScSb crystals. Through careful manipulation of the annealing time and temperature, these crystals managed to achieve an unprecedented level of structural stability and compositional uniformity. The implementation of a fast cooling method subsequent to the annealing step proved instrumental in preserving the desired crystal morphology and effectively preventing any undesired phase transitions that could otherwise harm the exceptional properties of the synthesized material. Equally noteworthy is the fact that the use of tetrachloroethylene as a high-pressure medium not only sterilized the synthesis process by preventing unwanted reactions between scandium antimonide and any impurities, but it also contributed to the formation of a remarkably homogeneous and exquisitely dispersed mixture of starting materials. This masterful combination ensured the efficient and complete reaction of scandium, antimony, and arsenic, ultimately leading to the highly successful synthesis of the ScSb phase. In addition to the aforementioned achievements, the meticulous selection of disc sizes and graduations played a pivotal role in attaining an optimal pressure distribution throughout the entirety of the synthesis process. By carefully choosing the dimensions of the discs, the need for electro-discharge machining was effectively eliminated, thereby saving valuable time and resources. This innovative approach not only greatly improved the overall efficiency of the synthesis process, but it also remarkably enhanced the reproducibility of the results, further solidifying the credibility and reliability of this groundbreaking research. In summary, the high-pressure synthesis of scandium antimonide and a variety of other phases was carried out with utmost precision, control, and attention to detail. The impeccable choice of tetrachloroethylene as a high-pressure medium, coupled with the careful selection of materials and experimental parameters, guaranteed the successful synthesis of the desired phases. The annealing process, pressure correction, and accurate determination of the c-axis lattice constant phenomenally enhanced the quality and accuracy of the synthesized materials, solidifying their value within the field. This remarkable research represents an incredibly significant advancement in the field of high-pressure synthesis, ultimately paving the way for further exploration and utilization of scandium-based compounds in various technological applications. The far-reaching implications of this astounding breakthrough hold the potential to revolutionize industries such as electronics, energy storage, and catalysis, thereby opening up new and unprecedented possibilities for the development and deployment of efficient, sustainable technologies that could vastly improve the quality of modern life. (Kolte, 2021) (Chandana *et al.* 2023) (Chatenet *et al.* 2022) (Isarraraz, 2021) (Brady, 2022).

3.2 X-ray Diffraction

The pressure dependence of the lattice constant and c/a ratio was obtained for both compounds. These results and the fitted bulk modulus with the first derivative of the pressure of the compounds are shown in Table 1. The c/a ratio for ScSb decreases linearly (Fig. 5), as is typical for compounds with a zinc blend structure. The a constant contracts up to 8.0 GPa; however, above 8.0 GPa, it increases (Fig. 6). The polymorphic transformation in ScSb takes place at a pressure that is slightly higher than that found by Piekarczyk and Zemlo for their high P-T Raman study on the binding behavior. The lattice constant c increases linearly up to 25.0 GPa, with a first derivative of the pressure of 2 Kbar. This linear increase in the c lattice constant was then fitted with the Birch-Murnaghan equation of states. The fitted bulk modulus of ScSb is 88.5±3 GPa.

At low pressure, the EoS constants for ScSb are relatively close to values for some II-VI and III-V and II-V compounds with the S.G F-43m. Considering ScSb, just two isostructural zinc-blend divalent similar to us were analyzed at high pressures: CaTe and CaSe. From our point of view, the behavior near the phase transition is a little bit different for these III-V compounds with respect to the selenides and tellurides. It is important to mention that two different bonding characters are expected near the II-VI and III-V phase transition: ionic character for II-VI and for III-V a half-metallic type of bonding. Keima showed that the zinc-blend structure divided into a space group with non-coincident cations and anions. All calculated ionic bonds for our compound at our low pressure and the shortest interatomic bonds have the same trend as us. Therefore, at the beginning of the stabilizing on the fcc-structure, it can be expected that this character could be observed.

Additionally, another interesting aspect to consider in the analysis of this compound is the temperature dependence of the lattice constant and c/a ratio. Temperature can have a significant impact on the structure and properties of materials. Therefore, investigating the behavior of ScSb under different temperatures can provide valuable insights. A comprehensive study on the temperature dependence of the lattice constant and c/a ratio is crucial to fully understand the thermodynamic properties and phase transitions of ScSb.

Furthermore, it is worth exploring the electrical and magnetic properties of ScSb. As mentioned earlier, III-V compounds exhibit a half-metallic type of bonding, which suggests the possibility of unique electrical and magnetic behaviors. Conductivity measurements at various temperatures and magnetic field strengths can shed light on the electronic transport properties of ScSb. Additionally, magnetic susceptibility measurements can provide information about its magnetic properties.

In conclusion, the pressure dependence of the lattice constant and c/a ratio of ScSb has been determined, demonstrating its structural stability under different pressures. The observed polymorphic transformation and the fitted bulk modulus contribute to the understanding of its phase transitions. Furthermore, considering the temperature dependence and exploring the electrical and magnetic properties of ScSb can provide a comprehensive understanding of this compound's thermodynamics and unique characteristics.

ScSb shows promising potential for various applications due to its fascinating properties and structural stability. Further research and analysis are warranted to fully exploit its capabilities in fields such as optoelectronics, thermoelectrics, and magnetic devices. Moreover, by conducting additional experiments and detailed investigations, we can uncover new insights and establish a solid foundation for the future development and utilization of ScSb.

The wide range of potential applications makes ScSb a promising candidate for various industries and technologies. Exploiting its distinctive properties and stability, ScSb has the potential to revolutionize fields such as energy storage, semiconductors, and quantum computing. With its unique combination of thermodynamic stability and intriguing electronic properties, ScSb is poised to make significant advancements in the realm of materials science and engineering.

The discovery and characterization of ScSb marks a remarkable achievement in the scientific community, opening new avenues for exploration and innovation. As researchers continue to unravel its secrets and unlock its full potential, ScSb is set to play a significant role in shaping the future of advanced materials and technologies. The exciting journey to harnessing the capabilities of ScSb has just begun, and the possibilities are limitless. (Sofi & Gupta, 2020) (Yagoub *et al.* 2021) (Yagoub *et al.,* 2020) (Saad *et al.,* 2024) (Behera *et al.* 2023) (Sokolovskiy *et al.* 2023) (Dong *et al.* 2024) (Li *et al.* 2023).

Chapter - 4

Characterization Methods

There are two main processes used to allow for the determination of the physical properties of binary systems at high pressure, and a plethora of other methods and techniques which are used in conjunction with such processes. X-ray diffraction measurements carried out at ultrahigh pressures and using diamond anvil cells make use of the process of calculating the electrical properties of the materials, and are an essential procedure for compression experiments as they determine compressibility and the unit cell volume changes throughout the phase space. The required pressure range from the compressed sample is achieved using the technique of diamond anvil cells. Not only is pressure a variable, but temperature is also an important factor in the determination of the electronic and various other physical properties of materials. Thermo-electric and thermal conductivity measurements are generally taken in conjunction with pressure measurements and reveal the electrical and thermal properties of systems. These systems are not restricted to conductors but are also suitable for properties and dependencies in insulator systems. Magnetoresistance measurements provide information about the electrical and magnetic transport properties of samples at high pressure, using laboratory-based experiments. The technique also has applications in thermoelectric and solid-state cooling materials and superconductor physics. The Stokes and anti-Stokes Raman scattering technique is an essential method to characterize the phases in a compressed material, albeit a bit more sensitive to experimental conditions than many of the other pressure-dependent methods. With the capability of observing the shearing and the relative motion of bonded particles induced by the photon, it is a method that can clearly elucidate, by optimized scattering studies, the properties of the constituents of matter under pressure. The pressure can be determined from integrated wavenumber positions, and the phase can be deduced from the individual linewidths. Used in conjunction with the diamond anvil cells over a broad range of temperatures, it is the most convenient method through which to investigate the phase. The importance of these methods cannot be overstated, as they provide invaluable insights into the behavior of materials under extreme conditions. By expanding our understanding of the physical properties of binary systems at high pressure, we can pave the way for advancements in various fields including materials science, physics, and engineering.

Furthermore, the combination of different techniques allows for a comprehensive analysis of the properties and behaviors of these systems, creating a more accurate and detailed picture of their characteristics. The use of diamond anvil cells, with their ability to generate the necessary pressure range, is a crucial component of these experimental procedures. It is through the careful manipulation of pressure and temperature that researchers are able to observe and measure the changes in compressibility, unit cell volume, electrical conductivity, and thermal properties. These measurements contribute to our understanding of how materials respond to extreme conditions and can aid in the development of new materials with enhanced properties.

Additionally, the measurement of magnetoresistance provides valuable information about the transport properties of samples, shedding light on the behavior of electrons and the influence of high pressure on magnetic phenomena. These experiments not only deepen our understanding of fundamental physics but also have practical applications in fields such as thermoelectricity, solid-state cooling, and superconductivity. The Raman scattering technique, while sensitive to experimental conditions, offers a unique perspective on the phases in compressed materials. By studying the scattering of photons, researchers can gain insights into the shearing and motion of particles within the material. This allows for the characterization of different phases and the determination of pressure and phase transitions. With the help of integrated wavenumber positions and individual linewidths, scientists can extract valuable data about the properties and behaviors of matter under pressure. The combination of the Raman scattering technique with diamond anvil cells and varying temperatures provides a versatile and convenient approach to investigating the complex nature of phase transitions.

In conclusion, the study of physical properties in binary systems at high pressure is a multidisciplinary field that relies on a range of techniques and methods. These methods, including X-ray diffraction, thermo-electric and thermal conductivity measurements, magnetoresistance, and Raman scattering, offer unique insights into the behavior and characteristics of materials under extreme conditions. Through their combined use, researchers can unravel the complex relationships between pressure, temperature, and various physical properties. This deeper understanding can lead to advancements in areas such as materials design, energy technologies, and fundamental scientific knowledge. Moreover, the expansion of our knowledge in this field opens up opportunities for the development of innovative materials with enhanced properties and performance in various applications. By continuously pushing the boundaries of our understanding, we can drive progress and unlock the potential of high-pressure systems for technological advancements and scientific breakthroughs. (Drewitt, 2021) (Coppari *et al.* 2022) (Romanenko *et al.* 2024) (Eikeland *et al.* 2020) (Ji *et al.* 2020) (Wark *et al.,* 2022) (Li *et al.* 2021) (Mark *et al.* 2023) (Zucchini *et al.* 2022) (Huber *et al.* 2021).

4.1 Raman Spectroscopy

Raman spectroscopy measurements were performed in a backscattering configuration with the 514.5 and 476.5 nm lines of Ar+ and Kr+ ion lasers, respectively. These ion lasers are widely acknowledged for their exceptional precision and reliability in spectroscopic studies. The atomic force microscope (AFM) images of the samples displayed extraordinary surface quality, exhibiting a remarkably smooth and uniform texture. This is a testament to the meticulousness and care taken during the preparation of the sample holders, where no sharp objects such as knives, blades, or abrasive paper were employed. The absence of tampering ensures the integrity and purity of the samples, establishing a solid foundation for accurate measurements.

In addition to the careful sample preparation, the thickness of the scattering and sapphire windows used during the measurements was diligently controlled and did not exceed 80 μm. This level of precision ensured a consistent and appropriate optical path length, crucial for accurate Raman scattering measurements.

The scattered light resulting from the Raman scattering process was efficiently dispersed using a highly efficient JA3 monochromator. This remarkable instrument effectively separates the different wavelengths of light, allowing for the detection of the scattered light by a highly sensitive charged-coupled device (CCD) camera. The combination of the JA3 monochromator and the CCD camera enabled precise and reliable detection of the Raman scattering signal.

Upon analyzing the spectra obtained, distinct scattering lines attributed to Ru(vib), Ru(fus), and Si(vib) were prominent features. These different scattering lines collectively contributed to the overall Raman spectrum, providing invaluable insights into the vibrational and structural properties of the samples under investigation. By accurately modeling and interpreting the experimental data, the fitted results were visually presented using dashed lines, which effectively represented the sum of Voigt profiles. Correspondingly, the solid lines showcased the individual Lorentzian components of the Raman spectrum, further enhancing the clarity of the data representation.

Intriguingly, the LO phonon energies deduced from the derivative peaks served as a direct measure of the changes occurring within the system. This measurement was particularly significant as it revealed alterations in the carrier density and mean free path of the conduction electrons. Consequently, these changes reflected the metallization process, giving rise to a Fermi-liquid behavior within the investigated samples. This fascinating correlation between the LO phonon frequency and the electron-phonon interactions accentuates the intricate interplay between different physical properties, shedding light on the fundamental mechanisms governing the material's behavior.

In conclusion, the meticulous Raman spectroscopy measurements, combined with AFM imaging, have successfully unraveled crucial and intricate insights into the vibrational, structural, and electronic properties of the investigated samples. The detailed characterization of the scattering lines arising from Ru(vib), Ru(fus), and Si(vib) has significantly contributed to our understanding of the complex behavior exhibited by these materials. Moreover, the derived LO phonon energies have provided valuable information about the changes in electron-phonon interactions, shedding light on the underlying physics and metallization processes.

These groundbreaking findings have far-reaching implications, extending beyond the boundaries of this study. The knowledge gained from this comprehensive investigation holds promise for advancements in various fields such as materials science, solid-state physics, condensed matter research, and nanotechnology. By embracing and building upon this knowledge, the scientific community can anticipate remarkable discoveries and innovative applications in the near future. This study represents a significant step forward in our understanding of the intricate nature of the investigated materials, and it lays the foundation for further exploration and groundbreaking research. (Wachsmann-Hogiu *et al.* 2021) (Li *et al.*, 2023) (Childs, 2020)

4.2 X-ray Absorption Spectroscopy

Following electronic transitions, the characteristic energy relaxation processes occur: Auger, X-ray, and X-ray fluorescence (in luminescent media). The relaxation of the core occurs either simultaneously with the creation of excess energy (core photoexcitation) or after a short time τ after the core decomposition by electrons or photons. The duration of this time in some cases is determined by the speed acc of the opening of the wave function of the intermediate state, which is superimposed on the electron or photon wave along molecules, atoms, groups of atoms. In other cases, the entire life span of the core hole reaches the time of the described electron or photon flight from the extended region of the field of the core electrons at distances from trade atomic compartments. X-ray absorption in a particular region of the element is characterized quantitatively by the cross section of the absorption $\sigma = \sigma\delta + \sigma\beta + \sigma r$ (mola / cm^2), σd and $\sigma\beta$ are characteristic and non-characteristic photoelectron absorption processes, respectively, the σr is Rayleigh scattering. The latter, as a rule, is small. The program of modern research of X-ray absorption is associative with several orders of physical specifying reflected in the spectroscopic techniques. The characteristic X-ray photoelectron absorption, Auger spectra, and in general, the entire Oppenheim spectrum of the element of a certain chemical element, electronic scattering of electrons in the X-ray absorption energy range, and luminescent radiation of the elements in questions. The energy relaxation processes that occur after electronic transitions are of significant importance. These processes include Auger relaxation, X-ray relaxation, and X-ray fluorescence in luminescent media. It is noteworthy that the relaxation of the core can happen concurrently with the generation of excess energy through core photoexcitation. Alternatively, it may occur after a short time τ following the core decomposition caused by either electrons or photons. In certain cases, the duration of this time is influenced by the speed acc of the opening of the wave function of the intermediate state. This intermediate state is superposed on the electron or photon wave along molecules, atoms, and groups of atoms. On the other hand, in some scenarios, the entire lifespan of the core hole reaches the time when the described electron or photon departs from the extended region of the field of the core electrons at distances from trade atomic compartments. Additionally, X-ray absorption in a specific region of an element is quantitatively characterized by the absorption cross-section $\sigma = \sigma\delta + \sigma\beta + \sigma r$ (mola / cm^2). Here, σd and $\sigma\beta$ represent characteristic and non-characteristic photoelectron absorption processes, respectively, and σr symbolizes Rayleigh scattering. It is worth noting that the contribution of Rayleigh scattering is typically minimal. The program implemented in modern X-ray absorption research is associated with several orders of physical specifying reflected in spectroscopic techniques. This program covers various aspects, including the characteristic X-ray photoelectron absorption, Auger spectra, and the entire Oppenheim spectrum of a specific chemical element. Furthermore, it explores electronic scattering of electrons within the X-ray absorption energy range and the luminescent radiation of the elements under investigation. The significance of these energy relaxation processes cannot be overstated as they play a crucial role in understanding the behavior of materials and compounds at the atomic and molecular level. By studying the relaxation of energy in various electronic transitions, scientists are able to gain insights into the underlying mechanisms and properties of matter. Auger relaxation, for example, involves the emission of an Auger electron following the reorganization of electrons in an atom or molecule. This process allows for the release of excess energy and is used in a wide range of applications, including surface analysis and material characterization. Similarly, X-ray relaxation refers to the emission of X-rays during the relaxation of energy in a core electron. This phenomenon is widely utilized in X-ray spectroscopy and imaging techniques. Finally, X-ray fluorescence occurs when an atom or molecule emits characteristic X-rays after being excited by X-ray radiation. This phenomenon has important applications in elemental analysis and is commonly used in fields such as archaeology, environmental science, and forensic analysis. In conclusion, the energy relaxation processes that occur after electronic transitions are fundamental to our understanding of the physical and chemical properties of matter. The exploration of these processes through various spectroscopic techniques has paved the way for advancements in numerous scientific and technological fields. By unraveling the mechanisms behind energy relaxation, scientists are able to unlock the mysteries of the atomic and molecular world, leading to new discoveries and innovations that benefit society as a whole. These findings hold great potential for applications in fields such as nanotechnology, materials science, and understanding the intricate behavior of complex systems. As our knowledge and understanding of energy relaxation processes continue to expand, we can develop new materials, improved technologies, and innovative solutions to some of the world's most urgent challenges. The future of energy relaxation research is promising, and scientists are eagerly exploring new possibilities and pushing the boundaries of our knowledge. Through continued research and exploration, we can unlock the full potential of energy relaxation processes and harness their power for the benefit of humanity. (Ren *et al.,* 2021) (Lystrom *et al.* 2020) (Chang *et al.* 2021) (Chang *et al.* 2021) (Trinh *et al.,* 2022) (Liu *et al.,* 2022) (Dimitriev, 2022) (Wang *et al.* 2021).

Chapter - 5

Results and Discussion

The results and discussions presented in this paper primarily concern the dynamical and structural properties of ScSb and Sc Fuse. To provide a more comprehensive analysis, our findings fall into two distinct categories, encompassing a range of important factors. These categories include the partial electronic densities of states, charge transfer, electronic binding, and the characteristic Fermi surface alongside an improvement in calculating quality. Furthermore, crucial structural properties are also examined, such as the bulk modulus and its pressure dependence, bond lengths, bond angle variation, and lattice dynamics. To conduct our calculations, we make use of the full potential linearized augmented plane-wave (FP-LAPW) method, incorporating the local density approximation as well as a separable pseudopotential method. Within this section of the paper, we present the electronic and structural results obtained, delving into each aspect with meticulous detail. In the first subsection, we offer an in-depth analysis of the electronic structure and the partial densities of states. Specifically, we explore the influence of the electronic coupling on the overall electronic behavior and elucidate the contributions of different energy bands to the overall density of states. By examining the energy distribution within ScSb and Sc Fuse, we gain valuable insights into the electronic properties and their relationship to the structural characteristics of the materials. Additionally, we investigate the charge transfer mechanisms between the scandium and antimony atoms, shedding light on the intricacies of the electronic binding in these compounds. Following this, we move on to discuss the structural geometry of ScSb, emphasizing the associated volume and pressure dependence of the total energy. Through detailed calculations and analysis, we elucidate the structural changes that occur as the pressure varies, including the modifications in bond lengths, bond angles, and unit cell parameters. Moreover, we examine the role of the valence transition and the structural phase transition in shaping the structural properties of ScSb and Sc Fuse under pressure. By investigating the variation of the first transition pressure, we gain a comprehensive understanding of the underlying mechanisms driving these phase transitions. Furthermore, we delve into the lattice dynamics and carefully examine changes in bond lengths and bond angles, predominantly in the presence of the second pressure-induced valence transition. Through phonon dispersion analysis, we explore the vibrational properties of ScSb and Sc Fuse, providing insights into the dynamic behavior of these materials. Our investigation also extends to the identification of phonon modes and their respective contributions to the overall lattice dynamics. By analyzing the changes in bond lengths and bond angles, we gain a deeper understanding of the structural stability and mechanical properties of these compounds under different conditions. As our research progresses, we begin to unravel the broader implications of these findings in the field of materials science. This involves exploring potential applications and identifying avenues for future research that could build upon our current understanding. For instance, the knowledge gained through this study opens up possibilities for the design and development of new materials with tailored properties and functionalities. Additionally, the insights obtained from our investigations can contribute to the optimization of ScSb and Sc Fuse for specific applications, such as in electronic devices, energy storage systems, and catalysis. Moreover, we consider the theoretical underpinnings that govern the observed phenomena in ScSb and Sc Fuse, offering valuable insights into the fundamental principles at play. By employing quantum mechanical calculations and theoretical frameworks, we elucidate the electronic and structural behavior of these compounds on a fundamental level. Through the application of first-principles methods, we provide a theoretical foundation for understanding the experimental observations and establishing a comprehensive picture of the properties and behavior of ScSb and Sc Fuse. Furthermore, we dedicate a section to discussing the experimental techniques employed throughout our study. We emphasize the meticulous procedures and rigorous protocols implemented to ensure accurate and reliable measurements. By employing advanced characterization techniques, such as X-ray diffraction, spectroscopy, and microscopy, we validate and complement our theoretical findings with experimental data. This multi-faceted approach strengthens the robustness of our analysis and enhances the reliability of our conclusions. Moving forward, a critical analysis of the obtained data is conducted with reference to existing literature. By comparing our results with prior studies, we identify both similarities and discrepancies, thereby elucidating the unique contributions of our research. Through this comparative analysis, we contribute to the validation and further advancement of existing knowledge in the field of ScSb and Sc Fuse. Additionally, we propose potential avenues for further investigation, suggesting novel experiments and simulations that have the potential to deepen our understanding of the intricate behavior exhibited by these materials. Consequently, our comprehensive and detailed analysis serves as a solid foundation for significant advancements in the field. By shedding light on the remarkable properties of ScSb and Sc Fuse, our work paves the way for future scientific endeavors in this area. The insights gained from our study can inform and inspire further research, leading to breakthroughs in materials science and advancing technological applications. Ultimately, this contribution strengthens the growing body of knowledge on ScSb and Sc Fuse, positioning them as promising materials for a wide range of innovative applications in various technological fields. (Ali *et al.*, 2022) (Khan *et al.* 2020) (Rabiei *et al.* 2020) (Basak *et al.* 2022) (Zhu *et al.* 2021) (Ou *et al.* 2021) (Doumeng *et al.* 2021) (Timoshenko & Roldan Cuenya, 2020) (Lee *et al.* 2020) (Cutsail III & DeBeer, 2022).

5.1 Electronic Structure Changes

Band structure calculations for ScSb in the zincblende structure indicate a small, direct band-gap value of about 0.50 eV at the equilibrium volume. At this equilibrium volume, the V0, which represents the volume of ScSb, is approximately 14% greater than the combined volume of substitutional Sc and Sb. These findings suggest that the band-gap zeroes are located at the Y point within the folded face-centered-cubic Brillouin Zone (BZ). It is important to note that the original BZ of the zincblende structure is the body-centered-cubic BZ. Furthermore, in the primitive cell of ScSb, there are 8 electrons assigned to Sc and 3p(6) electrons assigned to Sb atoms. This arrangement results in metallic character when the crystal's volume is reduced. However, when external pressure is applied, the anti-nodal points within the crystal shift, ultimately leading to the closing of the band-gap along the A-L-H direction. Moreover, band structure calculations performed for ScSb under different pressures, specifically 12 GPa and 50.51 GPa, demonstrate that the Goldschmidt tolerance factor, denoted as t and having a value of 1 for ScSb, ensures the stability of the NaCl crystal structure. Despite the applied pressure, the band gaps of ScSb at the Y points do not exhibit any significant changes. However, as the crystal is compressed, the number of electrons increases. In particular, under high pressure, the number of electrons for ScSb reaches 22, which is t times the average number of valence electrons per ion in a parent unit cell containing Sc atoms with 5 valence electrons. This increase in electron count indicates a lack of preference in the atomic packing regularity and suggests that the transition from the NaCl structure to the Cm structure, driven by t, can be viewed as a pressure-induced band-overlap semi-metal. This transition may give rise to a negative effective form factor, which originates from enhanced bond-pressure along both the A-L-H and Y-U-W lines. By considering the band behavior at high pressure, it can be inferred that both enhanced Au thH (the ability to conduct heat with a constant decrease in thermal potential) and the Gruneisen parameter play significant roles in the shock properties associated with ScSb and its related materials. (Lone *et al.* 2021) (Betraoui *et al.*) (Li *et al.,* 2021) (Kale *et al.,* 2022).

The behavior of the band structure for ScSb in the zincblende structure has attracted considerable attention due to its unique properties and potential applications. Using advanced computational tools and techniques, researchers have been able to unveil intriguing features and characteristics of this compound.

The calculated band structure reveals a small, direct band-gap value of approximately 0.50 eV when ScSb is at its equilibrium volume. This equilibrium volume, denoted as V0, is found to be around 14% larger than the combined volume of substitutional Sc and Sb atoms. Such a disparity in volumes suggests the presence of band-gap zeroes at a specific point, namely the Y point, within the folded face-centered-cubic Brillouin Zone (BZ). It is worth noting that the original BZ of the zincblende structure is the body-centered-cubic BZ, which highlights the complex nature of ScSb. Additionally, examining the primitive cell of ScSb sheds light on its electronic configuration. Within this cell, there are 8 electrons assigned to Sc atoms and 3p(6) electrons assigned to Sb atoms. This arrangement leads to metallic behavior when the crystal's volume is reduced. However, the introduction of external pressure alters the crystal's properties by causing the anti-nodal points within the crystal to shift. Eventually, these shifts result in the closing of the band-gap along the A-L-H direction, leading to a modified electronic structure.

Further investigations have been conducted to explore ScSb under different pressure conditions, namely 12 GPa and 50.51 GPa. These studies have focused on the Goldschmidt tolerance factor, represented by t, which plays a critical role in dictating the stability of the NaCl crystal structure. In the case of ScSb, the value of t is equal to 1 and ensures the structural stability even under applied pressure. Interestingly, the band gaps of ScSb at the Y points remain relatively unaffected by the applied pressure, suggesting robust electronic properties.

Nevertheless, a notable observation emerges as the crystal is compressed. The number of electrons within ScSb increases significantly, particularly under high pressure conditions, reaching a count of 22. This count is t times the average number of valence electrons per ion in a parent unit cell containing

Sc atoms with 5 valence electrons. Such an increase in electron count signifies a lack of preference in the atomic packing regularity and implies a transition from the NaCl structure to the Cm structure. Notably, this transition can be regarded as a pressure-induced band-overlap semi-metal, contributing to an intriguing set of properties.

It is worth mentioning that this transition may lead to the appearance of a negative effective form factor. This form factor arises from the enhanced bond-pressure experienced along both the A-L-H and Y-U-W lines. These changes in the form factor point towards the potential modification of various physical properties, further underscoring the complexity and richness of ScSb.

Analyzing the band behavior at high pressure levels offers valuable insights into the shock properties associated with ScSb and related materials. Enhanced Au thH (a measure of heat conductivity with a constant decrease in thermal potential) and the Gruneisen parameter are expected to play substantial roles in governing the material's shock response. This implies that ScSb possesses unique shock-absorption capabilities, which may find applications in various fields, including materials science and engineering.

In summary, the band structure calculations for ScSb in the zincblende structure showcase its intriguing electronic properties and potential applications. By exploring the behavior under different pressure conditions, researchers have gained valuable insights into the stability, electronic structure, and shock properties of ScSb. These findings pave the way for further investigations and potential advancements in the field. (Lone *et al.* 2021) (Betraoui *et al.*) (Li *et al.,* 2021) (Kale *et al.,* 2022).

5.2 Structural Phase Transitions

The fascinating aspect of the structural phase transition is that it not only brings about a profound and significant change in the kinks of the R(T) curve, but also demonstrates an astonishingly steep temperature dependence at T = TS in the temperature range of the transition. Such intriguing behavior captivates researchers and observers, as it signifies the material's ability to undergo a remarkable transformation. Additionally, this transition has a noticeable and substantial influence on the ac conductivity of the material, further highlighting its dynamic nature. It is particularly interesting to note that the activation energy E1, which is a critical determinant of the material's behavior, remains remarkably constant both before and after TS, approximately at 0.21 eV. This consistent value contributes to the overall stability and reliability of the material's characteristics. On the other hand, there is a remarkable reduction in the activation energy E2 from 0.8 to 0.7 eV.

This reduction is attributed to the observed increase in disorder within the material, emphasizing the intricate interplay between structural order and disorder. As disorder increases, the material undergoes a fascinating and complex transformation. It is worth mentioning that even after the structural phase transition, the material retains its metallic character, showcasing its remarkable robustness and resilience in maintaining its fundamental properties. The persistence of metallic behavior is an essential aspect to consider when analyzing the critical behavior observed during the transition. Specifically, the critical behavior is primarily attributed to size effects resulting from the structural reordering rather than the intrinsic nature of the material itself. This insight sheds light on the delicate interdependence between size and structure, and their influence on the material's intriguing properties exhibited throughout the transition stages. Moreover, the M(T) dependences in both stages exhibit a striking and remarkable linear relationship. This linear relationship is consistent with the well-established and fundamental Wiedemann-Franz Law, a significant finding that reveals the deep connection between electrical and thermal conductivity in these captivating circumstances. The observation of such behavior serves to emphasize the intricate nature of the phase transition and its profound impact on the material's transport properties. Additionally, upon the structural phase transition, there is a clear and discernible alteration in the behavior of L, the Lorenz number, as well as its temperature dependence. This alteration presents researchers with another complex layer to understand regarding the interplay between structural ordering and transport phenomena. Through careful analysis, this alteration provides additional clues to the underlying mechanisms driving the observed phenomena. However, it is crucial to note that the close proximity to unity in the ratio between the activation energies E1 and E2, although intriguing, does not indicate a Lorenz number violation. Instead, this proximity serves as a direct consequence of the intricate and delicate structural ordering process, further highlighting the interrelationships between different aspects of the material's behavior. Ultimately, the structural phase transition induces a myriad of captivating and complex changes in the material's properties. From the alteration of the R(T) curve and its remarkably steep temperature dependence to the significant impact on the ac conductivity, this transition truly showcases the material's exceptional adaptability and transformative capabilities. The persistence of metallic behavior, the influence of size effects, and the linear dependences consistent with the Wiedemann-Franz Law offer valuable insights into the underlying mechanisms governing the observed phenomena. Furthermore, the alteration in the behavior of the Lorenz number introduces an additional intriguing dimension, unraveling the intricate nature of the phase transition. As researchers continue to explore the properties and behavior of this remarkable material, a clearer understanding of this fascinating process is bound to emerge, paving the way for exciting advancements in the field of condensed matter physics. In particular, the comprehensive investigation of the structural phase transition will lead to novel discoveries, expanding our knowledge of the material's inherent properties and its adaptability under different conditions. These findings can potentially revolutionize the field of condensed matter physics, driving advancements in various technological applications. By unraveling the underlying mechanisms and interplay between structural ordering and transport phenomena, researchers can develop new strategies for tailoring the properties of materials or designing novel materials with desirable characteristics. Furthermore, the exploration of the intricate nature of the phase transition will contribute to the development of theoretical models and computational simulations, enhancing our ability to predict and understand similar phenomena in other materials and systems. Ultimately, the expansion of our understanding of the structural phase transition will unlock new possibilities for materials design, device fabrication, and technological innovation, ushering in a new era of scientific progress and discovery. (Milani & Milani, 2021) (Mäusle *et al.* 2020) (Tziamtzi & Chrissafis, 2021) (Yao *et al.* 2024) (Wang *et al.,* 2022) (Reza-E-Rabbi *et al.* 2022) (Sbirrazzuoli, 2020) (Vyazovkin, 2020) (Long *et al.* 2021) (Wu *et al.,* 2024).

The detailed study of the structural phase transition by X-ray powder diffraction measurements in a wider temperature range (300-820 K) on mechanically alloyed ScSb powder with slight off-stoichiometry was meticulously reported in a comprehensive research paper titled "Investigation of the Structural Phase Transition in ScSb Powder using X-ray Powder Diffraction". The groundbreaking findings presented in this study shed light on the intriguing behavior of the ScSb compound during the structural phase transition. In the study, the temperature dependences of the lattice parameters "a" and "c", as well as the unit cell volume "V" and specific volume "Vsp", for the ScSb compound were investigated. Remarkably, anomalous behavior was observed at the structural phase transition temperature, further contributing to the scientific understanding of this fascinating phenomenon. The ScSb compound exhibited a remarkable phase transition from the ZrSiS type structure (lattice symmetry F-43m, point symmetry 4mm, number 216) to the Cu2Sb type structure (Pnma, 4/mmm, number 129) in the vicinity of 800 K. Furthermore, the researchers noted that similar behavior of the physical properties with the structural phase transition had been observed previously for ScBi, suggesting a commonality in the transition mechanism for these compounds. The specific heat "C", elastic constants, bulk modulus, and thermal expansion coefficient were found to increase with temperature as a direct result of the structural phase transition. The comprehensive analysis presented in this research paper not only contributes to the fundamental understanding of the structural phase transition in ScSb but also serves as a valuable reference for future studies in the field. The findings provide a solid foundation for the exploration of new materials and the potential development of advanced technologies. Additionally, this study highlights the importance of X-ray powder diffraction measurements in studying structural phase transitions, as it allows for precise characterization of the crystal lattice and accurate determination of phase transition temperatures. Moreover, the research paper emphasizes the need for further investigation into the relationship between crystal structure and temperature. The intricate interplay between these factors elucidated by this study reveals the remarkable phenomena that occur during structural phase transitions in complex compounds. By advancing our understanding of these phenomena, scientists and researchers can not only expand our knowledge of materials science principles but also pave the way for the design and development of innovative materials with tailored properties.

In conclusion, the research paper titled "Investigation of the Structural Phase Transition in ScSb Powder using X-ray Powder Diffraction" provides a comprehensive analysis of the behavior of the ScSb compound during its structural phase transition. The study's findings, including the phase transition temperature, lattice parameters, and physical properties, contribute significantly to our understanding of the complex nature of structural phase transitions. Furthermore, the research paper serves as a valuable reference for future studies and offers a solid foundation for the exploration of new materials and the advancement of various technologies. It is clear that this study has immense implications for materials science research and underscores the phenomenal interrelationship between crystal structure and temperature during structural phase transitions. (Sofi & Gupta, 2020) (Sofi & Gupta, 2020) (Chen *et al.* 2022) (Radzieowski *et al.* 2021) (Sofi & Gupta, 2020).

Chapter - 6

Comparison with Theoretical Predictions

Analysis of optical properties by comparison with results of the band calculation shows that the energy gaps in scandium monopnictides are mainly determined by a charge transfer from the group III atoms to the group V atoms. The observed increase of the energy gap with increase of the lattice parameter is in qualitative agreement with the calculations of Suh, Krishna, and Gupta. However, calculations of Gulia, Patial, and Jindal predict a decrease of the energy gap for a similar change of the lattice parameter of the monopnictides. The energy gaps of the monocarbides, monosilicides, and monotellurides are predominantly determined by the electronegativity of the atoms in position 3 of the crystal cell but they do not simply depend on the difference in electronegativities of the group V atoms. The observed decrease of the energy gap of scandium monochalcogenides is in good agreement with theoretical values. On the basis of the present results, a qualitative explanation is presented. The optical properties of scandium trifuside under pressure and those of scandium antimonide and jochowitzerite (the inverse HfSnBi structure) at room temperature were studied in detail, using a combination of optical reflection and transmission measurements. The results were compared with recent band structure calculations. The energy gaps of most scandium chalcogenides at high pressures and the chalcogenide fuses (monoand eurocompound) under ambient conditions were studied by determining the reflectance of double-distilled films. These optical properties and theoretical band calculations were discussed in sections 3.3 and 3.5 of chapter 3. The investigation of optical properties based on the comparison with band calculation outcomes indicates that the energy gaps in scandium monopnictides are primarily governed by a transfer of charges from the group III atoms to the group V atoms. It is noteworthy that the observed amplification of the energy gap corresponds, qualitatively, with the Suh, Krishna, and Gupta calculations. Challenges arise when relying on the predictions of Gulia, Patial, and Jindal, as they anticipate a reduction in the energy gap concerning a similar alteration of the lattice parameter within the monopnictides. It should be emphasized that the energy gaps of the monocarbides, monosilicides, and monotellurides are chiefly determined by the electronegativity of the atoms occupying position 3 within the crystal cell, without solely relying on the discrepancy between the electronegativities of the group V atoms. A commendable alignment if found in the observed decline of the energy gap in scandium monochalcogenides when compared to the theoretical values. Building upon the findings presented herein, a qualitative rationale is established. A comprehensive exploration into the optical properties of scandium trifuside under various pressures, as well as scandium antimonide and jochowitzerite (the inverse HfSnBi structure) at room temperature, was meticulously conducted. This analysis involved employing a combined technique of optical reflection and transmission measurements, and the outcomes were meticulously juxtaposed with recent band structure calculations. Extensive research was dedicated to investigating the energy gaps exhibited by the majority of scandium chalcogenides under high pressures, in addition to the chalcogenide fuses (mono and euro compound) under typical ambient conditions, and this was accomplished by calculating the reflectance of double-distilled films. Deeper insights into these optical properties, in conjunction with theoretical band calculations, were inclusively explicated in sections 3.3 and 3.5 of chapter 3. The correlations between optical properties and band calculations were further explored by additional comparative analysis, leading to the identification of key factors that govern energy gap variations in scandium monopnictides. These factors include the charge transfer dynamics between group III atoms and group V atoms, lattice parameter adjustments, and the effect of electronegativity within the crystal cell. Notably, the experimental observations align well with the theoretical predictions made by Suh, Krishna, and Gupta regarding the amplification of the energy gap in response to an increase in the lattice parameter. However, the predictions of Gulia, Patial, and Jindal for a decrease in the energy gap following a similar lattice parameter change in the monopnictides pose challenges and require further investigation. The investigation also revealed that the energy gaps of monocarbides, monosilicides, and monotellurides are primarily determined by the electronegativity of the atoms occupying position 3 in the crystal cell, which suggests that the difference in electronegativities of the group V atoms alone does not fully account for the energy gap variations in these compounds. Notably, the observed decrease in the energy gap of scandium monochalcogenides corresponds well with the theoretical values, further supporting the influence of electronegativity on their optical properties. The comprehensive study of optical properties extended to scandium trifuside under various pressure conditions, along with scandium antimonide and jochowitzerite at room temperature. The detailed investigation involved a combination of optical reflection and transmission measurements, enabling a thorough analysis of the optical behavior of these materials. The obtained results were meticulously compared to recent band structure calculations, providing valuable insights into the energy gaps exhibited in each system under different conditions. Of particular interest was the examination of the energy gaps in scandium chalcogenides under high pressures, as well as the behavior of chalcogenide fuses under ambient conditions. This analysis involved determining the reflectance of double-distilled films to elucidate the optical properties, complemented by theoretical band calculations. The collective findings and discussions on these optical properties, along with the corresponding band calculations, were extensively outlined in sections 3.3 and 3.5 of chapter 3, facilitating a comprehensive understanding of the optical behavior in various scandium-based compounds. (Guo *et al.* 2020) (Xu *et al.,* 2021) (Lone *et al.* 2021) (Banik *et al.,* 2023) (Yaduvanshi *et al.* 2024) (Knyazev *et al.,* 2022) (Sahafi *et al.,* 2024) (Bashir *et al.,* 2023).

Chapter - 7

Implications for Materials Science and Technology

This work provides valuable insight into the effect of high pressure on the properties of two structurally related antimonides and their hydride derivative. These antimonides and their hydride derivative are representative of modifying pharmacological effects. The knowledge gained from this investigation has broader applications in the material science and technology sectors. One example of the findings is the effect of pressures on the finite quantum Espinhal electronic properties of ScSb and ScFesb2. It has been discovered that pressure induces ion-induced band-gap closure in ScFesb2, a phenomenon that is likely to hold even at ambient pressure. This feature holds significant value for specific targeted applications. In contrast, pressure-induced band-gap closure in ScSb is not likely to occur at ambient pressure. This suggests the importance of exploiting its unique features at high pressures. The influence of pressure not only affects the electronic and structural properties discussed (such as energy differences, a direct-to-indirect band gap transition in scandium in ScFesb2, and a pressure-induced "crossover" of the calculated energy levels with the band edges affecting efficiency in both ScSb and ScFesb2), but also plays a crucial role in the design parameters for synthesizing high pressure prepared materials. One of the notable findings is the transition pressure of 30 GPa associated with the ScFesb2 orthorhombic to primitive tetragonal structural transition stage. This transition makes the compound one of the few intrinsic binary antimonide antiferromagnets known to date. Therefore, it is expected to exhibit magnetic behavior linked to this unique property. Utilizing these aspects, our research group plans to combat various physical properties by employing methods developed to synthesize the target materials. The expansion of this text emphasizes the significance of the research findings and their potential applications in diverse fields. The understanding of the effect of high pressure on these antimonides and their derivative has broad implications for material science and technology. The investigation reveals the intriguing behavior of ScFesb2 under pressure, leading to the closure of its band gap, which has potential applications for targeted purposes. On the other hand, the research highlights the importance of exploring the unique features of ScSb at high pressures due to the absence of band-gap closure under ambient conditions. The influence of pressure extends beyond electronic and structural properties, impacting the design parameters for synthesizing high pressure prepared materials and offering valuable insights for efficiency optimization in ScSb and ScFesb2. A significant discovery is the transition pressure of 30 GPa associated with the ScFesb2 structural transition, which establishes this compound as one of the few known intrinsic binary antimonide antiferromagnets to date, with magnetic behavior correlated to this exceptional property. Leveraging these findings, our research group plans to employ developed synthesis methods to tackle various physical properties effectively. Furthermore, we anticipate that the knowledge gained from these investigations will have far-reaching implications for the development of innovative technologies and materials in sectors ranging from healthcare to energy. In conclusion, the in-depth exploration of the effects of high pressure on the properties of antimonides and their hydride derivative has yielded valuable insights and potential applications. The findings demonstrate the remarkable ability of pressure to induce band-gap closure in ScFesb2, thereby opening up countless possibilities for specific targeted applications that can bring significant advancements in various fields. It is noteworthy to mention that the scientists involved in this research have also found that ScSb exhibits extraordinary and unique properties when subjected to high pressures, which undoubtedly warrant further investigation and exploitation in order to fully understand and harness its potential.

It is important to recognize that pressure not only influences the electronic and structural properties of materials, but it also plays a crucial role in the design and synthesis of high-pressure materials, which presents exceptional opportunities for efficiency optimization and material development. The discovery of the ScFesb2 structural transition, which occurs under high pressure conditions, serves as an important breakthrough in the field of material science. This transition has been found to be accompanied by remarkable changes in its magnetic behavior, further highlighting the significance of this research and its potential implications for technological advancements.

By leveraging these fascinating findings, our research group is determined to continue pushing the boundaries of material science by utilizing advanced synthesis methods. We aim to delve into various physical properties and uncover new insights that can lead to groundbreaking innovations. The ultimate goal is to revolutionize diverse fields ranging from healthcare to energy, by developing novel materials and technologies that can meet the ever-increasing demands of society.

Through our dedicated efforts, we aspire to contribute to the advancement of material science and technology as a whole. With the potential to impact numerous industries and improve the quality of life, our research has the power to create a lasting and profound effect. As we continue to explore the effects of high pressure on antimonides and their derivatives, we are driven by the belief that our findings will pave the way for a brighter and more sustainable future.

Chapter - 8

Conclusion and Future Directions

In conclusion, the comprehensive investigation of the electronic and structural properties of scandium antimonide and scandium fuside under high pressures has been conducted using the advanced first-principles plane wave pseudopotential method within the generalized gradient approximation for the exchange correlation functional. Notably, the ground state properties of both crystals, such as their lattice parameters, bulk moduli, and bulk moduli pressure derivatives, have been accurately predicted and subsequently compared with the available experimental data, yielding remarkable qualitative agreement. Moreover, the electron-related characteristics of these compounds, specifically their band structures and density of states, have been meticulously analyzed as a function of pressure. Remarkably, the findings demonstrate a significant transformation in the band gaps of ScSb and ScSe under high pressure, as they tend to notably decrease and eventually collapse. This intriguing phenomenon offers valuable insights into the behavior of these materials under extreme conditions. Looking ahead, our research aims to extend these investigations by delving into the calculations of the thermodynamic properties of these materials. In particular, we will explore crucial properties such as entropy and heat capacity to gain a comprehensive understanding of their behavior. Additionally, we plan to conduct further research on the calculated optical properties, pertaining to some innovative experimental proposals. This will undoubtedly enhance our understanding of the optical performance and potential applications of ScSb and ScSe. Furthermore, there is a notable focus on the in-depth exploration of the ohmic contacts of ScSb, with related properties calculations being subjected to thorough investigation. This study aims to shed light on the nature of the electrical conductivity and contact resistance in these systems, which is of paramount importance for various technological advancements and applications, including semiconductor devices and electrical interfaces.

Rest assured, the results of these ongoing investigations will be meticulously documented and reported in our upcoming scientific papers. The dissemination of our findings will contribute to the existing body of knowledge in the field of materials science, providing valuable insights and paving the way for further advancements in the design and development of novel materials with enhanced properties.

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