
Superconducting Hydrides and Covalent Bonding: A Survey

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Abstract

The exploration of superconducting hydrides presents a transformative potential for high-temperature superconductivity, emphasizing the synthesis of hydrogen-rich compounds with sp^3 covalent bonds under low-pressure conditions. This survey paper systematically reviews the field, highlighting the significance of superconducting hydrides in achieving elevated superconducting transition temperatures and their potential applications in energy transmission and storage. The study delves into the challenges of high-pressure synthesis, offering insights into innovative low-pressure techniques and the strategic design of covalent bonds to optimize superconducting properties. Theoretical models, including Bardeen-Cooper-Schrieffer (BCS) theory and Density Functional Theory (DFT), are central to understanding electron-phonon interactions and guiding the discovery of novel superconductors. The survey also explores the role of sp^3 covalent bonds in superhard materials, underscoring their contribution to mechanical strength and stability. The findings emphasize the need for interdisciplinary approaches, leveraging computational methods and experimental validation to overcome existing challenges and enhance the practical applicability of superconducting hydrides. Future research directions focus on refining theoretical models, expanding the exploration of ternary and quaternary hydrides, and optimizing synthesis conditions to achieve superconductivity at ambient pressures. This comprehensive review not only synthesizes current knowledge but also identifies pathways for advancing the field, paving the way for innovative applications and deeper insights into high-temperature superconductivity.

1 Introduction

1.1 Significance of Superconducting Hydrides

Superconducting hydrides are crucial in the pursuit of high-temperature superconductivity, showcasing transformative potential across various technological applications. Their significance is highlighted by the capability to achieve superconductivity at elevated temperatures, particularly in yttrium-based ternary hydrides, which have demonstrated high-temperature superconductivity [1]. The exploration of metallic hydrogen, especially in its liquid state, further emphasizes their potential to revolutionize the field by enabling superconductivity under previously unattainable conditions [2].

Recent advancements indicate that superconducting hydrides can achieve warm and light superconductivity at ambient pressures, bridging critical gaps in our understanding of their stability and superconducting properties [3]. This is particularly relevant for carbon compounds with a sodalite structure, which may facilitate high-temperature superconductivity at lower pressures compared to traditional hydrogen compounds [4]. The discovery of the La_4H_{23} phase, characterized by high superconducting transition temperatures and robust electron-phonon interactions, exemplifies the promise of these materials [5].

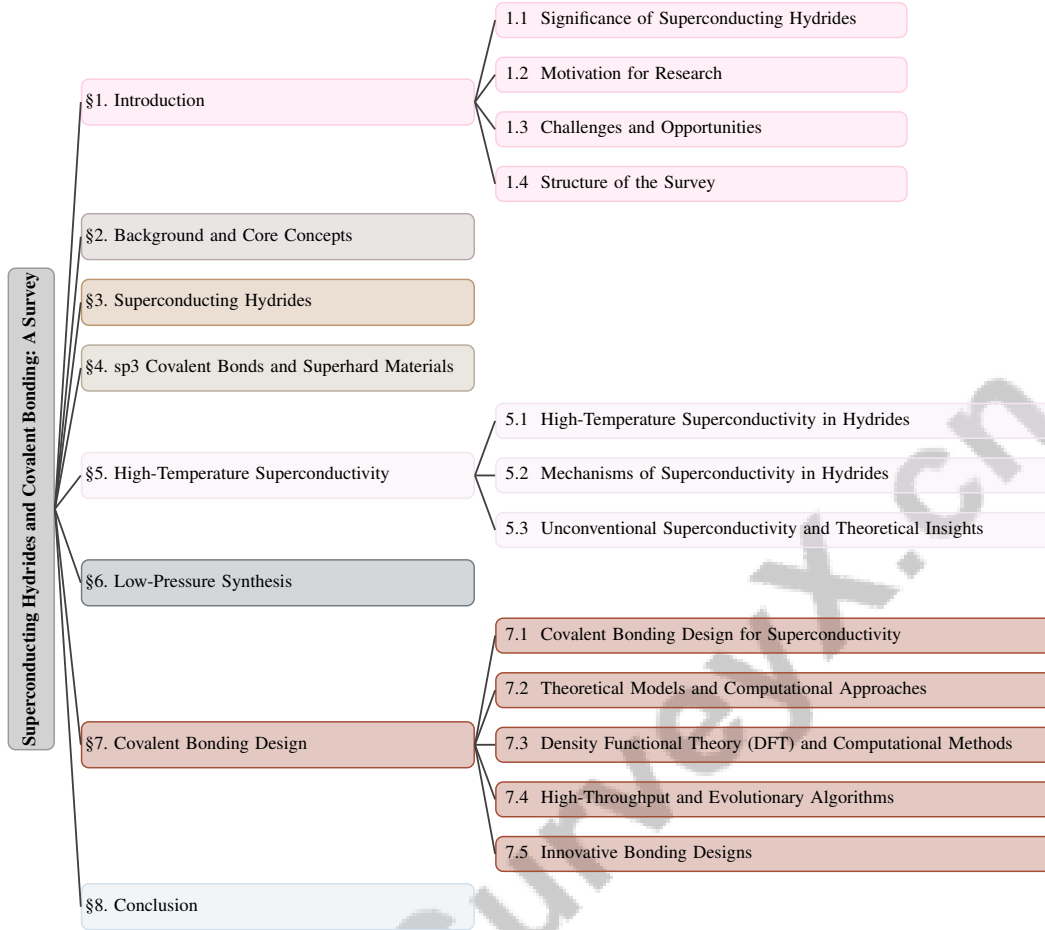


Figure 1: chapter structure

The potential applications of superconducting hydrides extend to achieving superconductivity at lower pressures, which is essential for practical deployment in energy transmission and storage technologies [6]. The identification of superconductivity in compounds such as $C_{60} + y$, with critical temperatures surpassing 100 K, further illustrates the vast potential of these materials in expanding the range of high-temperature superconductors [7]. Moreover, hydrides have achieved superconductivity at temperatures exceeding 200 K under high pressure, marking a significant milestone in the field [8].

The rising interest in polyhydrides is propelled by their potential for high-temperature superconductivity, promising future technological innovations [9]. Carbonaceous sulfur hydride (C-S-H) showcases the applications of superconducting hydrides in energy transmission and magnetic levitation, emphasizing their transformative impact on modern technology [10]. Additionally, uranium polyhydrides have emerged as candidates for high-temperature superconductivity at moderate pressures, further advancing superconductivity research [11]. These developments underscore the critical role of superconducting hydrides in enhancing our understanding of high-temperature superconductivity and paving the way for innovative applications across various technological domains.

1.2 Motivation for Research

The investigation of superconducting hydrides is driven by the goal of achieving superconductivity at lower pressures, a crucial factor for practical technological applications. Traditional superconductors require extreme pressures to maintain their superconducting phases, posing a significant barrier to widespread implementation [12]. The breakthrough discovery of high-temperature superconductivity in materials like H_3S has challenged existing paradigms, revealing the potential for superconductivity under more accessible pressure conditions [8]. This paradigm shift has intensified interest in hydrides that can sustain superconductivity with less stringent pressure requirements.

The synthesis of europium superhydrides, particularly those with clathrate structures and strongly correlated electronic properties, exemplifies the motivation for studying these materials due to their potential superconductivity [13]. The pursuit of uranium hydrides is similarly motivated by recent findings of high-temperature superconductivity in hydrogen-rich compounds, prompting the exploration of novel uranium hydrides [11]. These efforts highlight the necessity to expand the search for new superconductors beyond conventional systems.

A critical motivation remains the challenge of achieving superconductivity at or near room temperature, a long-standing goal, particularly within hydrogen-dominant alloys [10]. The inability to predict critical temperatures (T_c) in metal hydrides based on current electronic structure information has resulted in missed opportunities for discovering new superconductors [14]. Addressing these predictive limitations is essential for designing superconductors with higher T_c , especially given the absence of a comprehensive theoretical framework for room temperature superconductivity.

The quest to enhance superconducting transition temperatures at ambient pressure necessitates innovative approaches to navigate the complexity and diversity of ternary hydrides, which may hold the key to more practical superconducting conditions [15]. The study of materials like $C_{60} + y$, which exhibit high-temperature superconductivity, underscores the importance of understanding these mechanisms, particularly given their similarities with cuprate superconductors [7].

Ultimately, the motivation to explore superconducting hydrides is rooted in the ambition to surpass the limitations of existing hydride and lightweight element-based superconductors, which are not yet viable for effective operation at ambient pressure. By advancing the understanding of charge carrier behavior in high- T_c materials and examining the impact of strong long-range interactions, researchers aim to unlock new possibilities for high-temperature superconductivity. The potential of hafnium polyhydrides to exceed current superconducting temperatures further exemplifies the promising nature of these materials in advancing the field [9].

1.3 Challenges and Opportunities

The study and application of superconducting hydrides encounter numerous challenges, primarily due to the extreme pressures required to stabilize their superconducting phases, often exceeding 100 GPa, which presents significant barriers to experimental feasibility and practical deployment [10]. The synthesis of metallic hydrogen, a potential room-temperature superconductor, exemplifies these challenges, as it necessitates such high pressures that practical realization remains elusive [16]. Moreover, the complex chemistry of uranium polyhydrides complicates the prediction of stable phases and their superconducting characteristics under varying pressure conditions [11].

A critical obstacle is the limited understanding of how pressure influences the superconducting properties of titanium hydrides, particularly regarding phonon behavior and electron-phonon coupling [17]. This knowledge gap is compounded by the challenges of synthesizing stable hydride compounds at high pressures and the limitations of current experimental techniques, which often struggle to capture the nuances of these systems [8]. Additionally, the low superconducting transition temperatures of existing 5d transition metal hydrides, which have yet to surpass the liquid nitrogen temperature, highlight a significant hurdle in the quest for practical high-temperature superconductors [9].

Despite these challenges, substantial opportunities for advancement exist within the field. The exploration of ternary hydrides offers a promising avenue for enhancing superconducting properties beyond those of binary systems. By developing charge transfer mechanisms that maintain structural integrity while reducing the critical pressure for superconductivity, researchers can design materials capable of achieving superconductivity under more practical conditions [15]. Advances in computational techniques, such as machine learning and evolutionary algorithms, present potential for predicting phase transitions and superconducting properties, facilitating the discovery of novel superconductors with enhanced characteristics [18].

The ongoing quest for ambient-pressure superconductivity at elevated temperatures is driving significant advancements in materials science, particularly through innovative approaches like pressure-quenching techniques and machine-learning-assisted searches for new superconducting hydrides. Recent breakthroughs have demonstrated the potential to retain superconducting transition temperatures (T_c) of up to 37 K in modified FeSe and have identified numerous hydride compounds with T_c values exceeding 20 K, some even surpassing 70 K. These developments promise to enhance the

efficiency of energy transmission and storage technologies and pave the way for the synthesis of new superconductors, such as SrNHBC, which could achieve T_c values as high as 115 K at ambient pressure, significantly broadening the practical applications of superconductivity [19, 20, 21, 22]. By overcoming current challenges and leveraging new insights into the mechanisms and materials involved, the field of superconducting hydrides is poised for transformative technological advancements.

1.4 Structure of the Survey

This survey on superconducting hydrides is systematically structured to provide a comprehensive exploration of the field, addressing foundational theories and cutting-edge research. The survey begins with an introduction that highlights the significance of superconducting hydrides in achieving high-temperature superconductivity, emphasizing their potential applications and the motivation for ongoing research. Following the introduction, the paper explores the essential background and fundamental concepts necessary for understanding superconducting hydrides, emphasizing the significance of sp^3 covalent bonds in enhancing superconductivity, as well as the unique characteristics of superhard materials that contribute to the stability and performance of these high-temperature superconductors [23, 24].

The core of the survey is dedicated to an in-depth examination of superconducting hydrides, categorizing existing research based on chemical composition, structural diversity, and superconducting properties. This section also analyzes hydrogen-rich compounds and their covalent bonding, drawing insights from recent theoretical and experimental studies. The survey further explores the contribution of sp^3 covalent bonds to the mechanical properties of superhard materials, focusing on boron-rich and B-C-N compounds, as well as the impact of C-N bonds on material properties [25].

Subsequent sections analyze the mechanisms of high-temperature superconductivity in hydrides, discussing both conventional and unconventional theories and providing new perspectives on the underlying mechanisms [26]. The survey also addresses the challenges and techniques associated with low-pressure synthesis, reviewing experimental evidence and synthesis methods that support the feasibility of achieving superconductivity under more accessible conditions.

The survey concludes with a comprehensive discussion on covalent bonding design strategies aimed at enhancing superconducting properties. It emphasizes the importance of theoretical models and computational approaches, including first-principles calculations and innovative bonding designs, to optimize critical temperatures in superconducting materials, particularly in the context of high-pressure hydrides and novel compounds like lanthanum-yttrium ternary hydrides and europium superhydrides. The analysis integrates insights from recent advancements in material synthesis and the manipulation of ionic character in bonding to further improve superconductivity [19, 27, 24, 28, 29]. This comprehensive structure ensures that the survey synthesizes existing knowledge while identifying future research directions, offering a roadmap for advancing the field of superconducting hydrides. The following sections are organized as shown in Figure 1.

2 Background and Core Concepts

2.1 Fundamental Theories of Superconductivity

The study of superconducting hydrides is deeply rooted in several theoretical frameworks that elucidate the mechanisms of superconductivity. Central to this is the Bardeen-Cooper-Schrieffer (BCS) theory, which attributes superconductivity to the formation of Cooper pairs via phonon-mediated interactions, a phenomenon particularly relevant to hydrides due to their pronounced electron-phonon coupling, especially in hydrogen-rich variants [30]. The dynamics of protons within clathrate structures further highlight the significance of electron-phonon interactions in achieving high-temperature superconductivity [31].

Density Functional Theory (DFT) serves as a pivotal tool in the theoretical analysis of superconducting hydrides, providing insights into their electronic structures and enabling predictions of superconducting properties across varied conditions [32]. The integration of DFT with evolutionary crystal structure prediction methods, like the USPEX algorithm, is crucial for navigating the phase spaces of hydrides, thus aiding in the identification of stable superconducting phases [33].

The Ginzburg-Landau theory offers a macroscopic perspective on superconductivity, focusing on order parameters and coherence lengths, which are vital for analyzing the impact of structural and electronic variations on superconducting properties [31]. Additionally, theories of unconventional superconductivity, which explore diverse pairing mechanisms and electron correlations, provide a broader understanding of the superconducting phenomena observed in hydrides [34].

Theoretical models also explore coherence and transport properties in disordered systems, essential for understanding the superconducting behavior of hydrides [7]. Complementing these models are ab initio crystal structure prediction techniques, which estimate superconducting properties and guide the design of materials with improved superconducting characteristics [3].

2.2 sp³ Covalent Bonds and Material Properties

The role of sp³ covalent bonds is critical in defining the mechanical properties of superhard materials, significantly impacting their strength and stability. These bonds, characterized by tetrahedral coordination, are fundamental to the atomic structure of superhard materials such as diamond and cubic boron nitride, conferring exceptional hardness and resistance to deformation [25]. The robustness of sp³ covalent bonds arises from the substantial overlap of atomic orbitals, resulting in a high degree of electron sharing and a stable electronic configuration.

In hydrogen-rich compounds, sp³ covalent bonds are vital for achieving mechanical properties that support high-temperature superconductivity. The incorporation of hydrogen often leads to novel phases with enhanced hardness, as hydrogen's small size and high electronegativity promote the formation of dense, tightly bonded networks [35]. This is evident in carbonaceous sulfur hydride (C-S-H) and similar compounds, where the synergy between covalent bonding and hydrogen integration results in materials that combine superhard characteristics with superconducting potential [10].

The strategic design of materials with sp³ covalent bonds involves manipulating atomic arrangements to optimize mechanical properties. For instance, incorporating boron and nitrogen into carbon matrices can yield boron-rich and B-C-N compounds, which exhibit superior hardness due to robust sp³ covalent bonds [25]. These compounds not only display enhanced mechanical properties but also offer potential pathways to superconductivity by stabilizing specific electronic and structural configurations.

Furthermore, the study of C-N bonds within these materials highlights the importance of sp³ hybridization in achieving desired material properties. Nitrogen's ability to form sp³ hybridized bonds with carbon creates strong networks that enhance the overall hardness and stability of the material, making them suitable candidates for superhard applications [25]. This is particularly relevant in the design of new superconducting materials, where the mechanical integrity provided by sp³ covalent bonds is essential for maintaining structural stability under varying temperature and pressure conditions.

The exploration of superconducting hydrides has revealed a complex interplay of various factors that contribute to their unique properties. In particular, the hierarchical categorization of key concepts plays a crucial role in understanding this field. As illustrated in Figure 2, the figure presents a comprehensive overview of these concepts, focusing on essential aspects such as chemical composition, structural diversity, and superconducting properties. It further underscores the significance of hydrogen-rich compounds and covalent bonding in this context. By highlighting the relationships and advancements within each category, the figure emphasizes the synthesis of novel hydrides, the pursuit of high-temperature superconductivity, and the potential of hydrogen-rich compounds to enhance superconducting characteristics. This visual representation not only aids in conceptual clarity but also enhances the narrative flow of our discussion, providing a foundational framework for the subsequent analysis.

3 Superconducting Hydrides

3.1 Chemical Composition and Structural Diversity

Superconducting hydrides exhibit a wide array of chemical compositions and structural configurations, each contributing uniquely to their superconducting properties. The synthesis of complex hydrides such as Mg₂IrH₆, anticipated to exhibit superconductivity at ambient pressure, highlights the impor-

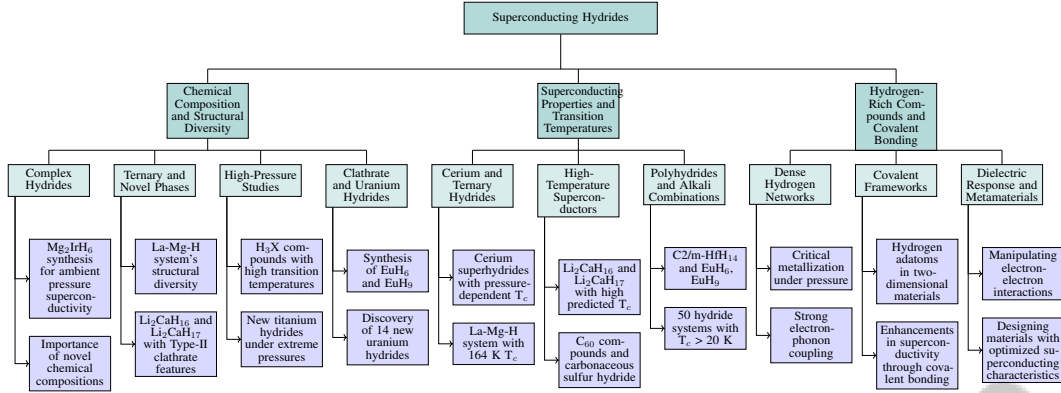


Figure 2: This figure illustrates the hierarchical categorization of key concepts in superconducting hydrides, focusing on chemical composition, structural diversity, superconducting properties, and the role of hydrogen-rich compounds and covalent bonding. It highlights the relationships and advancements within each category, emphasizing the synthesis of novel hydrides, high-temperature superconductivity, and the potential of hydrogen-rich compounds to enhance superconducting characteristics.

tance of exploring novel chemical compositions for practical applications [36]. This underscores the need to identify compounds that can maintain superconductivity without extreme conditions.

Ternary hydride systems, such as La-Mg-H, demonstrate extensive structural diversity, offering promising paths for discovering new superconductors with unique attributes [37]. Novel phases like $\text{Li}_2\text{CaH}_{16}$ and $\text{Li}_2\text{CaH}_{17}$, with structural features similar to Type-II clathrates, suggest complex bonding interactions that could enhance superconducting capabilities [15].

High-pressure studies of hydrides like H_3X ($\text{X}=\text{As, Se, Br, Sb, Te, I}$) show potential to exceed the superconducting transition temperature of traditional compounds like H_3S , emphasizing the critical role of electronic structure in achieving high-temperature superconductivity [38]. This is complemented by the identification of new titanium hydrides with high critical temperatures, expanding the range of superconducting materials under extreme pressures [17].

The synthesis of clathrate superhydrides, including EuH_6 and EuH_9 , marks significant progress in the structural diversity of superconducting hydrides, demonstrating the potential of clathrate frameworks to support novel superconducting phases [13]. Furthermore, the discovery of 14 new uranium hydrides enriches the chemical landscape, providing insights into the structural possibilities within superconducting hydrides [11].

Between 2015 and 2021, notable advancements were made in the discovery and characterization of superconducting hydrides, with numerous compounds synthesized for their superconducting properties [8]. These developments highlight the critical role of chemical composition and structural diversity in advancing the field of superconducting hydrides, paving the way for materials with optimized superconducting properties.

3.2 Superconducting Properties and Transition Temperatures

The superconducting properties and transition temperatures (T_c) of hydrides are pivotal to advancing high-temperature superconductivity. The SC-I phase of cerium superhydrides achieves a maximum critical temperature of 115 K at 95 GPa, while the SC-II phase shows a dome-like $T_c(\text{P})$ dependence, peaking at approximately 100 K at 130 GPa [12]. This underscores the importance of pressure-dependent structural transitions in optimizing superconducting properties.

Predicted critical temperatures for $\text{Li}_2\text{CaH}_{16}$ and $\text{Li}_2\text{CaH}_{17}$ reach 330 K and 370 K, respectively, under high pressures, highlighting the potential of structural tuning for achieving near-room-temperature superconductivity [15]. Similarly, the ternary hydride La-Mg-H exhibits a critical temperature of 164 K at high pressure, enhancing our understanding of superconducting properties in complex hydride systems [37].

C₆₀ compounds with sodalite structures achieve superconductivity at approximately 100 K at pressures exceeding 30 GPa, underscoring the role of structural diversity in facilitating high-temperature superconductivity [7]. Carbonaceous sulfur hydride exhibits superconductivity with a transition temperature of 260 K at 133 GPa, marking significant advancements in high-temperature superconductors [10].

The onset of superconductivity at T_c 83 K in C2/m-HfH₁₄ at 243 GPa illustrates the potential of polyhydrides to achieve high critical temperatures [9]. The successful synthesis of EuH₆ and EuH₉ positions them as promising candidates for high-temperature superconductors, with implications for future research into strongly-correlated superhydrides [13].

Recent research has identified around 50 hydride systems with transition temperatures exceeding 20 K, some surpassing 70 K, showcasing a variety of crystal structures, dimensionalities, and hydrogen arrangements. Many of these compounds consist of combinations of alkali or alkali-earth elements with noble metals, indicating a consistent chemical composition that could guide future experimental efforts towards high-temperature superconductivity. The majority of these hydride systems exhibit slight thermodynamic instability, suggesting that their synthesis may require conditions beyond ambient equilibrium [23, 22]. Continued exploration of these materials through experimental and theoretical approaches promises to unveil new pathways for achieving high-temperature superconductivity under more accessible conditions.

3.3 Hydrogen-Rich Compounds and Covalent Bonding

Exploring hydrogen-rich compounds is crucial for understanding superconductivity mechanisms, particularly due to their ability to form dense, metallic hydrogen networks that facilitate strong electron-phonon coupling. The critical metallization of hydrogen under pressure transitions it from an insulating to a metallic state, enabling superconductivity [39]. This behavior is essential for developing hydrogen-rich compounds capable of achieving superconductivity at significantly higher temperatures than traditional materials.

Incorporating hydrogen into covalent frameworks introduces new electron-phonon coupling channels that can enhance superconducting properties. This is particularly evident in two-dimensional materials, where hydrogen adatoms play a crucial role in opening novel coupling pathways, boosting superconductivity [40]. Such enhancements arise from hydrogen's ability to modify the electronic structure and vibrational modes of the host material, leading to increased superconducting transition temperatures.

Covalent bonding in hydrogen-rich compounds is crucial for structural stability and enhances superconducting potential. Recent findings suggest that optimizing the ionic character of bonds can lead to even higher critical temperatures under extreme pressure conditions [23, 24, 1, 29]. The formation of strong covalent bonds, often characterized by sp³ hybridization, contributes to the mechanical robustness of these materials, enabling them to withstand the extreme pressures necessary for superconductivity. This structural integrity is essential for maintaining the conditions required for superconductivity, as it prevents lattice collapse in high-pressure environments.

Manipulating dielectric response functions in metamaterials offers an innovative approach to enhancing electron-electron interactions, which can be leveraged to improve the superconducting properties of hydrogen-rich compounds [41]. By tailoring these interactions, researchers can potentially design materials with optimized superconducting characteristics, further advancing the field of high-temperature superconductivity.

4 sp³ Covalent Bonds and Superhard Materials

The investigation of sp³ covalent bonds is crucial for understanding the synthesis and properties of superhard materials, as these bonds substantially enhance mechanical strength and stability. Superhard materials are categorized based on synthesis techniques and intrinsic properties related to sp³ hybridization. Two primary categories are identified: one includes light, inexpensive main group elements requiring extreme pressures and temperatures, while the other involves transition metals combined with light elements, generally synthesized at high temperatures. However, the latter faces challenges due to the high cost and scarcity of transition metals. High-throughput first-principle calculations aid in identifying optimal compositions for new superhard materials, focusing

on mechanical performance, resource availability, and sustainability, with a particular interest in ultra-incompressible carbon nitride (CN) compounds, which may rival diamond in hardness due to robust C-N bonds [42, 43].

4.1 Classes of Superhard Materials

Superhard materials are primarily divided into those synthesized under high-pressure and high-temperature conditions and those combining transition metals with light main group elements [42]. The first class includes diamond and cubic boron nitride, known for exceptional hardness, produced by mimicking Earth's extreme conditions. Their mechanical properties are attributed to sp³ covalent bonds that form a robust atomic framework essential for resisting deformation.

The second class, involving transition metals combined with light elements like boron, carbon, and nitrogen, provides an alternative route to superhardness, generally requiring only high reaction temperatures. This class is more accessible compared to the first, which relies solely on light, inexpensive main group elements and extreme synthesis conditions. However, the use of transition metals raises concerns about cost and scarcity, necessitating a balance between synthetic feasibility and mechanical properties. Advances in high-throughput first-principle calculations and machine learning models have identified specific compositions, such as BCN, BCN, and BCN, with hardness values exceeding 40 GPa, potentially synthesized using low-temperature plasma methods [44, 25, 42, 45]. These compounds often feature complex crystal structures where sp³ covalent bonding enhances hardness and stability, contributing to dense, tightly bonded networks capable of withstanding significant mechanical stress.

Advancements in computational techniques, particularly machine learning models like random forests, have enabled the prediction of mechanical properties in these materials without extensive computational resources [45]. These models allow researchers to efficiently explore the vast compositional space of potential superhard materials, accelerating the discovery and optimization of compounds with desirable mechanical characteristics. By leveraging these predictive capabilities, materials can be designed to maximize the contribution of sp³ covalent bonds to superhardness, advancing the development of new materials with superior mechanical properties.

4.2 Boron-Rich and B-C-N Compounds

Boron-rich and B-C-N compounds are pivotal in superhard material development, offering unique properties that enhance hardness and potential superconductivity. Boron-rich carbides, such as B₆C, exemplify this dual capability, serving as promising candidates for advanced technological applications due to robust boron networks that significantly contribute to mechanical strength and stability [44].

The synthesis of novel phases like the Pnnm CN phase underscores the potential of B-C-N compounds in achieving superhard characteristics. The stability and ultra-incompressibility of these phases, attributed to sp³ hybridization, highlight their importance in materials science [43]. However, the development of B-C-N compounds is challenged by the high cost and scarcity of transition metals, often necessary to enhance mechanical performance [42]. This necessitates a careful balance between synthetic accessibility and material performance, driving research towards more efficient synthesis methods and alternative compositions.

Recent advancements in computational techniques, particularly machine learning models, have facilitated the prediction of new superhard materials within the B-C-N system. These models can predict Vickers hardness values greater than 40 GPa, enabling exploration of extensive compositional spaces and accelerating the discovery of compounds with optimized mechanical properties [45]. By utilizing these predictive capabilities, researchers aim to design B-C-N compounds that maximize the contribution of sp³ covalent bonds, enhancing superhardness and expanding applicability in various technological domains.

4.3 C-N Bonds and Mechanical Properties

The mechanical properties of materials incorporating C-N bonds are significantly influenced by the nature of these bonds, particularly regarding superhard materials. C-N bonds are characterized by their strong covalent nature, often resulting in enhanced hardness and stability, crucial for applications

requiring materials that withstand extreme conditions. The synthesis of C-N compounds, such as the Pnnm CN phase, exemplifies the potential of these bonds to contribute to ultra-incompressibility and mechanical robustness [43].

The proposed direct synthesis method for C-N compounds offers a significant advantage by bypassing the need for chemical precursors, allowing for the production of stable materials with superior hardness. This innovative synthesis method streamlines the production of carbon-nitrogen (C-N) compounds, significantly increasing their availability for various technological applications, including superhard materials that could rival diamond in hardness. Utilizing high-pressure and high-temperature conditions facilitates the creation of novel materials with exceptional mechanical properties, while also considering sustainability and resource accessibility in the material selection process [25, 42, 43]. The resulting materials exhibit high structural integrity due to the sp³ hybridization of carbon and nitrogen atoms, forming a dense and tightly bonded network.

The mechanical properties imparted by C-N bonds are further enhanced by their ability to form complex crystal structures, contributing to the overall hardness and durability of the material. The integration of C-N bonds is particularly significant in developing superhard materials, as recent research demonstrates that compounds with C-N composition can achieve hardness levels comparable to diamond. This is due to the strong and relatively low-ionic nature of the C-N bond, which enhances performance under extreme conditions of high pressure and temperature. For instance, synthesizing sp³-hybridized carbon nitride (CN) at pressures exceeding 55 GPa and temperatures around 7000 K has resulted in a highly incompressible material, highlighting the potential of C-N compounds in creating superhard materials that can endure harsh environments. Ongoing studies into the mechanical properties and stability of various C-N and B-C-N compounds suggest a promising avenue for developing new materials that excel in hardness while exhibiting desirable thermal and mechanical characteristics [25, 45, 43, 42, 44].

5 High-Temperature Superconductivity

5.1 High-Temperature Superconductivity in Hydrides

High-temperature superconductivity (HTS) in hydrides is distinguished by their unique structural and electronic properties, positioning them as viable candidates for room-temperature superconductivity. Research into complex hydride systems, like La₄H₂₃, reveals strong electron-phonon coupling and unconventional superconducting traits, suggesting their potential to attain higher critical temperatures than known materials [8]. Studies on selenium hydrides, inspired by sulfur hydride discoveries, indicate similar superconducting properties [18]. Rare-earth hydrides potentially achieve superconductivity at reduced pressures, emphasizing the role of structural diversity in enhancing performance. Carbonaceous sulfur hydride shows conventional superconductivity at high critical temperatures under lower pressures [10], and clathrate superhydrides in sodalite-like structures further exhibit HTS potential [13].

Hafnium polyhydrides achieve higher critical temperatures under pressure [9], while uranium polyhydrides show a transition temperature of 54 K for UH₇ at 20 GPa, reflecting the diverse configurations contributing to superconductivity [11].

5.2 Mechanisms of Superconductivity in Hydrides

Superconductivity in hydrides is fundamentally linked to electron-phonon interactions and covalent bonding structures. The Bardeen-Cooper-Schrieffer (BCS) theory attributes superconductivity to Cooper pair formation via phonon-mediated interactions, particularly in hydrogen-rich compounds [46]. Innovations highlight phonon softening's role in superconductivity [46]. Density Functional Theory (DFT) and algorithms like USPEX predict stable hydride phases and superconducting properties by exploring energy surfaces across stoichiometries, as seen in the La-Mg-H system [17].

Predictive models aid in identifying new high-T_c superconductors within metal hydrides [14]. The superconductivity mechanisms in C₆₀ + y are examined through a percolative approach, revealing connectivity and transport properties [7]. Strong electron-phonon coupling and a high density of states near the Fermi level contribute to elevated T_c in compounds like carbonaceous sulfur hydride [10]. Future research should focus on synthesizing complex hydrides and utilizing advanced

techniques to study superconductivity at high pressures, including SQUID magnetometry for precise superconducting parameter determination [8, 47].

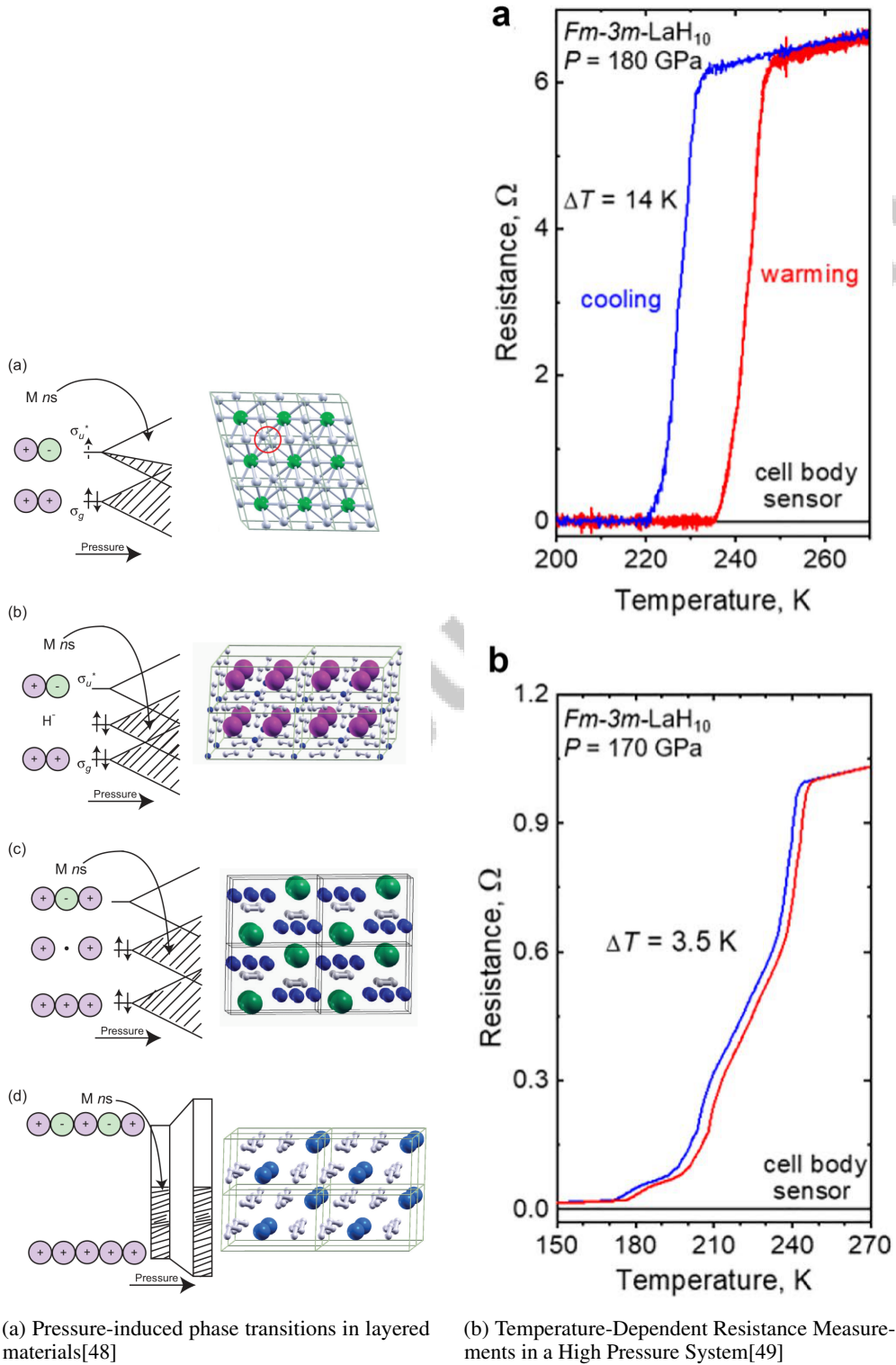


Figure 3: Examples of Mechanisms of Superconductivity in Hydrides

Figure 3 illustrates the significance of high-temperature superconductivity in hydrides for energy and magnetic applications. Superconductivity mechanisms are explored through pressure-induced phase transitions and temperature-dependent resistance studies. The first image shows how varying pressures induce structural changes, transitioning from metallic to semiconducting phases. The second image depicts resistance variations with temperature under different pressures, providing insights into superconducting transition temperatures [48, 49].

5.3 Unconventional Superconductivity and Theoretical Insights

Exploring unconventional superconductivity in hydrides has led to theoretical advancements, challenging existing paradigms. Binary hydrides under extreme pressure exhibit novel stoichiometries promoting superconductivity at elevated temperatures. Theoretical simulations predict superconducting hydrides with record-high transition temperatures, influenced by elements like alkali, rare earth, pnictogen, and chalcogen families [23, 50].

The anti-adiabatic multi-gap superconducting state contrasts with traditional theories, suggesting that the breakdown of the Born-Oppenheimer approximation is crucial for understanding superconductivity in hydrogen-rich compounds. This highlights the interplay between electronic and lattice dynamics essential for high critical temperatures.

Strong electron-phonon interactions are central to understanding hydride superconductivity, with simultaneous modeling of critical temperature and pressure emerging as a promising approach. This method identifies compounds with optimal properties by analyzing over 60,000 electronic structures, considering structural characteristics and electronic factors. This approach has expanded the search for high-temperature superconductors, identifying over one hundred layered compounds and fifty hydride systems with transition temperatures exceeding 20 K [33, 22].

Theoretical models emphasize the importance of strong repulsive interactions, proposing alternative mechanisms for electron pairing, including kinetic energy and localized interactions [51]. Local structural changes related to valence and spin order are crucial for superconductivity [52]. These insights suggest that local electronic environments and spin dynamics are significant in complex hydride systems.

The relationship between the superconducting state and the pseudogap is vital for understanding HTS. The interplay between charge density wave order and superconductivity requires advanced models to explain phase diagram discrepancies. Machine learning techniques help explore compositional phase space, identifying critical local minima and enhancing understanding of complex correlations. This is crucial for predicting superconducting transition temperatures and distinguishing structural polymorphisms under varying pressures. High-pressure synthesis reveals unique properties, emphasizing the need for sophisticated models to interpret material behavior under extreme conditions [25, 53].

6 Low-Pressure Synthesis

Category	Feature	Method
Low-Pressure Synthesis Techniques	Chemical Precursor Utilization	LaH10[46], HPS[12], NN-TCP[14]
Experimental Evidence and Synthesis Techniques	High-Pressure Techniques	DAC[13]

Table 1: This table provides a comprehensive summary of the synthesis methods for superconducting hydrides, categorizing them into low-pressure synthesis techniques and high-pressure experimental evidence. It highlights key features such as chemical precursor utilization and high-pressure techniques, referencing specific methodologies like LaH, HPS, NN-TCP, and DAC, which are crucial for advancing the field of superconducting hydrides.

The development of low-pressure synthesis methods represents a pivotal advancement in the synthesis of superconducting hydrides, providing an alternative to the conventional high-pressure approaches. This section delves into innovative strategies for synthesizing superconducting hydrides at reduced pressures, highlighting their potential to make these materials more accessible and practical. Table 1 presents an overview of synthesis techniques for superconducting hydrides, illustrating the distinctions between low-pressure and high-pressure methods and their respective features. Additionally, Table 3 offers a comparative overview of the methodologies employed in the synthesis of superconducting

hydrides, emphasizing the distinctions between low-pressure techniques and experimental high-pressure methods. The following subsection details various low-pressure synthesis techniques, demonstrating their effectiveness and significance in current research.

6.1 Low-Pressure Synthesis Techniques

Method Name	Synthesis Methods	Phase Stability	Material Composition
LaH10[46]	Diamond Anvil Cell	Pressure-induced Transition	Lanthanum Superhydride LaH10
DAC[13]	Laser-heating Techniques	Stable Clathrate Structures	Europium And Ammonia
HPS[12]	Ammonia Borane	Compositional Tuning	Cerium Superhydrides
NN-TCP[14]	Evolutionary Algorithms	Stable Hydride Phases	K-H, Ca-H

Table 2: Summary of low-pressure synthesis methods, phase stability, and material composition for various superconducting hydrides. The table highlights different synthesis techniques, including diamond anvil cell and evolutionary algorithms, and their impact on achieving stable hydride phases under reduced pressure conditions. It also details the composition of materials such as lanthanum superhydride and cerium superhydrides, underscoring the role of compositional tuning in phase stability.

Table 2 provides a comprehensive overview of the low-pressure synthesis techniques, phase stability, and material composition for superconducting hydrides, illustrating recent advancements in achieving stable phases under milder conditions. Low-pressure synthesis techniques for superconducting hydrides are crucial for circumventing the extreme conditions traditionally needed to stabilize their superconducting phases. Conventional methods, such as those used for LaH₁₀, often require pressures above 160 GPa [46]. Recent innovations have introduced precursor compounds and novel synthesis routes to promote hydrogen-rich phase formation under milder conditions. A key approach is the in situ generation of hydrogen from chemical precursors, facilitating controlled hydrogen release to react with metal precursors, forming the desired hydride phases. This method has been effectively employed in synthesizing europium clathrate superhydrides, using a mixture of europium and ammonia borane pressurized and laser-heated in a diamond anvil cell [13]. Similarly, cerium superhydrides synthesized at high pressures and temperatures, followed by resistance measurements, demonstrate the success of precursor-based methods in lowering pressure requirements [12].

Exploring phase diagrams, such as for the Li-Mg-H system, offers insights into potential low-pressure synthesis routes by identifying stable phases through compositional tuning [14]. This underscores the importance of phase stability and compositional adjustments in synthesizing superconducting hydrides at reduced pressures. Evolutionary algorithms targeting the K-H, Ca-H, and Ti-H systems have been effective in predicting stable hydride phases, guiding experiments towards feasible low-pressure synthesis pathways [14].

Future research aims to optimize synthesis parameters and explore chemical modifications for achieving superconductivity under lower pressures. Leveraging advanced synthesis techniques and strategic precursor selection broadens the range of materials for exploration and practical application in superconducting hydrides. Machine-learning-assisted searches of over 150,000 compounds have identified approximately 50 hydride systems with transition temperatures exceeding 20 K, some surpassing 70 K despite slight thermodynamic instability, indicating a need for non-ambient synthesis conditions. Discoveries of high-temperature superconductivity in metal hydrides like H₃S and lanthanum hydride open new avenues for understanding superconductivity mechanisms at elevated temperatures, particularly under extreme pressures. The consistent chemical composition in many of these compounds, typically involving alkali or alkali-earth elements with noble metals, suggests promising directions for future experimental investigations aimed at achieving room temperature superconductivity [54, 22]. These efforts aim to reduce high-pressure synthesis challenges, paving the way for new superconductivity discoveries.

6.2 Experimental Evidence and Synthesis Techniques

The experimental investigation of low-pressure synthesis techniques for superconducting hydrides is vital for advancing towards practical applications. Recent studies have shown the potential of various methods to achieve superconductivity under reduced pressures, fostering the development of new materials with improved superconducting properties. Diamond anvil cells have been crucial, providing the necessary high-pressure environments for synthesizing and studying hydrides. For

example, Mg_2IrH_5 synthesis was achieved at 0 to 30 GPa and temperatures between 450 K and 2500 K, demonstrating the feasibility of forming hydrogen-rich phases under moderate pressures [36].

High-pressure techniques, utilized in synthesizing H_3X hydrides, employ advanced computational tools like LAPW and Quantum-ESPRESSO to predict superconducting properties and guide experimental efforts [38]. These computational predictions are essential for identifying promising hydride phases and refining synthesis parameters. Evaluating superconducting critical temperatures for various hydride phases at pressures achievable in diamond anvil cells underscores the potential of these methods to discover new superconductors [55].

Experimental setups often incorporate X-ray diffraction for phase identification, as seen in synthesizing sodalite-like clathrate structures at 80 to 170 GPa and temperatures up to 2800 K [13]. This approach highlights the importance of precise experimental control to effectively explore hydride phase space. Additionally, synthesizing ultra-incompressible sp^3 hybridized carbon phases at over 70 GPa and temperatures above 7000 K exemplifies the capability of diamond anvil cells to facilitate superhard material formation [43].

Despite progress, a limitation of these studies is their reliance on theoretical calculations, which may not fully account for experimental variances or synthesis challenges [54]. Future experiments should verify trapped flux existence under varying conditions and explore properties in non-simply connected geometries, potentially providing new insights into the superconducting behavior of hydrides [56]. By advancing low-pressure synthesis techniques and leveraging experimental evidence, the field can continue to expand the boundaries of high-temperature superconductivity in hydrides, paving the way for new technological applications.

Feature	Low-Pressure Synthesis Techniques	Experimental Evidence and Synthesis Techniques
Pressure Range	Reduced Pressures	0 TO 30 Gpa
Synthesis Technique	Precursor-based Methods	Diamond Anvil Cells
Material Composition	Hydrogen-rich Phases	Hydrogen-rich Phases

Table 3: This table provides a comparative analysis of low-pressure synthesis techniques and experimental evidence for synthesizing superconducting hydrides. It highlights the differences in pressure ranges, synthesis methods, and material compositions between low-pressure and high-pressure approaches. The table underscores the potential of precursor-based methods and diamond anvil cells in achieving hydrogen-rich phases under varied pressure conditions.

7 Covalent Bonding Design

7.1 Covalent Bonding Design for Superconductivity

Covalent bonding design is pivotal in enhancing superconducting properties, leveraging advanced computational methods and synthesis techniques. Evolutionary algorithms and first-principles calculations, as applied to Y-Mg-H compounds, optimize superconducting characteristics by precisely controlling atomic interactions and structural configurations [1]. This approach underscores the importance of tailoring electronic environments for desired superconducting outcomes.

Research on ternary hydrides, such as La-Mg-H, indicates the potential for stable structures with enhanced superconducting properties at lower pressures, aligning with covalent bond design strategies [37]. The Gaspari-Gyorffy theory further clarifies the decoupling of electronic and phononic contributions to superconductivity [38].

Introducing hydrogen adatoms into two-dimensional superconductors offers a novel strategy to optimize superconducting properties by creating new electron-phonon coupling pathways [40]. This demonstrates hydrogen's transformative potential in enhancing electronic structures and increasing superconducting transition temperatures.

Machine learning and hybrid computational methods are essential for predicting and designing materials with superior superconducting properties. Enhancing machine learning models with additional features improves prediction accuracy, facilitating the discovery of new superconductors, particularly those with high structural symmetry and robust electron-phonon coupling, as seen in cerium superhydrides.

The exploration of uranium polyhydrides using evolutionary algorithms predicts and synthesizes new compounds with potential high-temperature superconducting capabilities, highlighting computational tools' role in guiding experimental efforts [11].

7.2 Theoretical Models and Computational Approaches

The integration of theoretical models and computational approaches significantly advances covalent bond design for superconductivity. Evolutionary algorithms like USPEX, combined with density functional theory (DFT), facilitate the exploration of stable superconducting compounds under varying pressure conditions [57]. This methodology is crucial for identifying stable phases and predicting critical temperatures in systems like YCeH_x and LaCeH_x [58].

New theoretical frameworks categorize existing research on hydride superconductors, emphasizing the predictive power of computational methods in identifying stable structures and superconducting properties [28]. Advanced techniques, including the minima hopping method and DFT, broaden the scope of potential superconductors by predicting superconducting properties at lower pressures [59].

High-throughput calculations and machine learning models increasingly evaluate the stability and superconducting properties of new compounds, showcasing the application of theoretical models in covalent bonding design [21]. Combining machine-learned moment tensor potentials with the stochastic self-consistent harmonic approximation (SSCHA) enhances the analysis of quantum effects, improving the predictive capabilities of these models [60].

Swarm-intelligence methods like CALYPSO uncover stable stoichiometries of hydrides, providing insights into structural configurations that support superconductivity [61]. These computational approaches, complemented by phonon calculations and DFT, assess the dynamic stability of potential superconductors, offering a comprehensive understanding of superconductivity's influencing factors [62].

Future research should explore hypervalent hydrides and develop new theoretical frameworks to identify superconductors with lower stable pressures, expanding the range of materials for practical applications [23]. Leveraging advanced computational methods and theoretical models will continue to push the boundaries of covalent bonding design, paving the way for new discoveries in high-temperature superconductivity.

7.3 Density Functional Theory (DFT) and Computational Methods

Density Functional Theory (DFT) is a cornerstone of computational materials science, providing a robust framework for predicting and analyzing superconducting materials' properties. In superconducting hydrides, DFT predicts stable compounds and explores electronic structures under various pressure conditions, exemplified by its application in the Ti-H system, where DFT and evolutionary algorithms navigate the potential energy landscape to identify stable hydride phases [17].

Integrating DFT with advanced computational techniques enables the systematic exploration of complex phase spaces, leading to the discovery of novel superconducting materials. This integration allows researchers to assess the stability and electronic characteristics of over one hundred newly identified layered compounds and approximately fifty hydride systems with transition temperatures exceeding 20 K. Analyzing the electronic structures provides insights into superconducting mechanisms that guide experimental synthesis aimed at discovering high-temperature superconductors [33, 22].

DFT's predictive power is enhanced by combining it with self-consistent phonon approaches and enhanced sampling techniques, facilitating precise calculations of electron-phonon coupling, essential for understanding superconducting transition temperatures in hydrogen-rich compounds like H₃S and LaH₁₀, synthesized under extreme high-pressure conditions. This coupling plays a pivotal role in high-temperature superconductivity emergence, as evidenced by their record transition temperatures and the complex interplay of phonon modes contributing to superconducting properties. Recent advancements in theoretical and experimental frameworks, including DFT and BCS-Eliashberg-Migdal theory, guide research aimed at optimizing superconducting performance in hydrides [63, 64, 65]. DFT's versatility in handling diverse material systems underscores its importance in high-temperature superconductor design and discovery.

Additionally, DFT is employed alongside particle swarm optimization algorithms, demonstrated in the CALYPSO method, to predict stable structures of compounds like tellurium hydrides under high pressures. This collaboration emphasizes the potential of DFT and advanced optimization algorithms in navigating the extensive compositional phase space of potential superconductors. By leveraging machine learning techniques to analyze structural representations and electronic properties, researchers can identify and predict new materials with superior superconducting characteristics, streamlining the search process and uncovering previously overlooked compounds like Ca(CuBrO), KCoF, and various hydride systems for further experimental exploration [33, 53, 22].

7.4 High-Throughput and Evolutionary Algorithms

High-throughput and evolutionary algorithms have revolutionized the design of superconducting materials, enabling efficient exploration of vast chemical spaces to identify stable structures and optimal bonding configurations that enhance superconductivity. High-throughput methods, especially when combined with machine learning models, facilitate rapid screening of potential superconductors by evaluating their electronic structures, phonon properties, and superconducting transition temperatures [45]. This accelerates the discovery process, allowing researchers to focus on promising candidates for experimental validation.

Evolutionary algorithms, such as USPEX, predict the crystal structures of superconducting hydrides under high-pressure conditions, simulating natural selection to refine candidate structures iteratively and identify low-energy configurations [17]. This synergy between evolutionary algorithms and DFT enhances predictive capabilities, allowing accurate assessments of electronic and phononic contributions to superconductivity.

Integrating high-throughput and evolutionary algorithms with advanced computational tools, such as particle swarm optimization and the minima hopping method, provides a comprehensive framework for superconducting material design. These methodologies systematically explore hypervalent hydrides and other complex systems, identifying stable stoichiometries and bonding configurations that support high-temperature superconductivity [61]. By combining these approaches with experimental validation, researchers can refine theoretical models and develop new materials with optimized superconducting properties.

7.5 Innovative Bonding Designs

Innovative bonding designs in superconducting materials are pushing the boundaries of traditional materials science, exploring new avenues for high-temperature superconductivity. These designs focus on strategically manipulating covalent bonds to enhance electron-phonon coupling and optimize structural configurations that support superconductivity. One approach involves exploring hypervalent bonding configurations, facilitating the formation of unconventional superconducting phases through greater flexibility in electron distribution and bonding interactions [61].

The integration of machine learning and high-throughput screening techniques accelerates the identification of novel bonding configurations that maximize superconducting properties. By leveraging large datasets and advanced algorithms, researchers can predict specific bonding arrangements' impact on superconducting transition temperatures, identifying promising candidates for experimental validation [45]. This approach not only expedites discovery but also provides insights into the fundamental mechanisms underlying superconductivity.

Experimental techniques, including in situ high-pressure synthesis and advanced characterization tools, validate innovative bonding designs by allowing researchers to observe the formation and stability of novel bonding configurations under extreme conditions. The synthesis of complex hydrides with unique bonding arrangements, such as those involving sp³ hybridization, exemplifies the potential of these designs to achieve high-temperature superconductivity under more accessible pressure conditions [17].

Investigating metamaterials and engineered nanostructures presents significant opportunities for developing innovative bonding designs, particularly in synthesizing superhard materials. These materials, which can exhibit unique properties like enhanced hardness and mechanical performance, often require specific conditions like high pressure and temperature for creation. By leveraging advanced computational methods and high-throughput data mining, researchers can identify optimal

compositions that balance mechanical performance with sustainability, paving the way for novel bonding strategies utilizing these advanced materials in practical applications [25, 42]. Manipulating dielectric properties and electronic environments within these materials can enhance electron-electron interactions and potentially achieve superconductivity at higher temperatures, underscoring the importance of interdisciplinary collaboration in advancing superconductivity, drawing principles from materials science, physics, and engineering to develop novel solutions.

8 Conclusion

8.1 Challenges and Future Directions

Superconducting hydrides present formidable challenges, particularly due to the necessity of high pressures for stabilizing their superconducting phases, which significantly hinders their practical application potential. The synthesis of compounds such as fcc-YH₁₀ exemplifies the intricate requirements needed to achieve superconductivity near ambient conditions, requiring meticulous control over synthesis parameters. To overcome these limitations, future research should pivot towards exploring alternative compounds and structural modifications. Additionally, investigating superconducting properties at reduced pressures and elevated temperatures is crucial, as the current high-pressure prerequisites pose substantial obstacles.

Refinement of theoretical models is imperative for accurately predicting hydride behavior and identifying alternative compositions that could lead to superconductivity. The limitations of the conventional BCS theory in explaining high T_c values indicate a pressing need for enhanced models and the exploration of other hydrogen-rich compounds. Delving into metamaterial geometries and diverse materials could further augment T_c , thereby opening new avenues for research.

Progress in computational methodologies is essential to efficiently navigate the quantum energy landscape, potentially leveraging machine-learned potentials. Machine learning techniques can refine structural representations and expand datasets, which is crucial for advancing the understanding of superconductivity across a wide array of materials. Additionally, exploring coupled quantum diffusion and superconductivity in an expanded range of superhydrides may provide insights into the underlying mechanisms.

The experimental synthesis of predicted hydrides remains a critical focus, with an emphasis on ternary hydrides to enhance superconducting properties. Optimizing synthesis conditions and exploring doping strategies in metal borohydrides could lead to significant advancements. The PQ method, which retains high T_c phases without high pressure, presents opportunities for broadening superconductivity applications.

Investigating the influence of quantum fluctuations and various metal atoms in enhancing hydrogen's contribution to T_c is also warranted. Future research should refine calculations of electron-phonon coupling and explore additional hydride compounds to identify materials with even higher superconducting temperatures. By addressing these challenges through innovative research directions, the field of superconducting hydrides can advance, paving the way for new technological applications and overcoming limitations in experimental reproducibility and synthesis conditions.

8.2 Experimental Validation and Future Directions

Experimental validation is crucial for advancing superconducting hydrides, serving as the bridge between theoretical predictions and practical applications. The synthesis and characterization of predicted hydrides are essential for verifying their superconducting properties under various conditions. This process not only validates theoretical models but also provides empirical data that refines these models, enhancing predictive accuracy for future discoveries.

Future research should prioritize the exploration of ternary and quaternary hydrides, as these compounds offer a fertile landscape for discovering new superconductors with potentially superior properties. Optimizing synthesis conditions, including pressure and temperature, is vital for stabilizing these complex hydrides and achieving high-temperature superconductivity. Advanced synthesis techniques, particularly precise control of quenching parameters, could enhance the superconducting properties of these materials.

Theoretical advancements are necessary to more accurately predict superconducting properties under varying conditions. Improved models that account for the intricate interplay of electron-phonon interactions and covalent bonding in hydrides can guide experimental efforts and streamline the discovery of new superconducting phases. Additionally, exploring the potential of the PQ technique in other materials could open new pathways for achieving superconductivity without extreme pressures, broadening the applicability of these materials.

Support from funding agencies is essential to sustain and accelerate research in hydride superconductivity. Such support can facilitate the development of new experimental setups, enhance computational resources, and foster interdisciplinary collaborations, ultimately driving innovation in the field. Addressing these research priorities and leveraging interdisciplinary approaches will enable the field of superconducting hydrides to make significant strides, paving the way for groundbreaking technological applications and deeper insights into the fundamental principles of superconductivity.

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