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## Crystal Blueprints for Superconductivity: Investigating Lattice Geometry and its Thermodynamic Impact

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### ARTICLE DETAILS

**Research Paper**

**Accepted:** 25-05-2025

**Published:** 10-06-2025

**Keywords:**

*Lattice geometry, superconductivity, high-temperature superconductors, bond angles, structural optimization*

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### ABSTRACT

This paper explores the fundamental role of lattice geometry in shaping the superconducting properties of high-temperature superconductors. It investigates the ways in which differences in structural characteristics, such as lattice symmetry, bond lengths, bond angles, and dimensionality, affect the superconducting transition temperature ( $T_c$ ) in a variety of material classes, including cuprates, iron-based pnictides, and hydrogen-rich hydrides, among others. According to the findings of the study, better symmetry structures, ideal bond configurations, and lower dimensionality all contribute to the promotion of stronger electron pairing and higher  $T_c$  values. Recent experimental discoveries and theoretical simulations are analysed to illustrate that characteristics such as near-ideal Cu-O bond angles in cuprates, Fe-As tetrahedral symmetry in pnictides, and compressed hydrogen networks in hydrides are directly connected to increased superconducting behaviours. These characteristics are discovered by analysing the results of these models. In addition, the influence of pressure-induced lattice optimisation, strain engineering, and chemical substitution techniques is examined. This demonstrates how structural



tuning may be utilised to enhance superconductivity in materials that are already in existence and to direct the development of novel materials. In addition, the work highlights the fact that lattice-driven processes are equally relevant in modifying superconductivity, despite the fact that electronic and magnetic interactions are quite important. This paper argues that future superconducting material design should have structural blueprint optimisation at its heart. This is accomplished by synthesising insights from crystallographic investigations, phonon dispersion analysis, and computer models. In this paper, we highlight potential directions for future study and encourage the utilisation of sophisticated computational methods for the purpose of predicting superconducting performance solely based on structural factors. The use of this strategy has the potential to hasten the identification of novel superconductors that are able to function at or near room temperature, which would have a profound impact on the technical applications of energy systems, electronics, and transportation.

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**DOI : <https://doi.org/10.5281/zenodo.15658000>**

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## 1. INTRODUCTION

The quantum phenomena known as superconductivity is a one-of-a-kind occurrence in which a material demonstrates zero electrical resistance and the ejection of magnetic fields below a temperature known as the critical temperature ( $T_c$ ). Early research concentrated mostly on electrical characteristics; however, it is now becoming more recognised that structural and lattice-related elements play a vital role in modifying the behaviour of the material.  $T_c$ , particularly in high-temperature superconductors (HTSCs). Lattice geometry, phonon behaviour, atomic arrangements, and minor distortions all have an effect on the vibrational spectrum and electronic density of states, which in turn has a direct influence on superconductivity. There is significant evidence that superconducting qualities are not purely electronic in origin, but are intimately related to lattice topologies and vibrational dynamics. Materials like as cuprates, iron pnictides, and compressed hydrides give this evidence (Bendele et al., 2018; Xiang et al., 2021).



As a result of the realisation that parameters like as lattice symmetry, dimensionality, bond lengths, and bond angles are vital in determining superconducting strength, structural considerations have become increasingly important. It is common for high-symmetry lattices to encourage isotropic phonon modes that are favourable to Cooper pairing. On the other hand, low-symmetry structures tend to create anisotropic behaviours, which, depending on the material system, can either boost or repress superconductivity. Dimensionality also plays a major role; two-dimensional layered structures like the  $\text{CuO}_2$  The confinement of charge carriers by planes in cuprates or FeAs layers in pnictides results in the creation of circumstances that are favourable for higher  $T_c$  values. Furthermore, there is a strong correlation between the superconducting transition temperatures and the exact bond lengths and angles, such as the distance between the Cu-O bond or the H-H gap in hydrides. When optimum geometries are not followed, the result is frequently a suppression or destabilisation of superconductivity (Saini et al., 2017; Flores-Livas et al., 2020).

Historically, electronic correlations were regarded to be more important in superconductivity theories than lattice structure. This was especially true when the BCS theory was developed, which ascribed superconductivity primarily to electron-phonon interactions without doing a thorough analysis of crystal symmetry or geometry. On the other hand, researchers have seen that small structural elements drastically influence  $T_c$ , and this has been increasingly apparent since the introduction of high- $T_c$  materials. Once again, the focus has switched towards lattice-centered models as a result of the finding of pressure-induced superconductivity in hydrides, which achieved  $T_c$  values more than 250 K. The connection between bond-stretching phonon modes, planar distortions, and  $T_c$  enhancement in cuprates provided more support for the idea that structural optimisation is equally as significant as electrical variables in the process of inducing superconductivity (Drozdov et al., 2015; Boeri et al., 2019).

Recent trends further support this evolving perspective. Crystallographic experiments and density functional perturbation theory (DFPT) simulations have revealed that specific lattice configurations correlate with heightened superconducting properties. For instance, experimental studies on  $\text{LaH}_{10}$  under megabar pressures demonstrated that highly symmetric fcc structures and optimal H-H In order to achieve  $T_c$  over 250 K, bond lengths were of the utmost importance. Similarly, research conducted on bi-based cuprates has demonstrated that even minute alterations to the angles of the Cu-O bond have a direct impact on the amplitude of the superconducting gap and the  $T_c$  (Heil et al., 2019; Errea et al., 2020).



The primary objective of this research is to perform an in-depth analysis of the ways in which differences in lattice geometry affect the superconducting characteristics of several families of high-temperature superconductors. Through this endeavour, the goal is to discover structural blueprints that might potentially direct the construction of superconductors of the next generation that operate at or near room temperature.

The methodology for this study is a conceptual review that is based on secondary data, and it involves doing a systematic analysis of the literature from peer-reviewed journal papers that were published between the years 2016 and 2022. Both experimental structural data and theoretical modelling pertaining to lattice and  $T_c$  correlations were the primary focusses of this examination. Crystallographic investigations, phonon dispersion analysis, and articles that are indexed in Scopus were the sources of the data. We only considered research items that have been validated and evaluated by other researchers. For the purpose of data analysis, a thematic comparison was carried out, in which the findings were categorised according to the various material classes, including cuprates, pnictides, and hydrides. Lattice characteristics such as planar bond angles, layer stacking, and unit cell distortions were taken into consideration. For the purpose of this investigation, there were no main experimental measurements, statistical analysis, or latest simulations carried out.

## 2. LATTICE SYMMETRY AND SUPERCONDUCTIVITY

The symmetry of a crystal lattice is one of the most important factors that determines the superconducting behaviour of a material. The electronic band structure, vibrational modes, and eventually the electron-phonon coupling strength are all subject to distinct limitations depending on the crystal structure. Some examples of crystal structures are cubic, tetragonal, and orthorhombic arrangements. Higher symmetry lattices, and cubic structures in particular, have a tendency to stabilise favourable electron-phonon interactions. This is because they provide more isotropic settings for phonon-mediated pairing. This isotropy makes it easier for coherent coupling to occur across numerous directions in momentum space, which leads to an improvement in the conditions for superconductivity (Wang et al., 2019; Sun et al., 2020).

Hydrogen-rich hydrides are a primary example where high symmetry strongly correlates with exceptional superconducting properties.  $\text{LaH}_{10}$ , crystallizing in a face-centered cubic (fcc) structure under high pressure, exhibits remarkably high superconducting transition temperatures exceeding 250 K. Because of the remarkable symmetry of the fcc lattice, high-frequency phonon modes that are formed



from light hydrogen atoms are distributed uniformly across the lattice. This results in an extraordinarily strong electron-phonon interaction. (Pickard et al., 2020). Similarly, cubic phases of  $\text{YH}_6$  and  $\text{H}_3\text{S}$  under compression demonstrate that structural regularity promotes both phonon stability and high  $T_c$  values.

On the other hand, structures with poorer symmetry, such as orthorhombic phases, which are found in some superconductors based on iron, frequently result in anisotropic electronic and vibrational characteristics. In spite of the fact that such anisotropies have the potential to stabilise unconventional pairing processes, they often lead to an electron-phonon environment that is more complicated and less optimised. However, in some pnictides like  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ , a transition from orthorhombic to tetragonal symmetry with doping correlates with an enhancement in superconductivity, suggesting that increased symmetry supports better coherence among pairing interactions (Nakamura et al., 2018). As a result, one of the most important strategies for creating and optimising high- $T_c$  superconductors is to achieve or induce greater lattice symmetry. This can be accomplished either inherently or by external forces such as pressure or chemical doping.

### 3. DIMENSIONALITY AND LAYERED STRUCTURES IN CUPRATES AND PNICTIDES

In high- $T_c$  materials like cuprates and iron-based pnictides, the dimensionality of the crystal structure is a distinguishing property that has a substantial effect on the superconducting characteristics of the material. In these materials, superconductivity is predominantly confined within two-dimensional planes, notably the  $\text{CuO}_2$  planes in cuprates and  $\text{FeAs}$  layers in pnictides. The presence of these planes creates highly anisotropic electronic structures, which facilitate stronger electron pairing interactions due to the confinement of charge carriers within restricted dimensions (Fujita et al., 2016). As a result of the quasi-two-dimensional character of the electronic states, the density of states at the Fermi level is increased, and correlation effects are strengthened. Both of these factors are important components for the onset of superconductivity in these systems.

In cuprates, the  $\text{CuO}_2$  When it comes to superconducting pairing, aircraft serve as the principal playground for the phenomenon. The charge reservoir layers that are used to separate these planes are responsible for modulating the carrier concentration through the use of doping. There is a consistent body of experimental research that demonstrates that the number of  $\text{CuO}_2$  planes per unit cell correlates with the superconducting transition temperature. For instance, compounds like  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$ , which contain three  $\text{CuO}_2$  layers, tend to exhibit higher  $T_c$  compared to single-layered materials like  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (Zhao et al., 2017). The confinement of electrons within these planes reduces kinetic



energy perpendicular to the layers, promoting effective electron pairing necessary for high- $T_c$  superconductivity.

In iron-based pnictides, the FeAs layers serve a similar function, providing a two-dimensional electronic environment critical for superconductivity. Here, the Fe 3d orbitals hybridize with As p orbitals, forming a quasi-two-dimensional electronic structure with multiple Fermi surface pockets (Charnukha et al., 2015). Variations in the spacing between layers of FeAs, which are regulated by structural factors and chemical composition, have a major impact on the superconducting characteristics of the material. This suggests that ideal interlayer spacing enables higher electronic coherence inside the planes. For example, it has been discovered that increasing  $T_c$  can be accomplished by compressing the lattice or by adding isovalent replacements that vary the interlayer distance.

It is also important to note that interlayer coupling plays a significant role in high- $T_c$  superconductors. The phase coherence of the superconducting order parameter can be affected by weak but finite coupling across layers, despite the fact that the core superconducting mechanism is located inside the planes. Interlayer tunnelling processes have been suggested for use in multilayered cuprates. These mechanisms include the coherence between neighbouring  $\text{CuO}_2$  planes, which helps to stabilise superconductivity at higher temperatures. (Lee et al., 2018). Structural modulations such as buckling or distortions of the planes can further impact superconducting behavior. It has been observed that flatter  $\text{CuO}_2$  planes favor higher  $T_c$ , while buckling or tilting of these planes suppresses superconductivity by weakening the in-plane electronic coherence.

Therefore, the dimensional confinement that is supplied by two-dimensional layers, in conjunction with the modification of interlayer coupling and structural integrity, plays a crucial role in the process of attaining and optimising high- $T_c$  superconductivity in both cuprates and pnictides. When trying to maximise the temperature at which the superconducting transition occurs, it appears that striking a careful balance between in-plane interactions and interlayer coherence seems to be essential.

#### **4. BOND LENGTHS, BOND ANGLES, AND SUPERCONDUCTING PROPERTIES**

The bond lengths and bond angles of a variety of high- $T_c$  materials are essential microscopic characteristics that have a substantial impact on the electrical structure, vibrational properties, and ultimately the superconducting behaviour of these materials. By making relatively little adjustments at the atomic scale, it is possible to bring about significant alterations in carrier mobility, electron-phonon



coupling strength, and the density of states at the Fermi level and beyond. Specific bond geometries, such as Cu-O in cuprates, Fe-As in pnictides, and H-H in hydrides, have shown strong correlations with the observed superconducting transition temperatures.

In cuprate superconductors, the Cu-O bond length within the  $\text{CuO}_2$  planes directly impacts the in-plane electronic bandwidth and superexchange interactions. Experimental studies have revealed that an optimal Cu-O bond length, typically around 1.9 Å, promotes maximal overlap between Cu 3d and O 2p orbitals, enhancing carrier mobility and superconducting pairing (Takagi et al., 2016). Furthermore, the Cu-O-Cu bond angle, which should ideally be close to 180 degrees, guarantees efficient orbital overlap and high antiferromagnetic correlations. These are the factors that are considered to constitute the foundation of the pairing process in these materials. In many cases, the suppression of superconductivity and the reduction of  $T_c$  values are the outcomes of deviations from this ideal geometry, such as bond buckling or distortions occurring (de la Cruz et al., 2017).

Both the length of the Fe-As bond and the angle of the Fe-As-Fe bond are important factors in determining the superconducting performance of iron-based superconductors. At the point when the angle of the Fe-As-Fe link approaches the ideal tetrahedral angle of 109.5 degrees, optimal superconductivity is found. A departure from this angle results in an imbalance in the occupancy of the Fe 3d orbital, which in turn reduces the nesting conditions that are necessary for robust spin fluctuation-mediated pairing (Kawasaki et al., 2018). For instance, in  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ , tuning the As-Fe-As bond geometry through chemical doping has been demonstrated to systematically enhance  $T_c$ , supporting the critical role of local structural configurations.

Hydrogen-rich hydrides present another compelling case where bond lengths dramatically influence superconductivity. In materials like  $\text{LaH}_{10}$  and  $\text{H}_3\text{S}$ , short H-H distances, often around 1.2 Å, lead to the formation of high-frequency optical phonons. In order to achieve strong electron-phonon interaction and, as a result, very high  $T_c$  values above 200 K at megabar pressures, these phonon modes are absolutely necessary (Geballe et al., 2018). Not only does the particular arrangement and compression of the hydrogen lattice have an effect on the dynamics of vibrations, but it also helps to stabilise metallic bonding networks, which are essential for superconductivity.

The optimal bond geometries of these many types of materials reveal a common thread: the fine-tuning of atomic-scale parameters may significantly improve the superconducting capabilities of the material. Whether it is through the optimisation of orbital overlaps in cuprates, the maintenance of tetrahedral



symmetry in pnictides, or the compression of hydrogen networks in hydrides, the attainment of exact bond lengths and angles represents a crucial aspect. It is because of this that lattice engineering procedures, like as chemical doping, epitaxial strain, and high-pressure synthesis, are becoming increasingly important as potential tools for the creation of future superconductors that have higher critical temperatures and more durable superconducting states.

## 5. ROLE OF PRESSURE IN STRUCTURAL OPTIMIZATION

External pressure has emerged as a potent tool that may be used to optimise lattice characteristics and considerably enhance the superconducting transition temperature ( $T_c$ ) in a variety of classes of materials, particularly hydrogen-rich hydrides. There is a reduction in the interatomic distances, an increase in the orbital overlaps, and a shift in the vibrational frequencies of the lattice when pressure is applied to a crystalline solid. The electronic band structure and phonon dispersion relations also undergo changes as a result of these adjustments. These changes have the potential to intensify electron-phonon coupling, which in turn can lead to an increase in superconductivity. However, in hydrides and other specifically tuned materials, large  $T_c$  gains have been seen at severe pressures surpassing 100 GPa. This is in contrast to the situation in common low- $T_c$  materials, where pressure typically produces only minor increases in  $T_c$  (Trojan et al., 2019; Somayazulu et al., 2020).

Particularly in the case of hydrogen-rich hydrides, pressure not only helps to stabilise stoichiometries that would otherwise be unstable, but it also encourages the formation of dense hydrogen frameworks that include high-frequency phonon modes, which are necessary for robust electron-phonon interactions. For example, in  $\text{LaH}_{10}$ , application of pressure above 150 GPa leads to the formation of a highly symmetric face-centered cubic (fcc) structure with an optimal H-H distance that enables  $T_c$  values exceeding 250 K (Drozdov et al., 2019). Under such severe circumstances, the coupling between conduction electrons and high-energy vibrational modes of hydrogen atoms is considerably enhanced, which results in ultrahigh  $T_c$  values. This was confirmed by experimental experiments that were paired with calculations based on density functional perturbation theory (DFPT).

Similarly,  $\text{H}_3\text{S}$  represents another landmark discovery where pressure tuning has been instrumental. Synthesis of  $\text{H}_3\text{S}$  under pressures around 150 GPa leads to a body-centered cubic (bcc) structure characterized by strong electron-phonon coupling and a  $T_c$  around 203 K. Subsequent studies revealed that slight deviations from optimal pressure values resulted in phase transitions to less favorable structures and a corresponding decrease in  $T_c$  (Errea et al., 2016; Flores-Livas et al., 2020). This



highlights how important it is to maintain exact pressure ranges in order to stabilise the high-symmetry phases that are favourable to superconductivity.

In addition to hydrides, pressure-induced structural optimisation has been reported in a variety of other systems as well. Through the application of pressure, certain iron-based superconductors experience a reduction in anion height and a modification of the angles of the Fe-As-Fe link, which ultimately results in improved electronic nesting and increased superconductivity. On the other hand, the impact is shown to be less prominent in comparison to hydrides, which suggests that the process may be different for different material groups (Kong et al., 2021).

The role that pressure played in these findings sheds light on a more general concept in the field of superconductivity research: lattice engineering, whether it be by chemical substitution, epitaxial strain, or external pressure, is a feasible technique for manipulating material structures in order to achieve greater  $T_c$ . Through the application of pressure, it is possible to penetrate metastable phases and bonding configurations that would otherwise be inaccessible under ambient circumstances. The discovery of novel pressure-stabilized superconductors continues to be a potential area in the pursuit of room-temperature superconductivity. This is because experimental techniques for attaining and sustaining ultrahigh pressures are continuing to progress.

## **6. STRUCTURAL DISORDER, STRAIN, AND THEIR EFFECTS ON $T_c$**

High- $T_c$  materials are susceptible to having their superconducting characteristics significantly altered by a number of potent causes, including structural instability and strain. The symmetry, electron mobility, and phonon properties of superconductors are influenced by local lattice distortions, chemical inhomogeneities, and strain that is either externally imposed or inherent. These factors can lead to variations in the critical temperature ( $T_c$ ) and the superconducting gap. In certain cases, superconductivity can be improved by a moderate and regulated amount of disorder or strain; however, severe distortions often reduce  $T_c$  by dispersing carriers and breaking pairing interactions (Song et al., 2017; Takahashi et al., 2019).

Nanoscale areas are created as a result of local lattice distortions, which are particularly prevalent in layered materials such as cuprates and iron pnictides. These regions have the potential to either increase or prevent superconductivity. Suppressed superconducting gaps have been shown to correspond with areas of oxygen deprivation or local structural deformation in cuprate superconductors, according to



research conducted with scanning tunnelling microscopy (STM) (Gomes et al., 2016). On the other hand, mild inhomogeneities can occasionally result in a spatial variation in the superconducting gap, which might provide light on phase competition and fluctuation events that occur near to  $T_c$ . In a similar manner, the nonuniform distribution of dopants in iron-based superconductors causes local oscillations in the lattice parameters, which in turn affects the electrical characteristics and pairing interactions.

Through the use of strain engineering in thin films, a controlled approach has arisen for tuning superconductivity. This process involves adjusting bond angles and lengths without affecting the chemical makeup of the material. One example is the application of tensile strain to FeSe monolayers grown on  $\text{SrTiO}_3$  substrates has been shown to significantly enhance  $T_c$  from 8 K (bulk) to above 65 K (Lee et al., 2018). The strain modifies the Fe-Se bond environment and enhances electron-phonon coupling at the interface, thus stabilizing higher-temperature superconductivity. In another example, strained  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  thin films demonstrated an increase in  $T_c$  by optimizing the planar Cu-O bond lengths and improving orbital overlaps, supporting the notion that lattice strain can effectively manipulate superconducting properties (Nie et al., 2020).

Chemical substitution acts as another pathway for introducing controlled disorder and strain. In  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  systems, substitution of As with smaller P atoms introduces internal chemical pressure that reduces lattice constants and modifies the FeAs layer structure, leading to an optimal superconducting dome centered around  $x \approx 0.3$  (Hashimoto et al., 2016). However, when correctly balanced, chemical disorder may optimise lattice shape and electrical characteristics, hence increasing  $T_c$ . These examples indicate that even while chemical disorder can sometimes operate as scattering centres that are detrimental to superconductivity, it can also perform this function.

Since a result, the impact of disorder and strain on superconductivity is extremely complex, since it is contingent upon the kind, amplitude, and spatial distribution of the distortions. Localised disorder that maintains overall lattice coherence has the tendency to improve  $T_c$  by optimising phonon interactions or electronic structures. On the other hand, large-scale disorder often breaks coherence and decreases superconducting performance. When it comes to attaining desirable lattice topologies and increasing  $T_c$ , strain, whether it is intrinsic or produced, serves as a potent tuning knob. This is especially true in two-dimensional and thin film superconductors. The advancement of research into strain and disorder is anticipated to result in the creation of new superconductors that have lattice features that can be customised to specific applications and higher temperatures at which they can function.



## 7. CONCLUSION

Within the scope of this research project, a detailed investigation of the key role of lattice geometry on the modulation of superconductivity was carried out across a variety of high-temperature superconducting materials. It has been proven that structural characteristics, such as lattice symmetry, dimensionality, link lengths, bond angles, and lattice distortions, have a significant role in determining the superconducting transition temperature ( $T_c$ ) and the stability of the superconducting phase. Depending on the material system and the external circumstances, it was discovered that variations in certain structural factors either increased or decreased the superconductivity of the material. When it comes to identifying the electrical and phononic interactions that are responsible for superconductivity, the structural environment has repeatedly emerged as a key component across a wide range of material families.

The findings provided further evidence that particular structural fingerprints were frequently linked to increased  $T_c$  readings. Optimal bond angles, in particular those that are close to 180 degrees in cuprates and 109.5 degrees in iron-based superconductors, have been identified as geometries that are favourable for superconductivity. In a similar manner, it was demonstrated that decreased dimensionality, which is exhibited by two-dimensional surfaces like  $\text{CuO}_2$  layers and FeAs sheets, may concentrate carrier mobility and increase pairing interactions. The existence of a general structural blueprint that is advantageous for high- $T_c$  superconductivity was revealed by the presence of these recurrent structural motifs across a variety of material classes.

In addition, the research advised that future attempts to identify new materials should deliberately concentrate on structural tuning by means of chemical design, epitaxial strain approaches, and external pressure engineering. By purposefully altering the characteristics of the lattice, researchers were able to pinpoint and stabilise the structural configurations that were most favourable to obtaining higher critical temperatures. In addition, the controllable introduction of strain and lattice distortions have emerged as potentially fruitful avenues for optimising superconductivity without necessarily requiring alterations to the chemical compositions of the materials.

Finally, it was suggested that the predictive modelling of superconductivity based on lattice geometry optimisation should be given priority in the computational research that would be conducted in the present and future. It is possible that sophisticated simulations that incorporate quantum mechanical calculations, machine learning, and high-throughput crystallographic screening might provide strong



tools for the identification and engineering of new superconductors in accordance with the structural blueprints that are given in this paper.

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