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# DFT+U HISOBLASH USULI YORDAMIDA $La_2CuO_4$ KUPRRATINING ENERGIYASI HAMDA KRISTALL TUZILISHINING GIDROSTATIK BOSIMGA BOG‘LIQ O‘ZGARISHINI O‘RGANISH

***Annotatsiya.*** *Ushbu ishda $La_2CuO_4$ kupratining strukturaviy va elektron xossalariga gidrostatik bosimning ta’siri zichlik funksional nazariyasi — Density Functional Theory (DFT) doirasida, DFT+U yondashuvi asosida o‘rganildi. Hisoblashlar Quantum ESPRESSO dasturiy paketi yordamida bajarildi. Olingan natijalar shuni ko‘rsatdiki, bosim ortishi bilan kristall panjara parametrlari va elementar yacheyka hajmi kamayadi, bu esa panjaraning siqilishini bildiradi. Shuningdek, deformatsiyaning anizotrop xarakterga ega ekanligi aniqlanib, c o‘qi bo‘ylab qisqarish a o‘qiga nisbatan kuchliroq ekanligi kuzatildi. Atomlararo itarilish kuchlarining ortishi natijasida bosim oshishi bilan tizimning umumiy energiyasi ham ortadi.*

***Kalit so‘zlar:*** *$La_2CuO_4$; DFT+U; gidrostatik bosim; elektron tuzilma; Fermi energiyasi; kupratlar.*

# ИССЛЕДОВАНИЕ ЗАВИСИМОСТИ ЭНЕРГИИ И КРИСТАЛЛИЧЕСКОЙ СТРУКТУРЫ КУПРАТА $La_2CuO_4$ ОТ ДАВЛЕНИЯ С ИСПОЛЬЗОВАНИЕМ МЕТОДА DFT+U

***Аннотация***. *В данной работе исследовано влияние гидростатического давления на структурные и электронные свойства купрата* $La_2CuO_4$ *с использованием DFT в рамках подхода DFT+U. Расчёты были выполнены с помощью программного пакета Quantum ESPRESSO. Полученные результаты показывают, что с увеличением давления параметры кристаллической решётки и объём элементарной ячейки уменьшаются, что свидетельствует о сжатии решётки. Наблюдается анизотропная деформация, при которой уменьшение вдоль оси* ***c*** *выражено сильнее, чем вдоль оси* ***a***. *Полная энергия системы увеличивается с ростом давления вследствие усиления межатомного отталкивания.*

***Ключевые слова***. $La_2CuO_4$*; DFT+U; гидростатическое давление; электронная структура; энергия Ферми; купраты.*

## INVESTIGATION OF THE PRESUURE DEPENDENT VARIATION OF THE ENERGY AND CRYSTAL STRUCTURE $La_2CuO_4$ CUPRATE USING THE DFT+U METHOD

***Abstract.*** *In this work, the effect of hydrostatic pressure on the structural and electronic properties of* $La_2CuO_4$ *cuprate was investigated using Density Functional Theory (DFT) within the DFT+U approach. The calculations were performed using the Quantum ESPRESSO package. The obtained results show that the lattice parameters and unit cell volume decrease with increasing pressure, indicating lattice compression. Anisotropic deformation was observed, with a more pronounced reduction along the c-axis compared to the a-axis. The total energy increases with pressure due to enhanced interatomic repulsion.*

***Keywords:*** $La_2CuO_4$*; DFT+U; hydrostatic pressure; electronic structure; Fermi energy; cuprates*

## Introduction

High-$T_c$ superconducting cuprates, particularly $La_2CuO_4$, belong to the class of strongly electron-electron correlated systems, in which the interplay between lattice structure and electronic properties plays a crucial role. The physical properties of these materials are highly sensitive to external parameters such as pressure, temperature, and doping [1]. Among these, hydrostatic pressure is an effective tool for tuning both structural and electronic characteristics without introducing chemical disorder.

The application of hydrostatic pressure leads to a reduction in lattice parameters, modifies interatomic distances, and consequently affects the electronic structure as well as the energetic stability of the system [2]. These structural changes can significantly influence orbital overlap and electron interactions, which are essential for understanding the behaviour of cuprate materials.

However, conventional Density Functional Theory (DFT) often fails to accurately describe strongly correlated systems due to its limitations in treating localized electron interactions. To overcome this issue, the DFT+U approach is widely employed, as it introduces an effective Hubbard $U$ parameter to better account for on-site Coulomb interactions [3]. In the case of $La_2CuO_4$, applying the Hubbard $U$ correction to Cu 3d orbitals provides a more realistic and reliable description of its electronic structure [4].

Hydrostatic pressure is also a key parameter for controlling electronic properties. As pressure increases, interatomic distances change, leading to enhanced orbital hybridization and redistribution of electronic charge density. As a result, significant modifications in the band structure and Fermi surface can occur. Recent studies have shown that cuprate materials may undergo notable electronic reconstruction under applied pressure, which directly impacts their physical properties [5].

In this work, we investigate the effect of hydrostatic pressure on the structural and electronic properties of $La_2CuO_4$ using the DFT+U method. Special attention is given to the evolution of lattice parameters, total energy, and Fermi

energy as a function of pressure, in order to better understand the relationship between structural compression and electronic behaviour.

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## Literature review

The study of high-temperature superconducting cuprates has been a central topic in condensed matter physics since the discovery of superconductivity in the La–Ba–Cu–O system by Bednorz and Müller. Among these materials, $La_2CuO_4$ is considered a prototypical parent compound of cuprate superconductors, exhibiting strong electron–electron correlations and antiferromagnetic insulating behavior. Understanding its structural and electronic properties is therefore essential for elucidating the mechanisms of high-Tc superconductivity.

Early theoretical investigations based on conventional Density Functional Theory (DFT) revealed significant limitations in describing the electronic structure of $La_2CuO_4$, particularly its insulating ground state. Standard DFT approaches, such as the Local Density Approximation (LDA), tend to underestimate electron correlation effects, often predicting a metallic state instead of the experimentally observed Mott insulating phase. To address this issue, the DFT+U method was introduced by Anisimov et al., incorporating an on-site Coulomb interaction term (Hubbard U) to better describe localized d-electrons. This approach has since become widely accepted for studying strongly correlated systems, including transition metal oxides and cuprates.

Subsequent studies have demonstrated that applying a Hubbard U parameter to Cu 3d orbitals significantly improves the accuracy of electronic structure calculations for $La_2CuO_4$. For instance, Pesant and Coté showed that DFT+U can successfully reproduce magnetic ordering and band gap behavior in doped

$La_2CuO_4$ systems. Similarly, Schluter and Hybertsen highlighted the importance of electron correlation effects in determining the renormalized electronic structure of this material.

In addition to electronic correlations, external parameters such as hydrostatic pressure play a crucial role in modifying the structural and electronic properties of cuprates. Experimental studies using neutron diffraction techniques have shown that pressure induces a reduction in lattice parameters and unit cell volume in $La_2CuO_4$, reflecting lattice compression and enhanced interatomic interactions. These structural changes are often anisotropic due to the layered nature of cuprates, with stronger compression observed along the c-axis compared to the ab-plane.

Pressure-induced modifications also strongly affect the electronic structure. Increased leads to enhanced orbital overlap, particularly between Cu 3d and O 2p orbitals, which are responsible for the electronic and transport properties of cuprates. Radaelli et al. reported that structural distortions under pressure can influence superconducting properties and electronic phase transitions in La-based cuprates. Furthermore, recent theoretical works suggest that pressure can induce significant changes in the Fermi surface and electronic band structure, potentially leading to electronic reconstruction phenomena.

Despite extensive research, the combined effect of hydrostatic pressure and strong electron correlation on the total energy, lattice deformation, and Fermi energy evolution in $La_2CuO_4$ remains an active area of investigation. In particular, the nonlinear behavior of electronic properties under pressure and their relationship with structural anisotropy require further detailed study using advanced computational methods such as DFT+U.

Therefore, building upon previous experimental and theoretical works, the present study aims to provide a systematic analysis of the pressure-dependent structural and electronic properties of $La_2CuO_4$, with special emphasis on total energy variation, anisotropic lattice compression, and Fermi energy evolution within the DFT+U framework.

## Methodology

The structural and electronic properties of $La_2CuO_4$ were investigated within the framework of Density Functional Theory (DFT) using the Quantum ESPRESSO simulation package. The exchange–correlation interaction was treated using the generalized gradient approximation (GGA+U) in the form of the Perdew–Burke–Ernzerhof (PBE) functional.

To properly describe the strong electron–electron correlation effects in the Cu 3d orbitals, the DFT+U method was employed within the Dudarev approach. The on-site Coulomb interaction parameter was set to U=12 eV for Cu atoms, which is commonly used for cuprate systems and provides a more realistic description of their electronic structure.

The interaction between valence electrons and ionic cores was described using ultrasoft pseudopotentials. First we checked convergence value of cut-off energy. The plane-wave basis set cutoff energy was set to 80 Ry for the wave functions, and a corresponding charge density cutoff (ecutrho) was chosen appropriately to ensure convergence. Brillouin zone integrations were performed using a Monkhorst–Pack k-point grid of 8×8×4, which is sufficient for layered cuprate structures.

The initial crystal structure of tetragonal $La_2CuO_4$ was taken from experimental data and fully optimized before further calculations. Structural optimization was performed using the variable-cell relaxation (vc-relax) scheme, allowing both atomic positions and lattice parameters to relax simultaneously.

The present GGA+U calculations yield a band gap of 1.8 eV for $La_2CuO_4$, which is consistent with previously reported theoretical and experimental values [7,11,12]. This result falls within the range of 1.4–2.0 eV established by Tyler et al., and is in close agreement with the value reported by Perry et al.

Hydrostatic pressure was applied in the range of 1–10 GPa to investigate its effect on structural and electronic properties. During optimization, the convergence thresholds for total energy and forces were set to standard values, ensuring reliable results.

Spin-polarized calculations were carried out to account for magnetic effects in $La_2CuO_4$, which is known to exhibit antiferromagnetic ordering. The self-consistent field (SCF) calculations were performed after structural optimization to obtain accurate total energies and Fermi energy values at each pressure point.

## Results and discussion

Figure 1 presents the spin-polarized electronic band structure of $La_2CuO_4$ calculated along the high-symmetry k-path Γ–X–M–Γ–Z–R–A–Z within the GGA+U framework. The band structure clearly reveals an insulating ground state, with a band gap of 1.8 eV opening between the valence band maximum and the conduction band minimum, consistent with the well-established charge-transfer insulating character of $La_2CuO_4$.

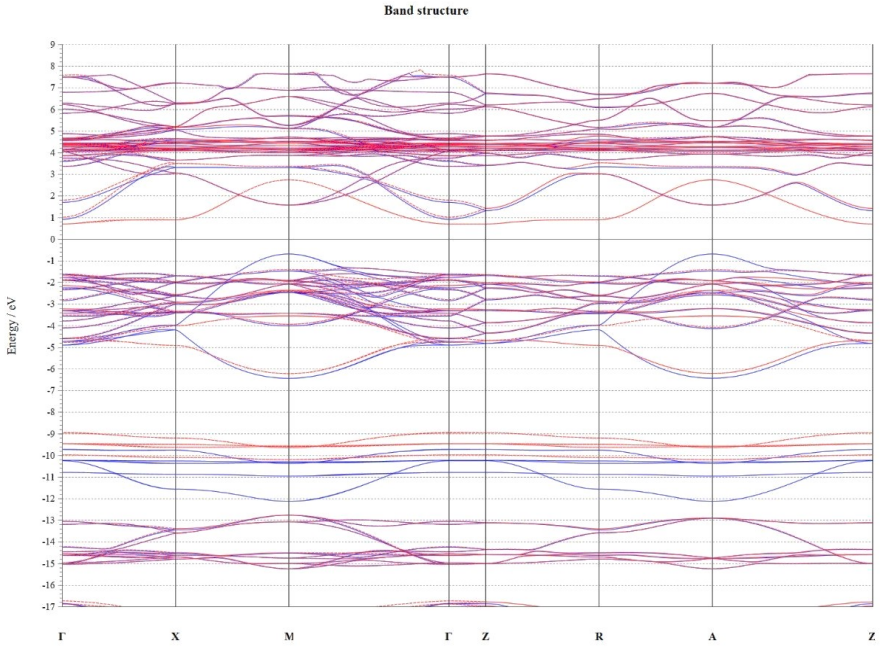
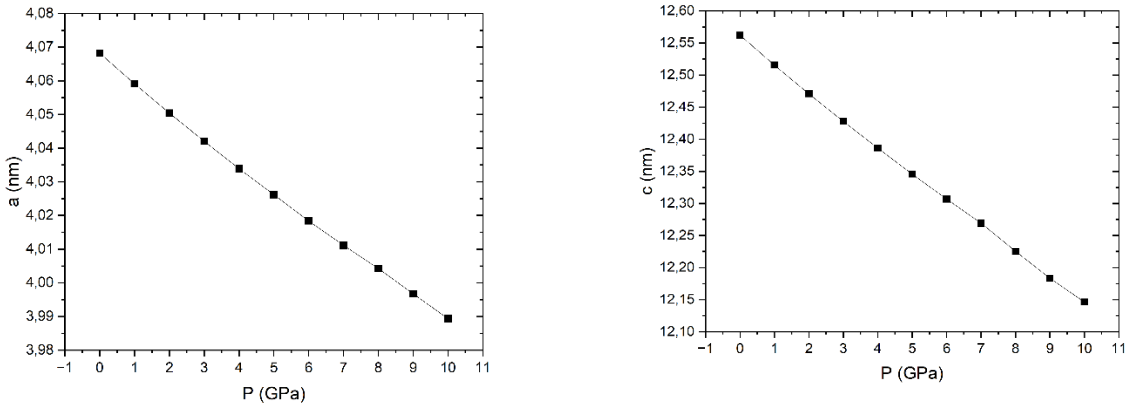



**Fig.1 – Band structure of $La_2CuO_4$**

The calculated structural parameters of $La_2CuO_4$ under hydrostatic pressure reveal a systematic contraction of the lattice. Specifically, the lattice parameter *a* decreases from approximately ~0.406 nm to ~0.398 nm, while the *c* parameter decreases from ~1.256 nm to ~1.214 nm (Fig.2 a,b). This trend is consistent with the well-known behavior of crystalline solids, where lattice parameters decrease under applied pressure due to the reduction of interatomic distances [2].




*a)* *b)*

**Fig.2 a,b. Effect of hydrostatic pressure on the (a) and (c) lattice parameters.**

Moreover, the reduction along the *c*-axis is more pronounced than along the *a*-axis, indicating anisotropic compression. This anisotropy is a characteristic feature of layered cuprate materials, where weaker interlayer interactions along the *c*-direction make it more compressible compared to the in-plane (*ab*) directions [5].

The pressure dependence of the lattice volume is shown in Fig.3. It is clearly observed that the volume decreases monotonically with increasing pressure. This behavior is consistent with classical equations of state and reflects the continuous compression of the crystal lattice [7]. The reduction in volume leads to shorter interatomic distances, which enhances the overlap between electronic orbitals and strengthens interatomic interactions [8].

The variation of total energy with pressure is presented in Fig.4. The results show that the total energy increases with increasing pressure. This can be attributed to the enhancement of repulsive interatomic interactions as atoms are forced closer together under compression [7]. As the interatomic distances decrease, the overlap between electron clouds increases, leading to a rise in the total energy of the system [8].

The calculated Fermi energy as a function of pressure is shown in Fig.5. Unlike structural parameters, the Fermi energy exhibits a nonlinear dependence on pressure. At low pressures (0–1 GPa), the Fermi energy changes only slightly,

increasing from approximately 10.55 eV to 10.68 eV. However, a pronounced rise occurs between 1 and 2 GPa, where $E_F$ abruptly increases to nearly 11.4 eV.

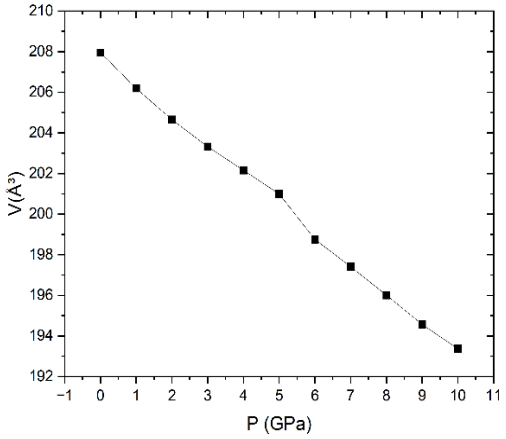



**Fig.3: Pressure-dependent variation of volume**

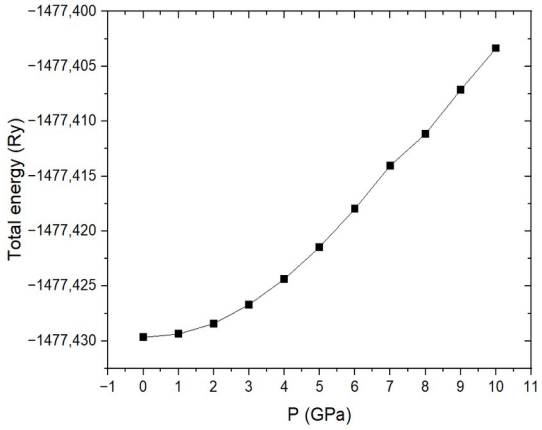



**Fig.4: Pressure-dependent variation of the total energy**

This sudden enhancement may indicate a significant modification in the electronic band structure, such as increased orbital overlap, redistribution of electronic states, or pressure-induced structural effects.

Beyond 2 GPa, the Fermi energy exhibits an almost linear increase with pressure. From 2 to 10 GPa, $E_F$ gradually rises from about 11.4 eV to 12.55 eV. The nearly linear behavior at higher pressures suggests a stable compression-induced modification of the electronic states and enhanced electronic density near the Fermi level.

The Fermi energy is a key parameter in determining the electronic properties of a material. It provides information about: (i) the highest occupied electronic state [4], (ii) the metallic or insulating nature of the system [9], (iii) the electron density and distribution of electronic states, and (iv) transport properties such as electrical conductivity [8].

The observed variation of the Fermi energy under pressure indicates significant modifications in the electronic structure. These include shifts in energy bands, increased orbital hybridization, and redistribution of electron density [8].

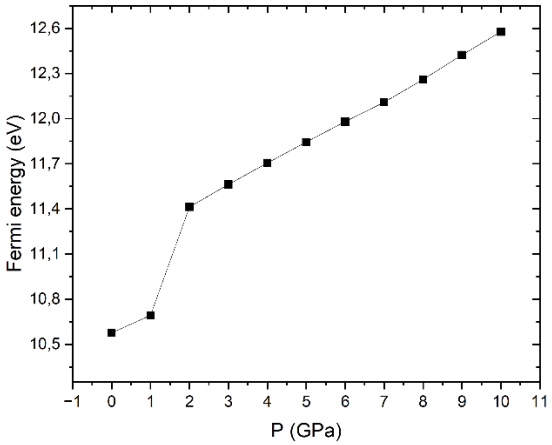



**Fig.5: Pressure-dependent variation of the Fermi energy**

The observed trend implies that pressure strongly affects the electronic properties of the material by altering interatomic distances and electron interactions. The continuous increase in the Fermi energy under compression may be associated with enhanced bandwidth, stronger hybridization between atomic orbitals, and changes in carrier concentration. Such behavior is commonly observed in strongly correlated and transition-metal oxide systems, where pressure tuning can significantly modify conductivity and superconducting properties. This behavior can be associated with changes in the interaction between Cu-3d and O-2p orbitals, which play a crucial role in determining the electronic properties of cuprates [10]. In summary, the results demonstrate a strong correlation between structural and electronic properties under pressure. The lattice compression leads to a decrease in volume, an increase in total energy, and a nontrivial evolution of the Fermi energy. The identified nonlinear behaviour of the Fermi level suggests the occurrence of pressure-induced electronic transitions, highlighting the complex nature of this material.

## Conclusion

The obtained results indicate that in $La_2CuO_4$, under the effect of hydrostatic pressure, the lattice parameters decrease while the total energy increases. These results confirm that, due to the layered structure of cuprates, they exhibit anisotropic deformation and significantly modifies the electronic structure. The observation of a maximum in the Fermi energy indicates the occurrence of

electronic reconstruction under this pressure. These results reveal the potential to tune the electronic properties of cuprate materials through external parameters.

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