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Investigation of the Electronic Structure of $HgBa_2CuO_4$ Cuprate Based on the DFT Approach

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Abstract. This study focuses on analyzing the electronic structure of the single-layer cuprate $HgBa_2CuO_4$ (Hg-1201) using the density functional theory (DFT) approach. The band structure and density of states (DOS) of the material were calculated using the Burai interface of the Quantum ESPRESSO package. The results reveal multiple energy bands near the Fermi level, with dominant contributions from Cu 3d and O 2p orbitals. These findings confirm the metallic or semimetallic nature of the compound and the central role of CuO_2 planes in high-temperature superconductivity. Furthermore, the presence of high DOS and low-dispersion bands supports the interpretation of Hg-1201 within the bipolaron condensation framework, explaining its elevated critical temperature (T_c). The results align with previous La_2CuO_4 studies and reinforce the potential of Hg-based single-layer cuprates in high-T_c superconductivity.

Keywords: High-T_c superconductivity; density functional theory; density of states and electronic band structure in Hg-based cuprates

I. INTRODUCTION

Since the discovery of high-temperature superconductivity (HTS) by Bednorz and Muller in 1986 [1], this field has become one of the central topics in modern condensed matter physics. Among HTS materials, copper-based cuprates have attracted particular attention because of their unique crystal structures and the strong electronic correlations that govern their superconducting behavior. A fundamental structural characteristic common to these compounds is the presence of CuO_2 planes, which are widely regarded as the key component that determines their electrical, magnetic, and superconducting properties [2]. Among various cuprates, Hg-1201 stands out due to its structural simplicity: it contains only a single CuO_2 layer and its relatively high critical temperature (T_c), which typically ranges from 90 to 94 K [3]. Hg-1201 crystallizes in a tetragonal structure, in contrast to the orthorhombic structure typically found in La_2CuO_4. This simpler, but highly effective crystal arrangement contributes to its elevated T_c. The compound adopts a tetragonal K_2NiF_4-type layered perovskite structure, in which Cu–O–Cu units form extended two-dimensional (2D) sheets (Fig. 1). These CuO_2 planes are the primary structural motif responsible for high-T_c superconductivity. Hg-1201 belongs to the Ruddlesden–Popper family of layered oxides, with the general formula $AO_n(ABO_3)$, characterized by alternating perovskite layers and rock-salt-type layers, with one BO_2 layer per formula unit [4].

The importance of CuO_2 planes has been experimentally confirmed in several single-layer cuprates, including $La_{2-x}Sr_xCuO_4$, $Tl_2Ba_2CuO_6$, $Bi_2Sr_2CuO_{6+\delta}$ and $HgBa_2CuO_4$ [4, 5]. The relationship between crystal structure and T_c is also explained by the bipolaron model, which suggests that strong electron–phonon interactions lead to the formation of intersite bipolarons. These bipolarons undergo Bose–Einstein condensation at low temperatures, giving rise to the superconducting state [6]. In this model, T_c is determined by the condensation temperature of the bipolaron gas (T_{BEC}), which depends on structural parameters such as the lattice height (h_0) and the Cu–O bond lengths [4, 7].

Modern computational techniques, especially density functional theory (DFT), offer powerful tools to investigate the electronic properties of such materials. DFT, which focuses on the electron density in many-body systems, has become a cornerstone of modern materials science [8]. Using software packages such as Quantum ESPRESSO, it is possible to calculate the electronic band structure and density of states (DOS), providing insights into whether a material behaves as a metal, semiconductor, or superconductor [8, 9]. For instance, DFT studies on La_2CuO_4 have revealed that only one band crosses the Fermi level, indicating

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the possibility of superconductivity at low temperatures [9, 10]. DOS analysis further shows that Cu $3d$ and O $2p$ orbitals dominate the states near the Fermi level. Applying a similar approach to Hg-1201 allows a detailed understanding of the electronic features underlying its high T_c. In this study, we investigate the electronic structure of $HgBa_2CuO_4$ using DFT. The results are compared with previously reported data for La_2CuO_4 and analyzed in terms of structural, electronic and phononic contributions to superconductivity [11]. This work aims to contribute to a deeper understanding of high-T_c superconductivity in single-layer cuprates.

II. METHODOLOGY

In this study, first-principles quantum mechanical calculations based on Density Functional Theory (DFT) were performed to explore the electronic properties of the high-temperature superconducting cuprate $HgBa_2CuO_{4+\delta}$ [12]. This approach allows for an accurate determination of the ground state electron density and provides a framework for analyzing the band structure and density of states (DOS), which are critical in understanding the material's superconducting behavior.

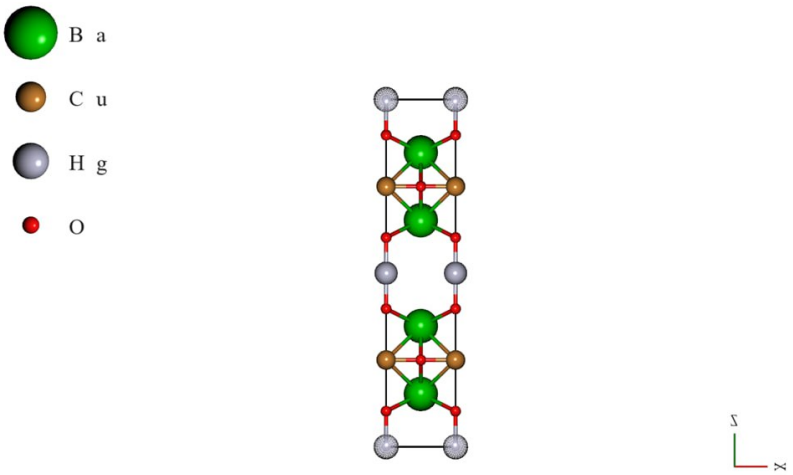


Figure 1. Crystal structure of $HgBa_2CuO_4$ (Hg-1201). The structure consists of a single CuO_2 plane per unit cell, separated by Hg and Ba layers. The Cu–O–Cu units form infinite two-dimensional sheets responsible for superconductivity. This tetragonal structure belongs to the Ruddlesden–Popper family and adopts a K_2NiF_4-type layered perovskite arrangement.

To perform these calculations, the Quantum ESPRESSO simulation suite was used via the Burai graphical user interface, which facilitates user-friendly control of structural optimization, self-consistent field (SCF) calculations, and electronic structure analysis. This method mirrors the computational workflow previously employed for La_2CuO_4, a model cuprate compound, as described by Mohanta et all. (2023) [9]. However, the present study focuses on the Hg-1201 system, which crystallizes in a simpler tetragonal structure, offering clearer insight into the physics of the cuprate plane without the complication of structural distortions seen in La_2CuO_4 [5, 13].

1. Computational parameters. The following settings and parameters were adopted for the DFT simulations [14].

- Exchange-correlation functional: The Perdew–Burke–Ernzerhof (PBE) formulation within the Generalized Gradient Approximation (GGA) was selected to account for electron exchange and correlation effects, consistent with both this and prior La_2CuO_4 studies
- Pseudopotentials: Ultrasoft pseudopotentials were utilized to effectively treat the interaction between core and valence electrons, allowing computational efficiency to be maintained without compromising accuracy.
- Plane-wave cut-off energy: Set to 60 Ry, ensuring the convergence of the wavefunctions.
- Charge density cut-off energy: Set to 600 Ry, providing an accurate representation of the charge distribution.
- Brillouin zone sampling: A Monkhorst–Pack k-point mesh of 6×6×6 was applied to accurately integrate the reciprocal space.

2. Structural Optimization. Structural optimization was conducted using SCF iterations until the total energy difference converged below 10^{-8} Ry [7, 15]. The initial atomic coordinates and lattice constants for Hg-1201 were retrieved from the

Atom	x	y	z
Hg	0.000000	0.000000	0.000000
Hg	0.000000	0.000000	9.827602
Ba	1.966857	1.966857	6.836050
Ba	1.966857	1.966857	2.991552
Ba	1.966857	1.966857	16.663652
Ba	1.966857	1.966857	12.819154
Cu	0.000000	0.000000	4.913801
Cu	0.000000	0.000000	14.741403
O	0.000000	0.000000	7.812659
O	0.000000	0.000000	2.014943
O	0.000000	1.966857	4.913801
O	1.966857	0.000000	4.913801
O	0.000000	0.000000	17.640261
O	0.000000	0.000000	11.842545
O	0.000000	1.966857	14.741403
O	1.966857	0.000000	14.741403

Table I. Atomic position of $HgBa_2CuO_4$

Inorganic Crystal Structure Database (ICSD) and corroborated by experimental reports. Unlike La_2CuO_4 , which undergoes a tetragonal-to-orthorhombic distortion, Hg-1201 remains in the tetragonal phase at ambient conditions, simplifying its electronic modeling.

3. Electronic Structure Calculations. After geometry optimization, the band structure was computed along a high-symmetry path in the Brillouin zone: Γ – X – M – Γ– Z – R – A – Z – X – R – M – A. This path was chosen to comprehensively sample the Brillouin zone and reveal features critical to the Fermi surface topology and electron dispersion relations. Additionally, Density of States (DOS) and Partial Density of States (PDOS) were calculated to quantify the contributions of specific atomic orbitals to the electronic states near the Fermi level. As in La_2CuO_4, the Cu 3d and O 2p orbitals dominate the electronic states in this region. This highlights the similar underlying CuO_2-plane physics between Hg-1201 and La_2CuO_4, despite differences in structure and superconducting critical temperatures[5, 16].

4. Comparison with La_2CuO_4-Based Studies While both Hg-1201 and La_2CuO_4 are layered cuprates with CuO_2 planes as the active superconducting layers, La_2CuO_4 crystallizes in a distorted orthorhombic structure, complicating the interpretation of its band structure. Conversely, the tetragonal symmetry of Hg-1201 enables a clearer and more symmetric energy band analysis. Moreover, Hg-1201 displays a higher superconducting transition temperature (T_c >90 K) compared to La_2CuO_4 ($T_c = 38$ K with doping), making it a more relevant subject for studying optimal high-T_c mechanisms [6, 17]. The present methodology builds upon and extends the techniques employed in the DFT study of La_2CuO_4 by incorporating more refined convergence criteria and examining a simpler yet more superconductively potent system.

III. RESULTS AND ANALYSIS

1. Band Structure Analysis. The electronic band structure of Hg-1201 was calculated using density functional theory (DFT) within the framework of the Burai interface, which is built atop the Quantum ESPRESSO platform. The structure of the band was evaluated along the high-symmetry path Γ – X – M – Γ– Z – R – A – Z – X – R – M – A in the Brillouin zone. The results reveal a broad distribution of electronic states extending from approximately –28 eV to +10 eV, with several bands crossing the Fermi level (set at 0 eV) [9, 17]. This feature clearly indicates metallic or semimetallic behavior, consistent with the existence of free charge carriers—an essential condition for high-T_c superconductivity.

The structure of the Hg-1201 band, calculated using the Burai interface along the high symmetry directions (Γ – X – M – Γ– Z – R – A – Z – X – R – M – A), reveals a complex distribution of electronic states over the energy range from –28 eV to +10 eV. Notably, the presence of multiple bands located near and crossing the Fermi level (set at 0 eV) suggests that the material exhibits semimetallic or weakly metallic behavior. This indicates the existence of free charge carriers, which is essential for high-T_c superconductivity [2,9].

Some of the bands exhibit low dispersion (i.e., relatively flat), indicating a partially localized character of the electronic states within Hg-1201. In particular, such flat bands observed in the Γ–X and M–Γ segments may favor the stable formation of bipolarons [9, 16]. Moreover, the presence of multiple dense branches at the top of the valence bands implies the likelihood of strong electron–phonon interactions.

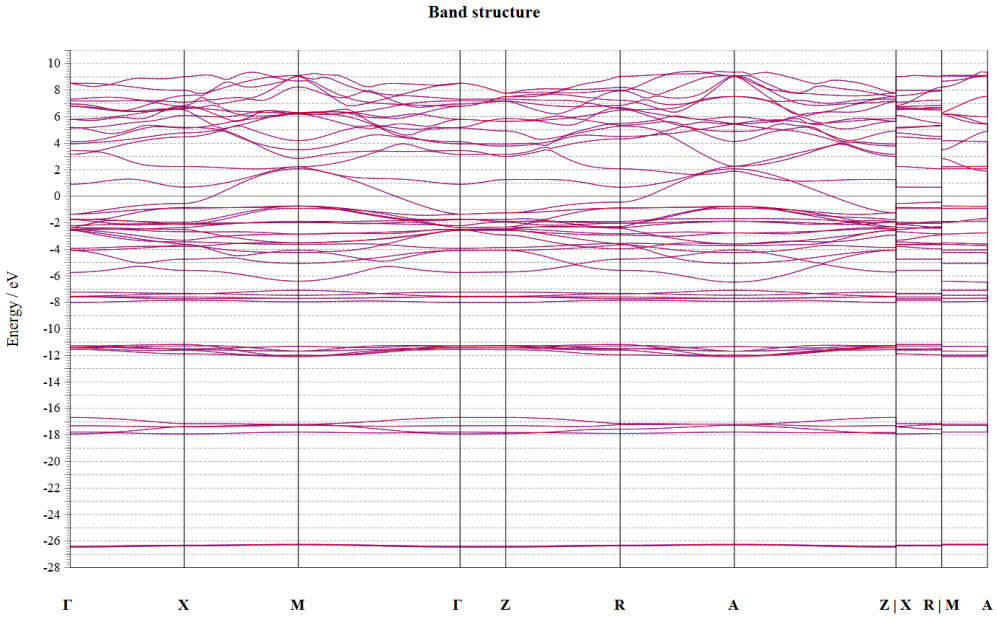


Figure 2. Band Diagram of $HgBa_2CuO_4$ Compound

2. Density of States (DOS) analysis. The DOS plot includes both the total density of states (Total DOS) and the element-resolved partial density of states (PDOS) contributions from Ba, Cu, Hg, and O atoms. The following observations were made from the data:

- Near the Fermi level, the Cu 3d and O 2p orbitals exhibit high density, highlighting the critical role of CuO_2 layers in electrical conductivity [4,9]
- The Hg and Ba orbitals contribute primarily to lower-energy states (around –25 eV and –10 eV), while they are nearly inactive near the Fermi level. This indicates that Hg and Ba ions primarily contribute to lattice stability
- The Total DOS at the Fermi level is nonzero, which confirms that Hg-1201 does not behave as a semiconductor, but rather shows metallic-like characteristics [2]

These observations are consistent with the results obtained for La_2CuO_4 based on DFT calculations, and they contribute to understanding the origins of the high T_c values observed in single-layer Hg-based cuprates [18]. Moreover, the presence of high density of states near the Fermi level and the existence of low-dispersion (flat) bands align with the Bose–Einstein condensation model involving bipolarons. In this framework, strong electron–phonon coupling leads to the formation of intersite bipolarons, whose condensation temperature determines the superconducting critical temperature T_c [6, 19]. The band structure and DOS calculations performed for Hg-1201 using the DFT approach confirm its metallic behavior and emphasize the crucial role of Cu–O layers in superconductivity [20]. These results support the theoretical framework of the bipolaron model and offer insight into the electronic factors responsible for the elevated T_c in single-layer Hg-based cuprates.

IV. CONCLUSION

In this study, we conducted a comprehensive first-principles investigation of the structural and electronic properties of the high-temperature superconductor $HgBa_2CuO_4$ using Density Functional Theory (DFT). The optimized crystal structure confirms the characteristic layered perovskite framework with well-defined CuO_2 planes, which play a central role in governing the superconducting behavior of the material[6, 9, 13].

Our electronic structure calculations reveal that states near the Fermi level originate primarily from hybridized Cu 3d(x^2-y^2) and O 2p orbitals, with flat bands and a pronounced two-dimensional character suggesting strong electronic correlations. The high density of states (DOS) at the Fermi level, particularly within the CuO_2 planes, provides favorable conditions for superconductivity and aligns well with experimental observations in cuprate systems[5, 7, 14].

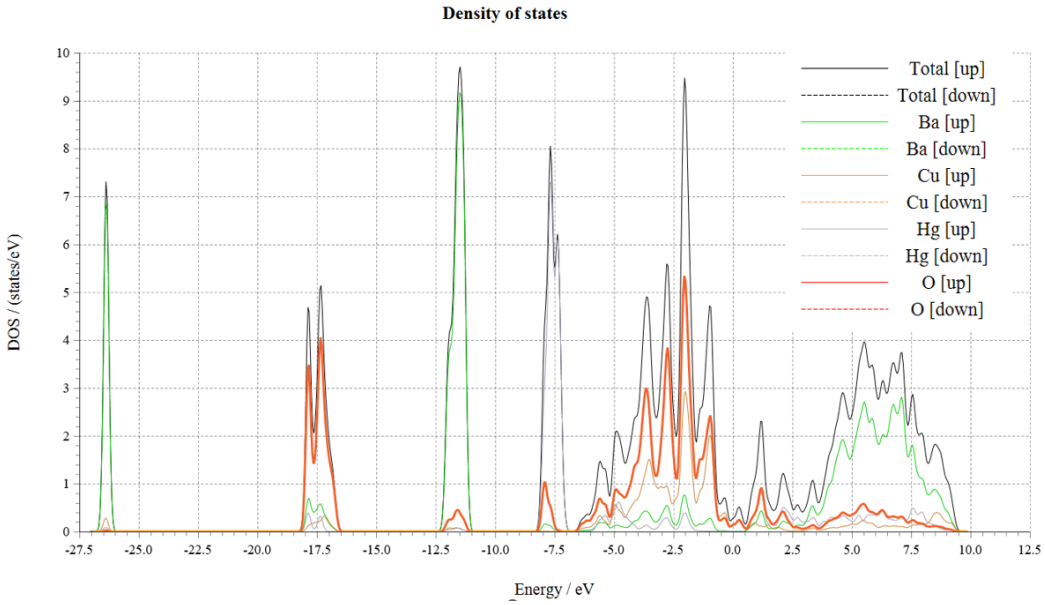


Figure 3. Density of states of $HgBa_2CuO_4$ compound

Furthermore, the analysis highlights the critical influence of structural parameters, especially the Cu-Oapex bond length, on the electronic structure and superconducting properties. The similarities between the electronic features of $HgBa_2CuO_4$ and other cuprates such as La_2CuO_4 further support the generality of the underlying mechanisms driving high-T_c superconductivity in single-layer cuprates[4, 16].

In general, our findings reinforce the pivotal role of Cu–O hybridization, the structural significance of the CuO_2 planes, and the importance of electronic correlations in allowing high temperature superconductivity in Hg-based cuprates. These insights provide a robust theoretical foundation for future studies focused on enhancing superconducting performance through structural engineering, doping, or application of external pressure. Incorporating many-body effects, spin–orbit coupling, and electron–phonon interactions in future work is essential to deepen the understanding of unconventional superconducting mechanisms in these complex materials.

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