

Electronic Properties of $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_x$ Ceramic via Computational Method

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ABSTRACT

The structural and normal-state electronic properties of $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_x$ (Y-247) high-temperature cuprate superconductor were investigated using first-principles density functional theory (DFT). Geometry optimizations were performed based on the experimentally reported orthorhombic structure using the local density approximation (LDA) and the Perdew–Burke–Ernzerhof generalized gradient approximation (GGA-PBE) with ultrasoft pseudopotentials. Both optimized structures preserved the orthorhombic symmetry, while the GGA-PBE results showed slightly better agreement with the selected experimental lattice parameters. Electronic band-structure calculations revealed multiple bands crossing the Fermi level, confirming the metallic character of Y-247 within the conventional DFT framework. The orbital-resolved density of states showed that the electronic states near the Fermi level are predominantly associated with Cu d and O p orbitals, highlighting the important contribution of Cu–O structural units to the electronic behavior of Y-247. Electron-density analysis further elucidated the spatial distribution of charge around these Cu–O units. The calculated energy separations of 1.44 eV and 0.91 eV, respectively correspond to selected electronic transitions above the Fermi level and therefore should not be interpreted as fundamental band gaps or as direct evidence of a superconducting pseudogap. Overall, the present results provide further insight into the structural characteristics and normal-state electronic behavior of Y-247. A more comprehensive description of superconducting pairing and strong Cu $3d$ electron-correlation effects, however, requires theoretical approaches beyond conventional LDA and GGA.

Keywords: Superconductor; computational and simulation; DFT; first principle theory; exchange correlation

INTRODUCTION

Superconductivity is a quantum phenomenon characterized by zero electrical resistance below a critical temperature (T_c). Superconductors are generally classified as either type-I or type-II based on their magnetic response and critical-field behavior. The yttrium–barium–copper–oxide (YBCO) compounds are type-II superconductors that have been extensively studied because of their relatively high critical temperatures and distinctive structural and electronic properties. The crystal structure and superconducting properties of YBCO compounds are strongly influenced by oxygen content and ordering within the crystal lattice, which determine whether the material adopts tetragonal or orthorhombic symmetry. Structurally, $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_x$ (Y-247) can be regarded as an intergrowth of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (Y-123) and $\text{Y}_2\text{Ba}_4\text{Cu}_8\text{O}_y$ (Y-124) structural blocks arranged alternately along the crystallographic c -axis. This structural arrangement produces different Cu–O coordination environments, which can significantly influence the electronic structure of the material [1,2,3].

First-principles calculations based on density functional theory (DFT) provide a powerful approach for investigating the structural and electronic properties of complex materials, including high-temperature superconductors. DFT describes the ground-state properties of a many-electron system in terms of its electron density, thereby avoiding the computational complexity associated with directly solving the many-electron Schrödinger equation [4]. This approach enables the determination of key material properties, including optimized crystal structures, electronic band structures, density of states and charge distributions.

In the present study, first-principles DFT calculations were performed to investigate the structural and electronic properties of Y-247 using the Cambridge Serial Total Energy Package (CASTEP) within the Materials Studio environment. The analysis focuses on structural optimization, electronic band structure, density of states and electron-density distribution to provide further insight into the electronic characteristics of Y-247 and the contribution of its Cu–O structural units.

METHODS

The crystal structure of Y-247 was constructed and analyzed using Materials Studio based on crystallographic parameters obtained from previously reported experimental data, including the lattice constants, space group, crystal system and atomic coordinates. Y-247 was identified as having an orthorhombic crystal structure with the Ammm space group [2]. These crystallographic parameters were used to generate the initial crystal model prior to structural optimization.

Geometry optimization was subsequently performed using the CASTEP module within the density functional theory (DFT) framework. The Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) were employed to evaluate the influence of the exchange–correlation functional on the optimized structural and electronic properties. The optimization process was performed to obtain a stable crystal configuration corresponding to the minimum total energy.

Following structural optimization, the electronic properties of Y-247 were investigated through calculations of the electronic band structure, density of states (DOS)

and electron-density distribution. These calculations were used to examine the electronic states near the Fermi level and to determine the contributions of the constituent atoms to the electronic behavior of the material. The calculated band structure and characteristic energy separation of Y-247 were subsequently compared with those of the $\text{YBa}_2\text{Cu}_3\text{O}_x$ (Y-123) phase to identify similarities and differences in the electronic characteristics of the two YBCO phases.

RESULTS AND DISCUSSION

Crystal Structure Parameters

Based on the crystallographic data reported in Ref. [2], the Y-247 crystal structure was constructed using Materials Studio. The structure of Y-247 along the crystallographic c -axis consists of alternating structural blocks containing single and double Cu–O chains. Structurally, Y-247 can also be regarded as an intergrowth of Y-123 and Y-124 blocks arranged alternately along the c -axis [5]. The Y-247 phase exhibits an orthorhombic crystal structure with reported lattice parameters of $a = 3.85 \text{ \AA}$, $b = 3.86 \text{ \AA}$ and $c = 50.29 \text{ \AA}$. These lattice parameters satisfy the orthorhombic condition, $a \neq b \neq c$. The constructed crystal structure was subsequently subjected to geometry optimization to obtain a stable atomic configuration prior to further electronic-structure calculations.

Table 1. Atomic coordinates of Y-247 crystal structure [2]

Atom	x	y	z
Ba1	1/2	1/2	0.04310
Ba2	1/2	1/2	0.18797
Y	1/2	1/2	0.11545
Cu1	0	0	0
Cu2	0	0	0.08293
Cu3	0	0	0.14831
Cu4	0	0	0.23012
O1	0	0	0.0353
O2	1/2	0	0.0871
O3	0	1/2	0.0865
O4	1/2	0	0.1430
O5	0	1/2	0.1432
O6	0	0	0.1937
O7	0	1/2	0.2328
O8	0	1/2	0
O9	1/2	0	0

Table 2. The orthorhombicity of Y-247 crystal structure from different experimentation

Reference	$a \text{ (\AA)}$	$b \text{ (\AA)}$	$c \text{ (\AA)}$
[2]	3.85	3.86	50.29
[5]	3.86	3.88	50.44
[6]	3.82	3.84	49.21

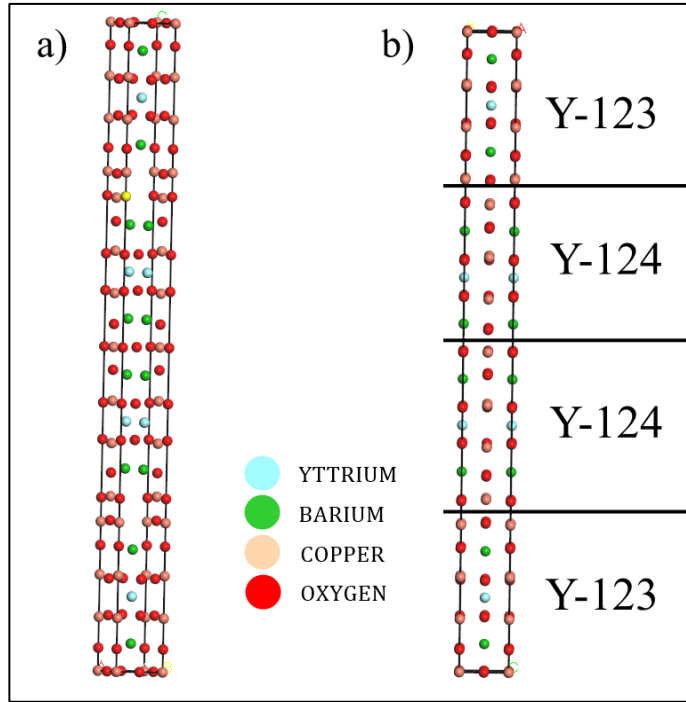


Figure 1. (a) Y-247 Crystal Structure generated in Material Studios using Bordet's atomic position along with the elements labelled and (b) Y-247 crystal structure with Y-123 and Y-124 labelled

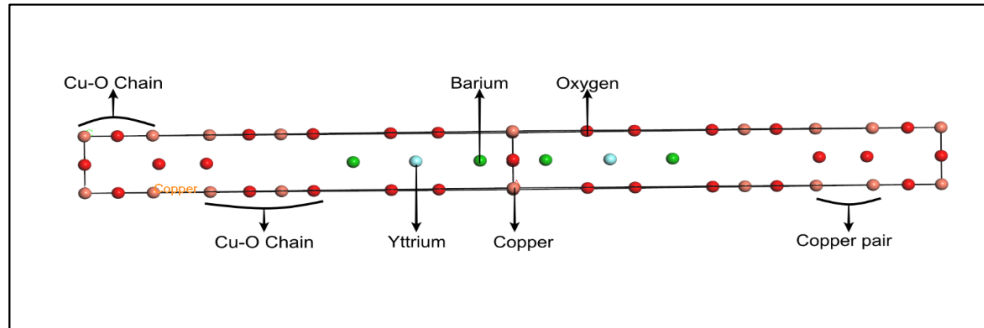


Figure 2. Y-247 crystal structure that have been optimized

Band Structure and Energy Band Gap of Y-247

From Figure 3, it can be seen that the electrons in the valence band (below 0 eV) cross the Fermi level (0 eV). A pseudogap is observed above the Fermi level [7]. The pseudogap plays a role in superconductors by influencing the electronic states and their interactions with electromagnetic radiation [8]. Based on Figure 4, the Local Density Approximation (LDA) produces a smaller energy gap of 0.91 eV compared with the Generalized Gradient Approximation (GGA), which produces an energy gap of 1.44 eV. The accuracy of the calculated energy gap depends on the choice of exchange-correlation functional. According to Jacob's ladder of DFT, as shown in Figure 5, LDA is located at

the lower level of the ladder and generally provides lower chemical accuracy compared with GGA. Basically, GGA is an improvement over the LDA exchange-correlation functional. LDA tends to suffer from an over binding problem, whereas GGA reduces this effect [9]. From Table 3, LDA underestimates the lattice parameters of the Y-247 structure, while GGA overestimates the lattice parameters. The use of GGA provides a more suitable basis for calculating other properties, such as the energy gap, phonon properties and density of states, compared with LDA [10]. Overall, GGA shows better agreement with the experimental structural parameters compared with LDA; therefore, GGA was selected for the subsequent calculations.

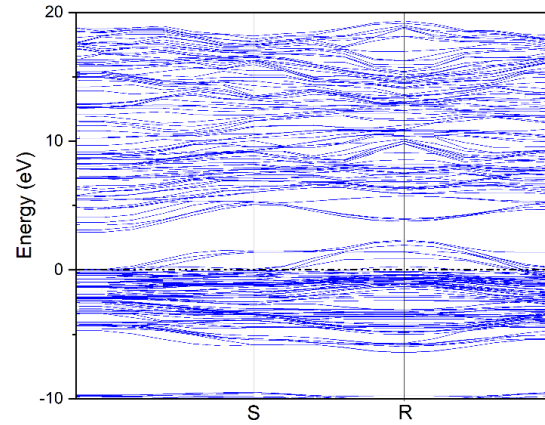


Figure 3. The electronic band structure of Y-247 with GGA exchange correlation

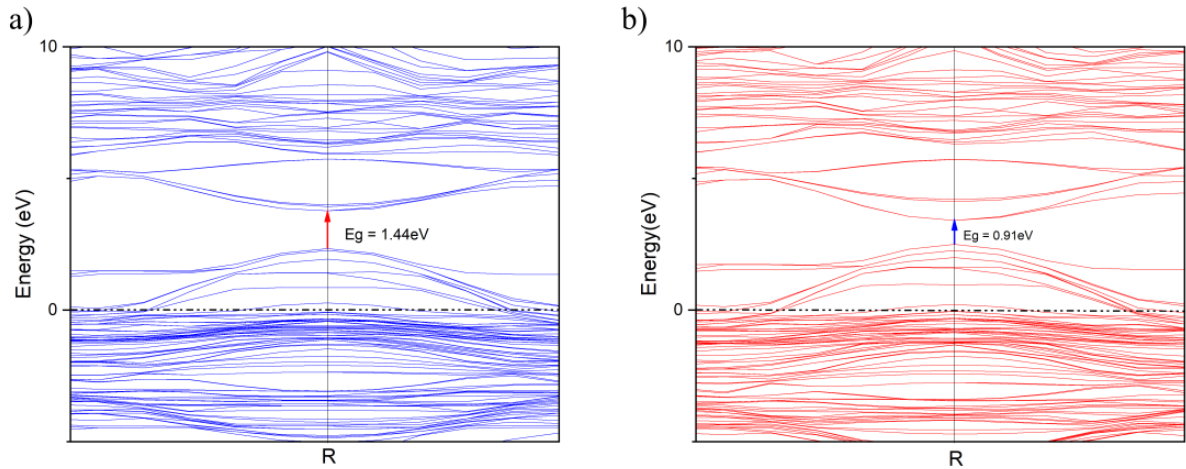


Figure 4. (a) Band structure with pseudogap of Y-247 with GGA exchange correlation and (b) band structure with pseudogap of Y-247 with LDA correlation

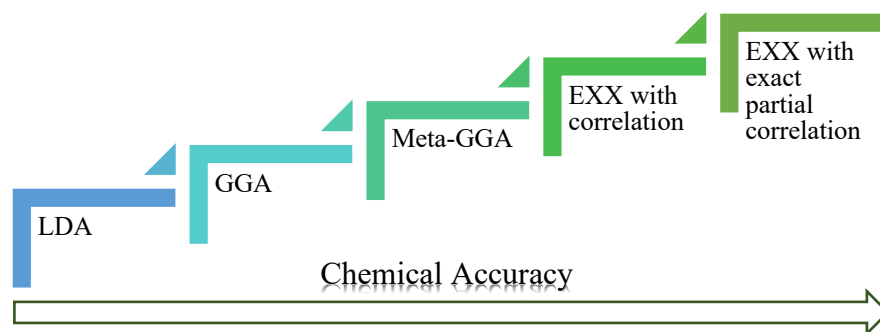


Figure 5. Jacob's Ladder for DFT accuracy. The more accurate the chemical, the time taken for calculation is also longer [9]

Table 3. Lattice parameters and volume of Y-247 crystal structure optimized using different exchange-correlation with its percentage error

	Lattice Parameters			Volume
	a (Å)	b (Å)	c (Å)	V (Å ³)
Experimental [2]	3.85	3.86	50.29	747.3597
LDA CA-PZ	3.817913	3.82638	48.70023	711.4838
	(-0.83%)	(-0.87%)	(-3.16%)	(-4.81%)
GGA-PBE	3.923868	3.91693	50.70356	779.2892
	(+1.92%)	(+1.47%)	(+0.82%)	(+4.27%)

Overestimate (+) underestimate (-)

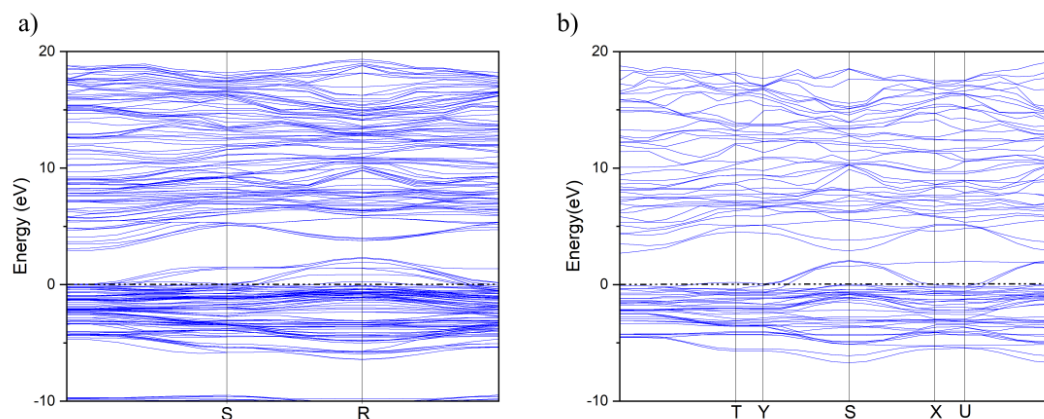


Figure 6. (a) Electronic band structure of Y-247 phase and (b) electronic band structure of Y-123 phase

Figure 6 shows that the Y-247 phase exhibits electronic characteristics similar to those of the Y-123 phase, with several valence-band states extending across the Fermi level. However, the two structures exhibit different energy separations between the selected valence- and conduction-band regions. The calculated energy separation for Y-247 is

approximately 1.44 eV, whereas that of Y-123 is approximately 0.83 eV. The band structure of Y-247 also appears to contain a greater number of electronic states than Y-123, which may be attributed to the larger number of atoms and the greater structural complexity of the Y-247 unit cell. The difference in the calculated energy separation between Y-247 and Y-123 may arise from several factors, particularly differences in crystal structure, Cu–O coordination, oxygen arrangement and the resulting electronic interactions. These structural differences may also contribute to their distinct superconducting properties.

Experimentally, Y-247 has been reported to exhibit a critical temperature, T_c , of approximately 40 K, whereas Y-123 typically exhibits a higher T_c of approximately 90 K [2,11,12]. The electronic states near the Fermi level are particularly important because they are closely associated with the charge-carrier behavior and superconducting properties of cuprate materials. In high-temperature cuprate superconductors, a suppression of the electronic density of states near the Fermi level may be associated with the pseudogap phenomenon. Unlike the superconducting energy gap, the pseudogap can persist above T_c in the normal state and remains an important subject of investigation in understanding the electronic behavior and superconducting mechanism of YBCO-based materials [1,12–14]. Therefore, the differences observed between the calculated electronic structures of Y-247 and Y-123 may provide useful insight into how their structural characteristics influence the electronic states relevant to superconductivity.

Density of States and Electron Density Differences

The density of states (DOS) was calculated to investigate the atomic orbital contributions and hybridization between Cu 3*d* and O 2*p* states in the $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_x$ superconductor using density functional theory (DFT) within the GGA exchange–correlation approximation. As shown in Figure 7, the *p* and *d* states exhibit the most significant contributions to the electronic density of states. The maximum DOS values for the *p*, *d* and *s* states are approximately 30.2, 23.4 and 21.2 electrons/eV, respectively. In addition, the *p* and *d* states are distributed close to the Fermi level, indicating their important contribution to the electronic properties of Y-247. In particular, the O 2*p* and Cu 3*d* orbitals contribute substantially to the electronic states near the Fermi level, reflecting strong Cu–O orbital hybridization. The Cu 3*d* orbitals are also associated with hole states arising from the Cu–O bonding network [8].

These results indicate that the Cu–O structural units in Y-247 play an important role in determining the electronic behavior associated with its superconducting properties. Figure 8 presents the calculated electron-density distribution, in which the reddish regions represent areas of higher electron density, whereas the blue regions correspond to lower electron density. A relatively high electron concentration is observed along the Cu–O chains, indicating significant electronic interaction between Cu and O atoms. The enhanced electron density around these Cu–O units suggests strong bonding interactions within the Cu–O network [15]. This observation is consistent with the DOS analysis, further emphasizing the important role of the Cu–O chains in the electronic structure of the Y-247 superconductor.

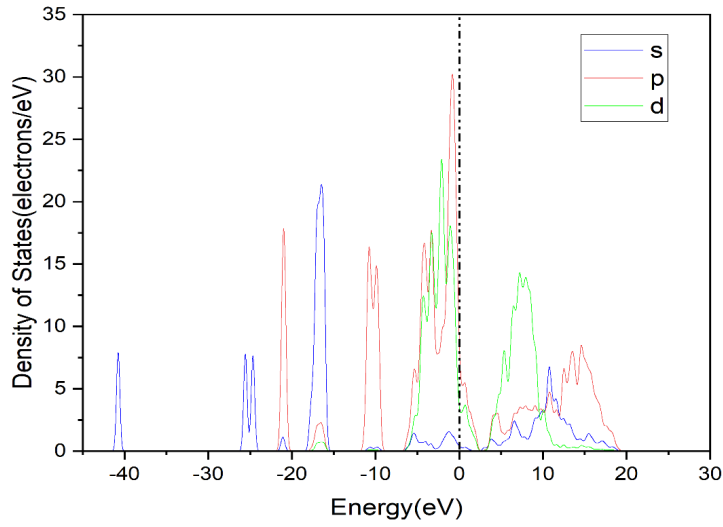


Figure 7. Density of states in Y-247 crystal structure

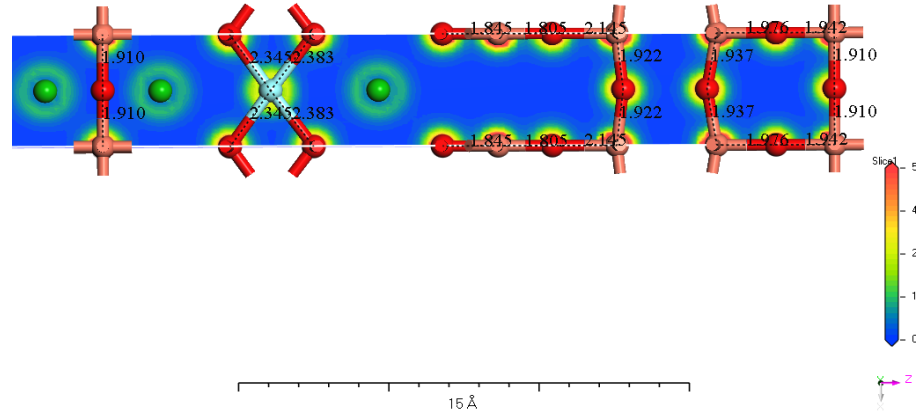


Figure 8. Cross section of optimized Y-247 crystal structure showing the electron density differences

CONCLUSIONS

The crystal structure of $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_x$ was successfully constructed and confirmed to consist of alternating Y-123- and Y-124-type structural blocks along the crystallographic direction. The calculated electronic band structure shows that several electronic states cross the Fermi level, indicating metallic behavior within the conventional DFT framework. An energy separation above the Fermi level was also observed for both Y-247 and Y-123, with calculated values of 1.44 eV and 0.83 eV, respectively. The difference between these values may be associated with differences in their crystal structures, atomic arrangements and resulting electronic environments. Comparison of the optimized lattice parameters obtained using the LDA and GGA exchange–correlation

functionals indicates that GGA provides better agreement with the selected experimental structural parameters. Therefore, the GGA approach was considered more appropriate for the subsequent analysis of the electronic properties of Y-247. The density-of-states analysis demonstrates that the Cu–O structural units play an important role in determining the electronic behavior of Y-247. Cu $3d$ and O $2p$ states contribute significantly near the Fermi level, indicating strong Cu–O orbital hybridization. The electron-density distribution further shows a relatively high electron concentration along the Cu–O chains, emphasizing the importance of these structural units in governing the electronic properties of the material. These results highlight the close relationship between the crystal structure, Cu–O electronic states and the characteristic electronic behavior of the Y-247 cuprate system.

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AUTHOR CONTRIBUTIONS

The manuscript was written through the contributions of all authors. SAS, NHH and MAH designed and organized this work. WAWR and MFO contributed to editing. MAH and SAS drafted the main ideas of the work. SAS, NHH and AH provided supervision. AH conducted the final review of the manuscript.

CONFLICT OF INTEREST

The authors declare no competing interests.

DATA AVAILABILITY

The simulation code and underlying datasets supporting this study are available from the corresponding author upon reasonable request.

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