

# The role of carbon (C) atoms on YBCO superconductor: DFT study

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In this study, we investigate the electronic properties of C-substituted YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> systems. In our study we use the full potential linearized augmented plane wave method within the density functional theory (DFT). We treat the exchange correlation energy using generalized gradient approach (GGA), Wu-Cohen GGA and local density approximation (LDA). The YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> has orthorhombic crystal system whose space group is *Pmmm* (47). The unit cell of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> contains 13 atoms. We have found that the band gap energies of all crystal systems do not depend linearly on the carbon concentration. In addition for YBa<sub>2</sub>Cu<sub>3</sub>O<sub>4</sub>C<sub>3</sub> crystal system, we show that the valence band and conduction band are overlapping. It means that, YBa<sub>2</sub>Cu<sub>3</sub>O<sub>4</sub>C<sub>3</sub> has metallic properties. The calculated electronic charge densities reveal that carbon atoms are bonded to copper atoms with strong covalent bonds. These bonds are similar to the bonds between copper and oxygen atoms. This theoretical work motivates further future studies.

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**Keywords:** Superconductors, DFT, FP-LAPW, Electronic properties

## 1. Introduction

High  $T_c$  superconductivity with transition temperatures above liquid nitrogen temperatures has attracted great attention of researchers. The REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> (RE-123) superconductors are useful for applications at the boiling point of liquid nitrogen [1]. It is considered that oxygen content in the CuO chain manages hole concentration in the CuO<sub>2</sub> planes [2-3]. Copper pairs are created in the CuO<sub>2</sub> planes. Superconductivity comes up in the CuO<sub>2</sub> layers of RE-123 superconductors. The YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> superconductor, as the first high  $T_c$  superconductor above 77 K (liquid nitrogen temperature), has been discovered in 1987 [4]. The transition temperature of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> superconductor depends on the oxygen content in the CuO chains. The transition temperature  $T_c$  decreases with decreasing oxygen content [5]. Superconductivity has been investigated experimentally and theoretically by many researchers [6-9].

Currently researchers are working on producing a higher critical temperature superconducting materials. It was reported that at temperature 155K or more superconductivity is possible in the Y–Ba–Cu–O–F system [10]. However, if it can be synthesized, this system is extremely unstable. Because of this, the nature of the electron states in high  $T_c$  superconductor plays a key role in understanding the properties and mechanism of superconductivity.

In this paper, we report the results of electronic properties of C-substituted YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> crystal. The electronic properties of C-substituted YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> systems have been studied using the full potential linearized augmented plane wave (FP-LAPW) method [11] within

the density functional theory (DFT) [12]. Section 2 of this paper deals with the computational method used in this study. Results and their discussion are presented in Section 3. Finally, a conclusion of the work is given in Section 4. The results of this work are hoped to be a guide and reference for future studies.

## 2. Computational details

We investigate the electronic properties of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub>C<sub>x</sub> ( $x=1, 2, 3$ ) systems using the WIEN2k [13-15] code within the framework of DFT. We treat the exchange correlation energy using generalized gradient approach (GGA) based on Perdew et al. [16], Wu-Cohen GGA [17] and local density approximation (LDA) [18]. In our study we take  $R_{MT}K_{MAX}$  parameter equal to 8.0. Here  $R_{MT}$  is the smallest atomic sphere radius in the unit cell and  $K_{MAX}$  is the magnitude of the largest K vector. The selected muffin-tin radii (a.u.) are 2.28, 2.50, 1.82, 1.57 and 1.55 for Y, Ba, Cu, O and C atoms respectively. We take a mesh of 100 k-points for the Brillouin zone integrations in the corresponding irreducible wedge. In addition, Brillouin zone integrations are performed on 6x6x2 k-points meshes for all compositions. Regarding Fourier expansion of charge density, magnitude of the largest vectors,  $G_{MAX}$  is equal to 12 for all systems. The cut-off energy for separating core from valence states is set to -6 Ry.

In order to replace C atoms with O atoms, the crystal structures are created using the P1 space group and supercell. The crystal structures of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub>C<sub>x</sub> systems are shown in Fig. 1. Atomic positions are given in Table 1.

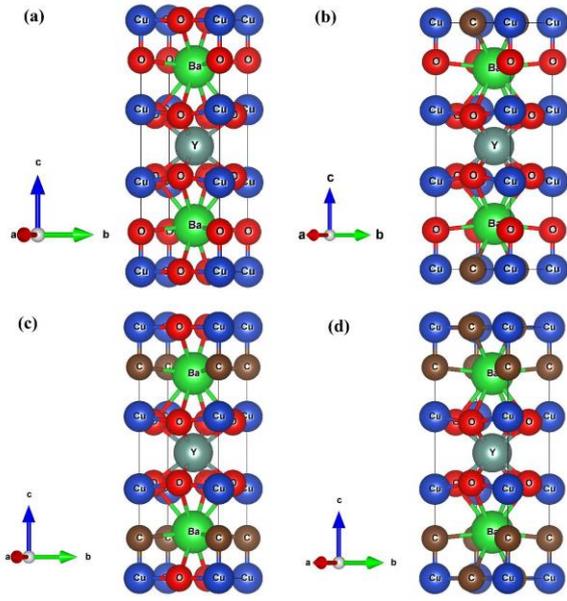


Fig. 1. The crystal structure of (a)  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (b)  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$  (c)  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$  (d)  $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$

Table 1. Atomic Positions of  $\text{YBa}_2\text{Cu}_3\text{O}_7$

Atom	x	y	z
Y	0.5	0.5	0.5
Ba	0.5	0.5	0.1843
Cu	0	0	0
Cu	0	0	0.3556
O	0	0.5	0
O	0.5	0	0.3779
O	0	0.5	0.379
O	0	0	0.159

### 3. Results and discussion

The  $\text{YBa}_2\text{Cu}_3\text{O}_7$  superconductor has orthorhombic crystal system whose space group is  $Pmmm$  (47). The unit cell of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  contain 13 atoms. We study the electronic properties of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ ,  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$ ,  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$  and  $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$  crystal systems. We calculate the band structure, the electronic total density of states (TDOS), partial density of states (PDOS) and electron charge density.

#### 3.1. The electronic properties of $\text{YBa}_2\text{Cu}_3\text{O}_7$

We start with the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  crystal structure. By using GGA, LDA and Wu-Cohen exchange potential the band structures of crystal systems are shown along high symmetry points. All methods, GGA, LDA and Wu-Cohen, show same behavior except for band gap energies

(Fig. 2). In all methods, the top of the valence band and bottom of the conduction band are positioned at the same symmetry point M for direct band gap. In addition, for indirect band gap, the top of the valence band is positioned at the symmetry point M, whereas the bottom of the conduction band is positioned at the symmetry point  $\Gamma$ . The band gap energies calculated using GGA, LDA and Wu-Cohen methods are given in Table 2. The other theoretical values of band gap energies are 0.74 eV [5], 1.09 eV [19], 1.06 eV [20] for indirect gap and 0.91 eV [5], 1.93 eV [19], 1.54 eV [20] for direct gap. The GGA method is in a good agreement with the other theoretical result.

The electronic density of states is defined as the number of the allowed states per unit energy. In Fig. 3, we illustrate the total and partial density of states of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  crystal system using GGA method. As can be seen from the Fig. 3 that TDOS exhibits very similar behavior to that of the band structure. From the figure we see that the valence band is divided into two sub-bands. The low energy sub-band extends from -11.29 eV to -10.07 eV. The p-states of Ba atoms mainly create these bands. The high energy sub-band extends from -7.16 eV to 1.92 eV. The d-states of Cu atoms and the p-states of O atoms mainly create these bands. This results show that the sub-band located between -7.16 eV to 1.92 eV is mainly dominated by Cu 3d-states and considerably mixed with O 2p-states indicating that there is a strong covalent bond between Cu and O atoms. Our results are in a good agreement with former studies in refs. [21-22]. The peaks in the conduction band between 2.69 eV and 13.31 eV mainly result from d states of Y and Ba atoms.

The electron charge density distribution is a common and well defined methodology to investigate the bonding nature and interactions between atoms. Therefore, we investigate the electron charge densities in the (020), (010) and Cu-O crystallographic plane which include all considered atoms. In Fig. 4 we show the contour plots of the electron charge densities distribution for  $\text{YBa}_2\text{Cu}_3\text{O}_7$ . The intensity of the charge density is shown in thermo-scale in which the red color represents the low charge density and the pink color represents the maximum intensity. From the figure we observe that the contour lines between Cu and O atoms are not spherical. The contours are deformed indicating that chemical bonds between Cu and O atoms inside the chains are strong covalent bonds. From (020) plane the electron distribution around Y and Ba atoms in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  is almost spherical indicating that the ionic bond is relatively more frequent than covalent bonds.

The case of ionicity is interesting since it can be related to the properties of the electron charge density. The ionicity, directly associated with the characteristics of the chemical bond, provides us with a means for explaining and classifying the properties of the systems. It is well known that the ionicity character is highly dependent on the total valence charge density. We calculate the ionicity parameter for all crystals adopting the empirical formula used in ref. [23]. In this empirical formula, the ionicity parameter is defined as,

$$f_i = \frac{1}{2} \left[ 1 - \cos \left( \pi \frac{E_{AS}}{E_{VB}} \right) \right] \quad (1)$$

where  $E_{AS}$  is the antisymmetric gap between the two lowest valence bands, and  $E_{VB}$  is the total valence band width. The calculated ionicity factors of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  are

given in Table 3 for GGA, LDA and Wu-Cohen methods. The ionicity parameters are 0.15, 0.16 and 0.17 for LDA, Wu-Cohen and GGA methods respectively. It means that the covalent bond is stronger than the ionic bond in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  crystal system.

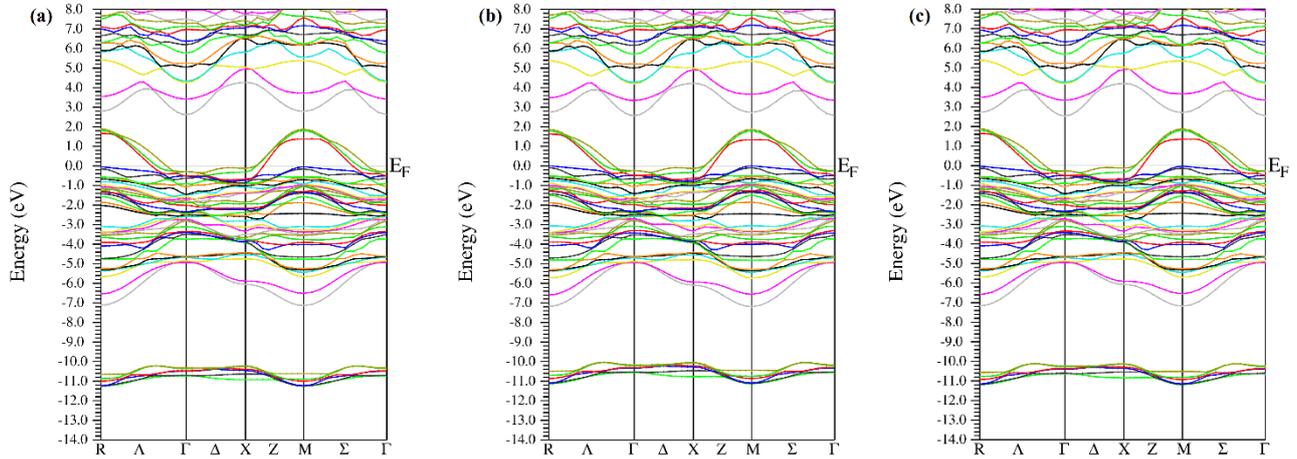


Fig. 2. The band structure of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , (a) GGA method, (b) LDA method and (c) Wu-Cohen method

Table 2. The obtained direct band gap ( $E_g$ ) and indirect band gap ( $E'_g$ ) for  $\text{YBa}_2\text{Cu}_3\text{O}_7$

Crystal System	GGA		LDA		Wu-Cohen	
	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)
$\text{YBa}_2\text{Cu}_3\text{O}_7$	0.90	0.74	0.87	0.71	0.83	0.66

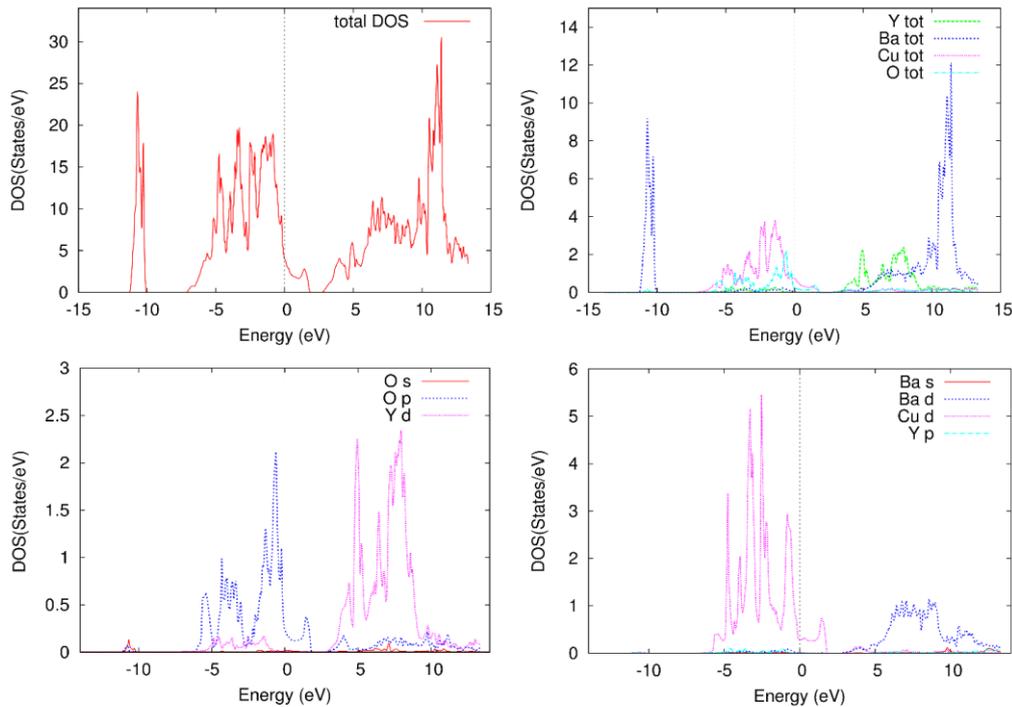


Fig. 3. Total and partial density of states of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  with GGA method

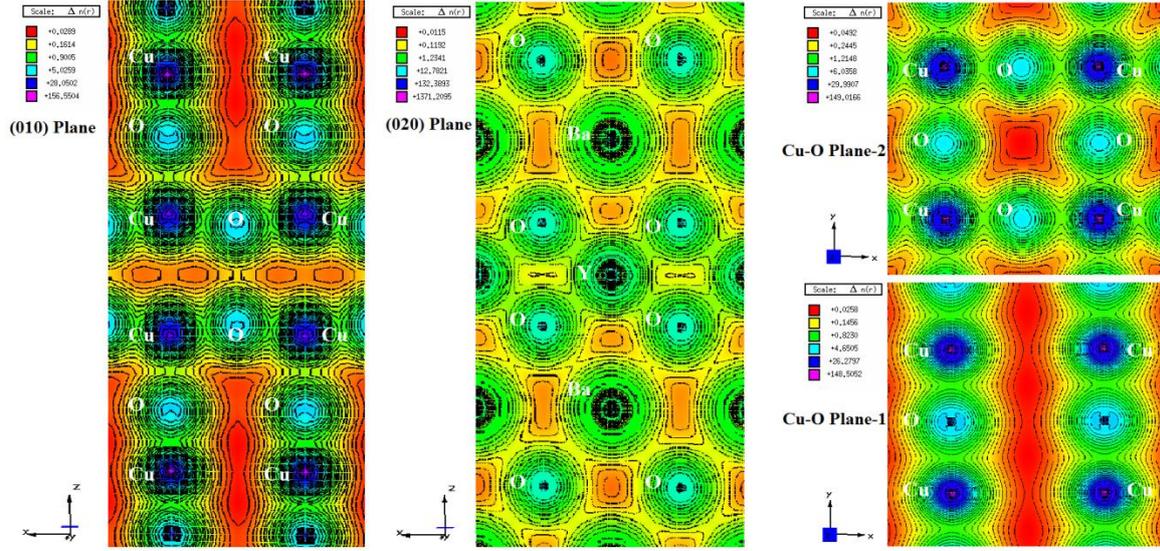


Fig. 4. Electron charge density contour plot for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  with GGA method

Table 3. The antisymmetric gap  $E_{AS}$  (eV), the total valance band width  $E_{VB}$  (eV) and ionicity factors ( $f_i$ ) for  $\text{YBa}_2\text{Cu}_3\text{O}_7$

Crystal System	GGA			LDA			Wu-Cohen		
	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$
$\text{YBa}_2\text{Cu}_3\text{O}_7$	3.10	11.26	0.17	2.86	11.14	0.15	2.94	11.20	0.16

### 3.2. The electronic properties of $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$

For a crystal system  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$  we remove one O atom from the point (0, 0.5, 0) and replace it by one C atom. The resultant band structures by using GGA, LDA and Wu-Cohen exchange potential are shown in Fig. 5 which exhibit same behavior except for band gap energies. The top of the valence band and the bottom of the conduction band are positioned at the same symmetry point M for direct band gap. On the other hand we find that for the indirect band gap, the top of the valence band is positioned at the symmetry point M and the bottom of the conduction band is positioned at symmetry point  $\Gamma$ . The replacement of O with C atom causes the decline of direct and indirect band gap energies. The decreasing of the band gap energies result from the p-states of C atom in the conduction band. The band gap energies calculated using GGA, LDA and Wu-Cohen methods are presented in Table 4.

In Fig. 6 we illustrate the total and partial density of states of  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$  crystal system using GGA method. As can be seen from the figure that TDOS exhibits very

similar behavior to that of the band structure. The valence band consists of three sub-bands. The low energy sub-band is positioned between -12.41 eV to -10.73 eV. This sub-band results from the p-states of Ba atoms and the s-states of C atoms. The s-states of C atoms mainly create the intermediate band between -9.85 eV and -8.63 eV. The p-states of Ba atoms and d-states of Cu atoms have a weak effect in this band. The high energy sub-band occurs between -7.32 eV to 2.03 eV. The d-states of Cu atoms, the p-states of O atoms and p-states of C atoms mainly create this band while the d-states of Y and Ba atoms rarely appear in this band. This results show that the sub-band located between -7.32 eV and 2.03 eV is mainly dominated by Cu 3d-states and is considerably mixed with O 2p-states indicating that there is a strong covalent bond between Cu and O atoms. Likewise, O 2-p states is considerably mixed C 2p-states indicating that there is a strong covalent bond between C and O atoms. In addition, the peaks in conduction band between 2.03 eV and 13.33 eV mainly result from d states of Y and Ba atoms. The effect of C atoms in the conduction band is very small.

Table 4. The obtained direct band gap ( $E_g$ ) and indirect band gap ( $E'_g$ ) for  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$

Crystal System	GGA		LDA		Wu-Cohen	
	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)
$\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$	0.20	0.53	0.17	0.48	0.13	0.45

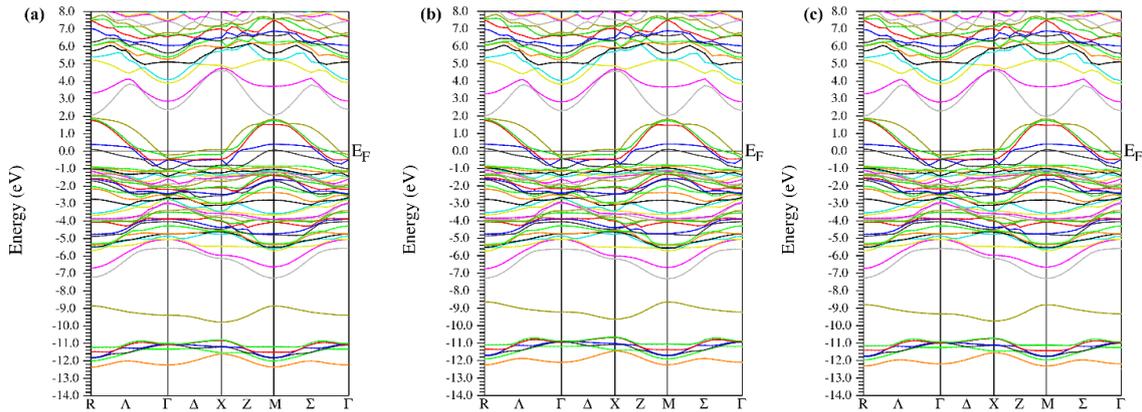


Fig. 5. The band structure of  $YBa_2Cu_3O_6C_1$ , (a) GGA method, (b) LDA method and (c) Wu-Cohen method

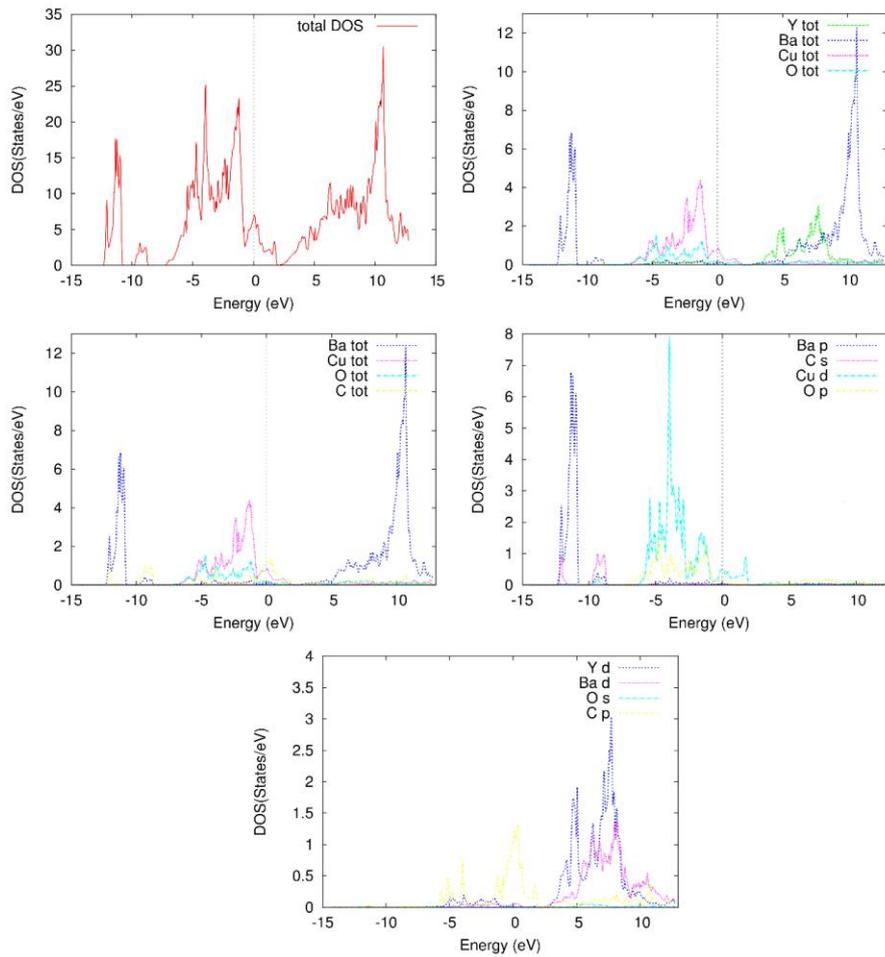


Fig. 6. Total and partial density of states of  $YBa_2Cu_3O_6C_1$  with GGA method

For the crystal system of  $YBa_2Cu_3O_6C_1$ , we calculate the electron charge densities in the (020), (100), Cu-O and Cu-C crystallographic plane which includes all considered atoms. The contour plots of the electron charge densities distribution for  $YBa_2Cu_3O_6C_1$  are shown in Fig. 7. The low and high charge density correspond to red color and pink color respectively. The contour lines between Cu and C atoms are not spherical. It means that there is strong

covalent bond between Cu and C atoms. From (020) plane the electron distribution around Y and Ba atoms in  $YBa_2Cu_3O_6C_1$  is almost spherical indicating that the bond is ionic which is relatively more frequent than covalent bonds. The ionicity parameter calculated for GGA, LDA and Wu-Cohen method are listed in Table 5. We see from the Table that, the covalent bond is dominant in  $YBa_2Cu_3O_6C_1$  crystal system.

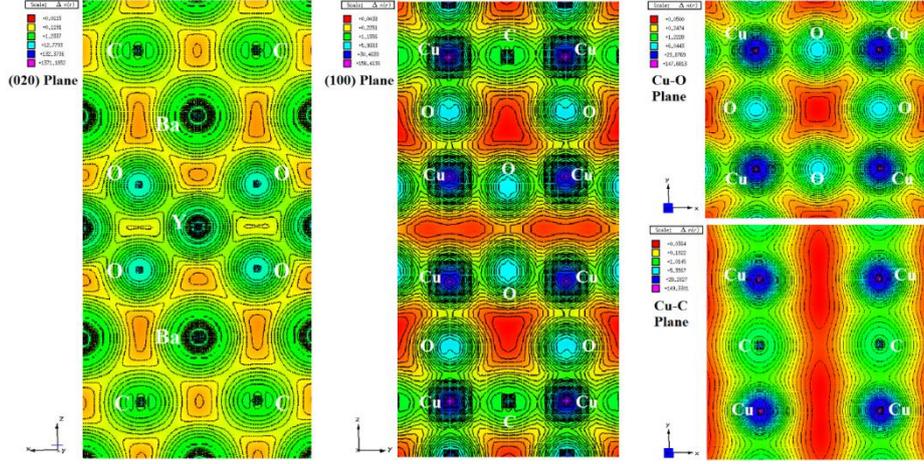


Fig. 7. Electron charge density contour plot for  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$  with GGA method

Table 5. The antisymmetric gap  $E_{AS}$  (eV), the total valance band width  $E_{VB}$  (eV) and ionicity factors ( $f_i$ ) for  $\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$

Crystal System	GGA			LDA			Wu-Cohen		
	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$
$\text{YBa}_2\text{Cu}_3\text{O}_6\text{C}_1$	3.57	10.83	0.19	3.34	12.25	0.17	3.40	12.33	0.18

### 3.3. The electronic properties of $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$

We turn to another crystal system  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$ . This crystal can be produced from the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  crystal system upon replacing two O atoms from the points (0, 0, 0.1590) and (0, 0, 0.8410) with two C atoms. The band structures are presented in Fig. 8. The band structures show the same characteristic properties for all methods. However, the direct and indirect band gap energies vary according to the using potential. The band gap energies calculated using GGA, LDA and Wu-Cohen methods are given in Table 6. As can be seen from Fig. 8 that the band gap energy is increased for direct and indirect band gaps. This can be explained due to the effect of the two C atoms. Explicitly, the p-states of C atom in the conduction band and the s and p states in the valence band cause the increase of the band gap energy.

The total and partial density of states of  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$  crystal system using GGA method are shown in Fig. 9. Clearly from Fig. 9 that, the valance band is composed of three sub-bands, which are low energy sub-band, intermediate sub-band and high energy sub-band. The p-

states of Ba atoms and the s-states of C atoms mainly create low energy sub-bands between -13.19 eV and -10.87 eV. The s-states of C atoms are influential in the formation of the intermediate band. In addition the p-states of Ba atoms and d-states of Cu atoms are rarely seen in this band. The energy range of the intermediate band is between -10.43 eV and -7.41 eV. The d-states of Cu atoms, the p-states of O atoms and the p-states of C atoms mainly create the high energy sub-band between -7.28 eV to 2.18 eV. It should be noted that the high energy sub-band are weakly affected by d-states of Y and Ba atoms. The PDOS results indicate that Cu 3d-states are considerably mixed with O 2p-states. Hence, we deduce that there is a strong covalent bond between Cu and O atoms. Likewise, there is a strong covalent bond between 2p-states of O and 2p-states of C atoms. The d states of Y and Ba atoms dominantly create the conduction band between 2.03 eV and 13.55 eV. The p-states of C atoms rarely affect the formation of the conduction band.

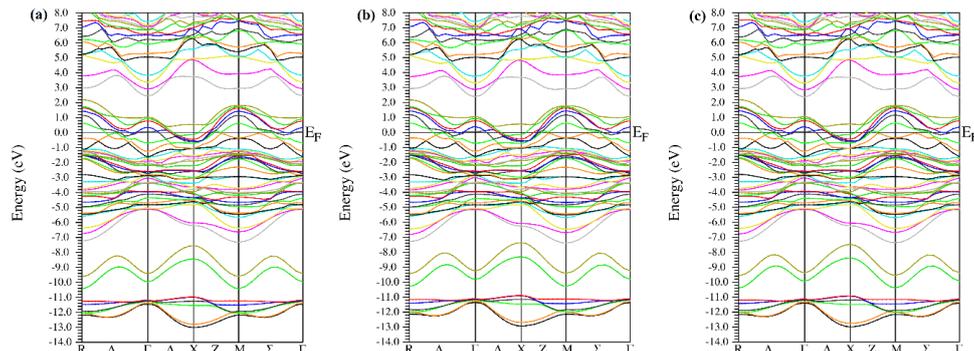


Fig. 8. The band structure of  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$ , (a) GGA method, (b) LDA method and (c) Wu-Cohen method

Table 6. The obtained direct band gap ( $E_g$ ) and indirect band gap ( $E'_g$ ) for  $YBa_2Cu_3O_5C_2$ 

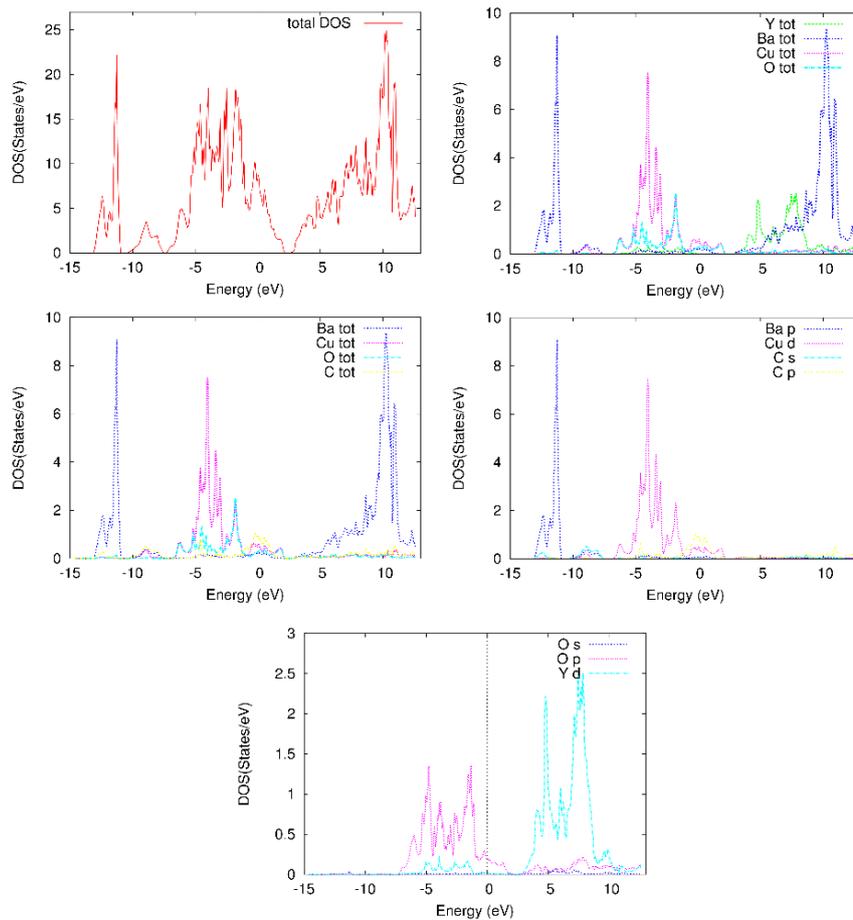
Crystal System	GGA		LDA		Wu-Cohen	
	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)	$E_g$ (eV)	$E'_g$ (eV)
$YBa_2Cu_3O_5C_2$	1.12	0.64	1.10	0.57	1.09	0.58

The electron charge density calculations are given in Fig. 10. In the figure we note that the contour lines between Cu and O atoms are not spherical. The deformation of the contours indicate that the chemical bonds between Cu and O atoms inside the chains are strong covalent bond. A similar deformation can be seen clearly between Cu and C atoms. The type of the bonds between Cu and C atoms are covalent. The electron distribution around Y and Ba atoms is almost spherical

which shows that the bonds between these atoms are ionic bonds. In Table 7 we list the calculated ionicity factors, using Eq. 1, corresponding to GGA, LDA and Wu-Cohen methods. The ionicity parameters for  $YBa_2Cu_3O_5C_2$  are 0.17, 0.17 and 0.18 for LDA, Wu-Cohen and GGA methods respectively. According to these results we conclude that the covalent bonds in  $YBa_2Cu_3O_5C_2$  crystal system are dominant than the ionic bonds.

Table 7. The antisymmetric gap  $E_{AS}$  (eV), the total valance band width  $E_{VB}$  (eV) and ionicity factors ( $f_i$ ) for  $YBa_2Cu_3O_5C_2$ 

Crystal System	GGA			LDA			Wu-Cohen		
	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$
$YBa_2Cu_3O_5C_2$	3.66	13.04	0.18	3.52	12.93	0.17	3.54	12.99	0.17

Fig. 9. Total and partial density of states of  $YBa_2Cu_3O_5C_2$  with GGA method

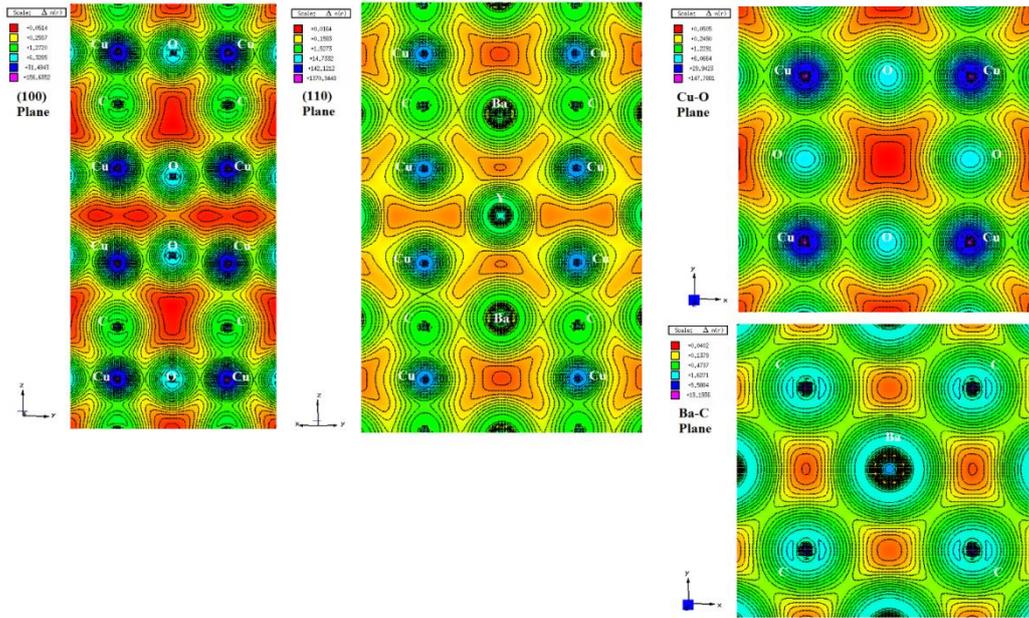


Fig. 10. Electron charge density contour plot for  $\text{YBa}_2\text{Cu}_3\text{O}_5\text{C}_2$  with GGA method

### 3.4. The electronic properties of $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$

Finally we consider the crystal system  $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$  which can be obtained from the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  crystal system upon replacing three O atoms from the points (0, 0, 0.1590), (0, 0, 0.8410) and (0, 0.5, 0) with three C atoms. The obtained band structures using GGA, LDA and Wu-Cohen exchange potential are shown Fig. 11. For direct band gap, we see from the figure that, for all methods, the top of the valence band and the bottom of the conduction band are overlapping at the same symmetry point M. Thus, this crystal system shows metallic properties. As can be seen from the figure that the band gap energy disappears for both direct and indirect band gaps. This can be understood as a result of replacing O with C atoms. The p-states of C atom in the conduction band and the s and p states in the valence band affect the band gap structures.

We discuss now the total and partial density of states of  $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$  crystal system using GGA method. They are plotted in Fig. 12. As can be seen from the figure that

the valence band has three sub-bands. The low energy sub-band is occurred between -13.06 eV to -10.78 eV. This band results from the p-states of Ba atoms and the s-states of C atoms. The s-states of C atoms mainly create the intermediate band between -10.56 eV and -7.52 eV. The p-states of Ba and d-states of Cu atoms rarely affect the formation of this band. The high energy sub-band extends from -7.30 eV to 2.25 eV. The d-states of Cu atoms, the p-states of O atoms and p-states of C atoms dominantly create this band. The contribution of the d-states of Y and Ba atoms to the formation of this band is small. The Cu 3d-states are considerably mixed with O 2p-states indicating that there is a strong covalent bond between Cu and O atoms. Likewise, O 2-p states are mixed with C 2p-states showing that there is a strong covalent bond between C and O atoms. In addition, the peaks in the conduction band between 2.25 eV and 12.45 eV mainly result from the d states of Y and Ba atoms. We note also that the p-states of C atoms rarely affect the formation of conduction band as in some other crystals.

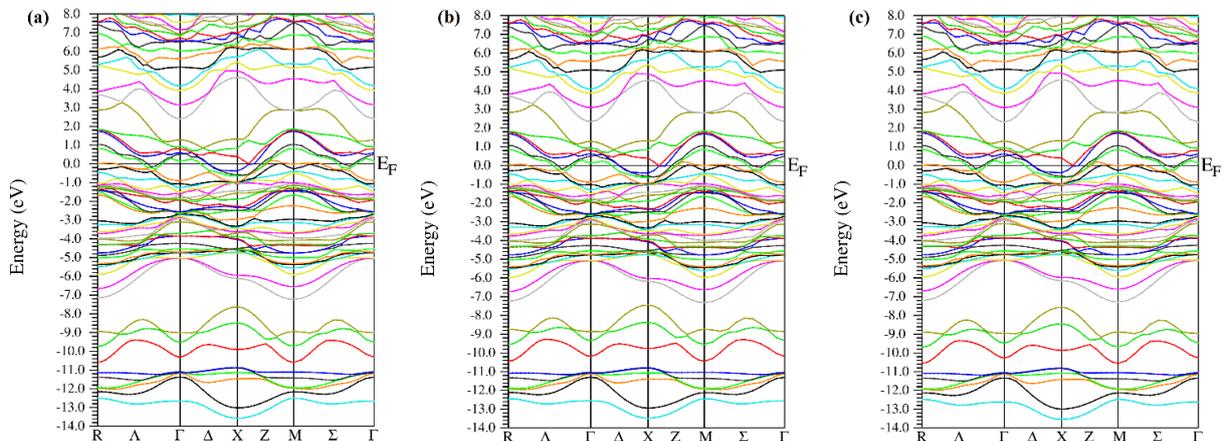


Fig. 11. The band structure of  $\text{YBa}_2\text{Cu}_3\text{O}_4\text{C}_3$ , (a) GGA method, (b) LDA method and (c) Wu-Cohen method

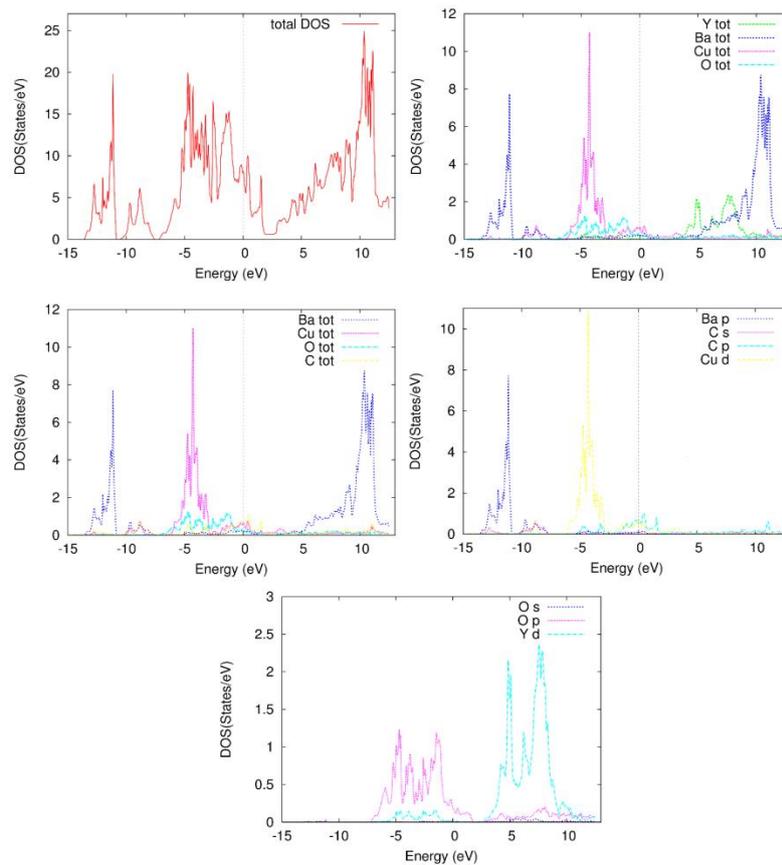


Fig. 12. Total and partial density of states of  $YBa_2Cu_3O_4C_3$  with GGA method

The plots of the electron charge densities are shown in Fig. 13 for (020), (100), Cu-O and Cu-C crystallographic planes. The plots show that the contour lines between Cu and O atoms are not spherical. It means that there is a deformation between Cu and O atoms inside the chains. This deformation implies that strong covalent bonds exist between Cu and O atoms. Moreover, similar features can be seen between Cu and C atoms indicating that there are also strong covalent bonds between Cu and C atoms. The electron distribution around Y and Ba atoms in  $YBa_2Cu_3O_4C_3$  is almost spherical. Because of this, the

ionic bond is relatively more frequent than the covalent bonds between the Y and Ba atoms. The calculated ionicity parameter using Eq. 1 shows that the covalent bond characteristic is more effective than the ionic bond characteristic in  $YBa_2Cu_3O_4C_3$  crystal system. The calculated ionicity factors are presented in Table 8 for GGA, LDA and Wu-Cohen methods. For all exchange potential the ionicity parameters are almost equal for  $YBa_2Cu_3O_4C_3$ . The ionicity parameters are 0.16, 0.16 and 0.17 for LDA, Wu-Cohen and GGA methods respectively.

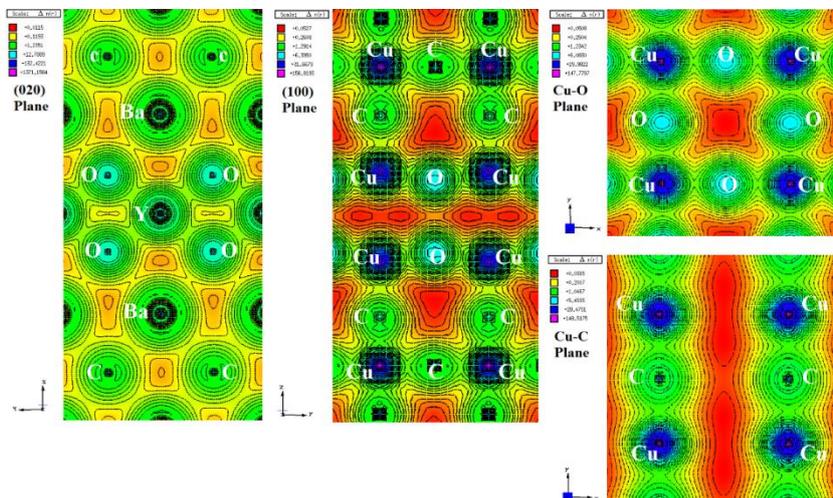


Fig. 13. Electron charge density contour plot for  $YBa_2Cu_3O_4C_3$  with GGA method

Table 8. The antisymmetric gap  $E_{AS}$  (eV), the total valance band width  $E_{VB}$  (eV) and ionicity factors ( $f_i$ ) for  $YBa_2Cu_3O_4C_3$ 

Crystal System	GGA			LDA			Wu-Cohen		
	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$	$E_{AS}$	$E_{VB}$	$f_i$
$YBa_2Cu_3O_4C_3$	3.63	13.59	0.17	3.49	13.50	0.16	3.55	13.56	0.16

#### 4. Conclusion

In this work, we have presented the electronic properties of  $YBa_2Cu_3O_7$ ,  $YBa_2Cu_3O_6C_1$ ,  $YBa_2Cu_3O_5C_2$  and  $YBa_2Cu_3O_4C_3$  crystal systems using the FP-LAPW method within DFT. We treated the exchange correlation energy using GGA, LDA and Wu-Cohen methods. Especially, we have calculated their band gap energies, total and partial densities of states and electronic charge densities. In all these crystal we have shown that replacing O atoms with C atoms results in some implications on the direct, indirect band gap energies and bonding nature between atoms in the crystals. We have shown that the valence band and the conduction band are overlapping for  $YBa_2Cu_3O_4C_3$  crystal system. This result shows that,  $YBa_2Cu_3O_4C_3$  has metallic properties. In addition we found that the direct and indirect band gap energies vary with the number of C atoms in the crystal. On the other hand TDOS and PDOS results showed that replacing C atoms with O atoms form the new intermediate sub-band in the valence band. The energy ranges of the sub-bands in the valence band vary with the number of C atoms in the crystal. The s-states of C atoms mainly create this intermediate band. Moreover high energy sub-band is mainly dominated by Cu 3d-states and is considerably mixed with O 2p-states indicating that there is a strong covalent bond between Cu and O atoms. Likewise, O 2-p states is considerably mixed C 2p-states indicating that there is a strong covalent bond between C and O atoms. The calculated electronic charge densities reveal that carbon atoms are bonded to copper atoms with strong covalent bonds. These bonds are similar to the bonds of copper and oxygen atoms. In addition the small changes are observed in the ionicity parameters in C doped crystal systems. This theoretical work is of great interest in superconductor research and motivates further future studies.

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