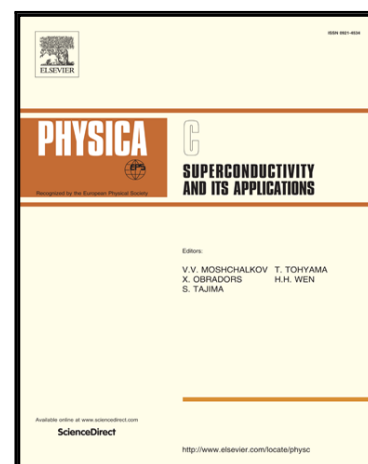


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Structural and electronic properties of Pb-doped $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$:
Comparison of LDA and GGA calculations

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HIGHLIGHTS

- We present for the first time the effects of Pb doping on structural and electronic properties of $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ (Bi2223) using GGA, compared with LDA results.
- We found the Pb concentration for which the Bi–O pockets disappear from the Fermi Surface in the Bi2223 compound using GGA and LDA, respectively.

Structural and electronic properties of Pb-doped Bi₂Sr₂Ca₂Cu₃O₁₀: Comparison of LDA and GGA calculations

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Abstract

We use Density Functional Theory to study the effects on the crystal structure and the electronic band structure of substituting Pb for Bi in Bi₂Sr₂Ca₂Cu₃O₁₀. We further use the Local Density Approximation (LDA) and the Generalized Gradient Approximation (GGA). The Virtual Crystal Approximation (VCA) was used to account for the substitution. We found that GGA reproduces better the lattice parameters although in both cases the internal coordinates were reproduced with some uncertainties. We further looked at the behavior of the so called Bi-O pockets, some electronic states that originate on the Bi-O planes and that appear on the Fermi surface (FS) in contradiction to the experimental evidence. We found that LDA and GGA differ on that subject. With 26% Pb and using LDA, the Bi-O pockets run away from the FS. But when GGA is used, it is needed up to 35% Pb to make the Bi-O pockets disappear from the FS. In the last case, once the Bi-O pockets are removed from the FS, we get a very good agreement with angular resolved photo-emission (ARPES) and nuclear magnetic resonance (NMR) experiments.

Keywords: Bi2223; Electronic structure; Band structure; Fermi surface.

I. INTRODUCTION

$\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ (Bi2223) is a member of the family of the Bi cuprates identified with the general formula $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{10}$ where n denotes the number of CuO_2 planes in the unit cell. Resistivity, susceptibility and magnetic experiments show that the critical superconducting temperature is $\sim 110 \text{ K}^{1,2}$. In spite of the fact that this compound seems to be very convenient for technological applications³⁻⁶ there are but very few theoretical papers on this compound. In particular, no theoretical studies on Bi2223 using Density Functional Theory (DFT) with the Generalized Gradient Approximation (GGA) have been reported so far.

Neutron diffraction and X-rays experiments on Bi2223 are consistent with an orthorhombic crystal structure (spatial groups A_{222} , A_{2mm} and $Fmmm$)⁷⁻⁹ and with the tetragonal crystal structure (spatial group $I4/mmm$)^{10,11}. Further, these structures were found to be more stable when the sample is doped with Pb⁹⁻¹³. Angle-resolved photo-emission spectroscopy (ARPES) experiments were reported¹⁴⁻¹⁷ and, in particular, Ideta *et al.*¹⁶ reported that the bands on the Fermi surface (FS) in the nodal direction that are associated with the Cu-O planes, unfold.

In a previous work¹⁸, we calculated the electronic properties of Bi2223 in the tetragonal phase ($I4/mmm$). We found the so-called Bi-O pockets^{19,20}, some electronic states associated with the Bi-O planes that appear at the FS as a small pockets around the anti-nodal $\bar{M}$ point on the irreducible Brillouin zone (IBZ). The appearance of the Bi-O pockets is in total disagreement with the experimental findings¹⁶. This problem has been reported in the literature for a very long time²¹⁻²⁶.

H. Lin *et al.* have found that in the parent $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_1\text{O}_8$ compound (Bi2221) the Bi-O pockets run away from the FS to higher energy values when Bi is replaced with Pb in concentrations higher than 22%^{19,20}. In this work, it is mentioned that the doping will result in the same effect in the parent Bi2201 and Bi2223 compounds but these results are not reported.

In this work, we report our study of the effects the Pb doping has on Bi2223. We use both the Local Density Approximation (LDA) and the Generalized Gradient Approximation (GGA) and compare the two results between them. On the overall, we found that the Bi-O pockets disappear from the FS when 26% Bi is replaced by Pb when the LDA is used and

with 35% when GGA is used. A small metallic character in the Bi-O bonds remains.

II. METHOD OF CALCULATION

To calculate the structural and electronic properties of the $\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ compound we used Linearized Augmented Plane Waves plus local orbitals with total potential²⁷ (LAPW+lo) as in the Wien2K code²⁸. Exchange and correlation effects are accounted for by the LDA and the GGA. For the GGA, we used the Perdew-Burke-Ernzerhof form²⁹. As a cut-off for the base functions we used $R_{mt}K_{max} = 8.0$ and for the expansion of the functions of the base within the atomic spheres a maximum angular momentum value $l_{max} = 12$ with $G_{max} = 20$ and a $14 \times 14 \times 14$ grid on the k-space which contains 288 point on the IBZ. The muffin-tin radii, R_{mt} (in atomic units), were 2.3 for Bi, 2.0 for Sr, 1.9 for Ca and Cu and 1.5 for O (1.6 in GGA).

To account for the Pb-Bi substitution, we used the Virtual Crystal Approximation (VCA) which has been shown to be a good approximation for a case like this³⁰. In a certain sense we can think of it as an effective atom Bi/Pb¹⁹.

Our calculations were done for Pb concentrations $x = 0.20$ and 0.26 using LDA and $x = 0.20$ and 0.35 when GGA was used. The Pb concentration of 0.20 was performed to reproduce the work of Zhu *et al.*¹⁰. The concentrations of 0.26 (LDA) and 0.35 (GGA) are the lowest concentrations of Pb that are able to reproduce the Bi2223 electronic properties reported by Ideta *et al.*¹⁶.

III. RESULTS AND DISCUSSION

A. Structural properties

We have considered Bi2223 doped with Pb with tetragonal structure (spatial group $I4/mmm$) (D_{4h}^{17}). The crystal structure consists of three Cu-O planes, one Cu1-O1 plane between two Cu2-O2 planes with Ca atoms between them. Each Cu2-O2 plane is followed by a Sr-O3 and Bi-O4 planes in that order. The crystal structure is shown in Fig.1.

We started from the experimental lattice parameters¹⁰ and optimized the ratio c/a by minimizing the total energy at constant volume. Then we relaxed the internal coordinates

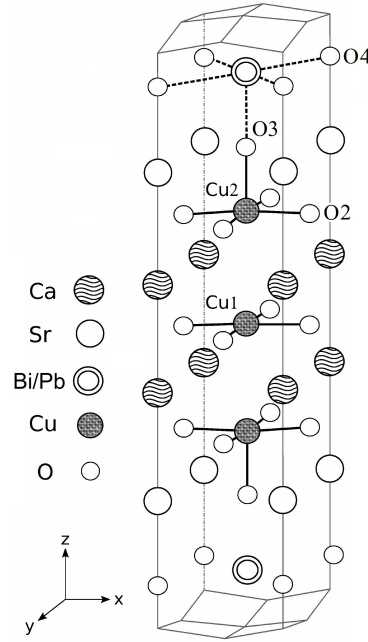


FIG. 1. The crystal structure of $\text{Bi}_{x-2}\text{Pb}_x\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ compound.

by minimizing the total forces using LDA (with $x = 0.20$ and 0.26) and GGA (with $x = 0.20$ and 0.35). See Table I.

As it is seen in the Table I, the calculated lattice parameters with both LDA and GGA agree well (up to at most a 1% difference) with the experimental parameters. Results with GGA agree even better since the difference with the experimental results is less than 0.2%. Notice also that the calculated values of a and c with LDA are overestimated as compared to experiment while the corresponding ones with GGA underestimate them.

It has been difficult to account accurately for the internal coordinates of the Cu2 and O2 ions in both cases, namely, using LDA or GGA. The differences with experiment are between 11% and 15% respectively. On the overall, nevertheless, GGA is slightly more accurate as compared to experiment in all cases, except O3. This last atom-position plays an important role since it can induce an almost-rigid displacement of the Bi-O bands toward higher energies with a null contribution at E_F around $\bar{M}$ point of IBZ, a result in agreement with the experiment. This compound contains alkaline earth metals (Sr, Ca) and 3d transitions metals (Cu) which have a better reproduction of its structural properties when GGA is used³².

In the next Table II, we show our calculated interatomic distances Bi/Pb-O3 ($d_{\text{Bi/Pb-O3}}$)

TABLE I. Optimized lattice parameters and atomic coordinates relaxed for $\text{Bi}_{x-2}\text{Pb}_x\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ with body-centered tetragonal structure and space group I4/mmm, for Pb concentrations of $x = 0.20$ and 0.26 (LDA) and $x = 0.20$ and 0.35 (GGA). The experimental values were taken from reference¹⁰. Our results appear in columns 3-6. The percentage difference with respect to the experiment is shown in parenthesis. The minus sign means that the calculation underestimates the experimental value.

Parameter	Lattice parameters in Å				
	Expt.	LDA*		GGA	
	x	x		x	
	0.20	0.20	0.26 [†]	0.20	0.35 [†]
a	3.823(9)	3.8058 (-0.4%)	3.8080 (-0.4%)	3.8187 (-0.1%)	3.8197(-0.1%)
c	37.074(5)	37.409 (0.9%)	37.369 (0.8%)	37.158 (0.2%)	37.139 (0.2%)
c/a	9.6976(2)	9.8295 (1.2%)	9.8133 (1.2%)	9.7305 (0.3%)	9.7229 (0.3%)
Atom	Atomic coordinates				
	Expt.	LDA*		GGA	
	x	x		x	
	0.20	0.20	0.26 [†]	0.20	0.35 [†]
$\text{Bi}_{(1-x)}\text{Pb}_x$	0.2109(6)	0.2034 (-3.6%)	0.2035 (-3.5%)	0.2088 (-1.0%)	0.2089 (-0.9%)
Sr	0.3557(2)	0.3693 (3.8%)	0.3685 (3.6%)	0.3656 (2.8%)	0.3650 (2.6%)
Ca	0.4553(8)	0.4576 (0.5%)	0.4572 (0.4%)	0.4564 (0.3%)	0.4562 (0.2%)
Cu1	0.0000	0.0000	0.0000	0.0000	0.0000
Cu2	0.0976(4)	0.0833 (-14.7%)	0.0840 (-13.9%)	0.0850 (-12.9%)	0.0855 (-12.4%)
O1	0.0000	0.0000	0.0000	0.0000	0.0000
O2	0.0964(2)	0.0834 (-13.5%)	0.0835 (-13.4%)	0.0855 (-11.4%)	0.0852 (-11.6%)
O3	0.1454(4)	0.1489 (2.4%)	0.1490 (2.5%)	0.1531 (5.3%)	0.1528 (5.1%)
O4	0.2890(2)	0.2992 (3.5%)	0.2992 (3.5%)	0.2928 (1.3%)	0.2936 (1.6%)

*Values were taken from a previous work³⁰.

[†] At this concentration the presence of Bi-O pockets on the Fermi surface of Bi2223 is not observed, reproducing correctly the experimental reports.¹⁶ (see below).

and Cu2-O3 (d_{Cu2-O3}) calculated with both LDA and GGA.

TABLE II. Our calculated interatomic distances in Å Bi/Pb-O3 ($d_{Bi/Pb-O3}$) and Cu2-O3 (d_{Cu2-O3}) calculated with both LDA ($x = 0.20$ and 0.26) and GGA ($x = 0.20$ and 0.35). The experimental values were taken from reference¹⁰.

	Expt.	LDA		GGA	
	x	x		x	
Distance	0.20	0.20	0.26	0.20	0.35
$d_{Bi/Pb-O3}$	2.428(15)	2.039	2.037	2.070	2.083
d_{Cu2-O3}	1.772(17)	2.454	2.429	2.529	2.499

$d_{Bi/Pb-O3}$ and d_{Cu2-O3} obtained using LDA differ from experiment in -0.39 Å³⁹ and 0.68 Å respectively as compared to experiment. Using GGA we obtain differences less than -0.36 Å and 0.76 Å. It is to be noticed that using GGA and $x = 0.35$ we get the more accurate result in the distance $d_{Bi/Pb-O3}$ but an important difference in the d_{Cu2-O3} . In a previous paper³¹ we stated that the position of O3 has an important influence in the electronic properties of this system.

B. Electronic properties

In Fig. 2 we illustrate the effects of Pb-doping on the electronic band structure and on the FS of the $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{10}$ compound calculated as we stated before with 20% and 26% Pb concentration using the LDA and with 20% and 35% using GGA.

By substituting only 20% of Bi with Pb, the Bi-O pockets appear in disagreement with experiment. We can observe that when the calculation is done with the GGA, the area occupied by the Bi-O pockets is bigger. We interpret this fact as a sign of a weakened interaction of between the Bi-O and Cu-O planes³⁰ but nevertheless it is not enough to reproduce the experimental electronic properties reported in the literature¹⁶. In both cases, using LDA or GGA, we obtain that the states that contribute at the FS are Cu $d_{x^2-y^2}$ -O $p_{x,y}$, Cu d_{z^2} -O p_z and Bi $p_{x,y,z}$ -O $p_{x,y,z}$.

So, by doping with Pb the Bi2212¹⁹ or Bi2223³⁰ a quasi-rigid shift of the Bi-O bands away from the FS is produced. Then an optimal doping should exist that eliminates the

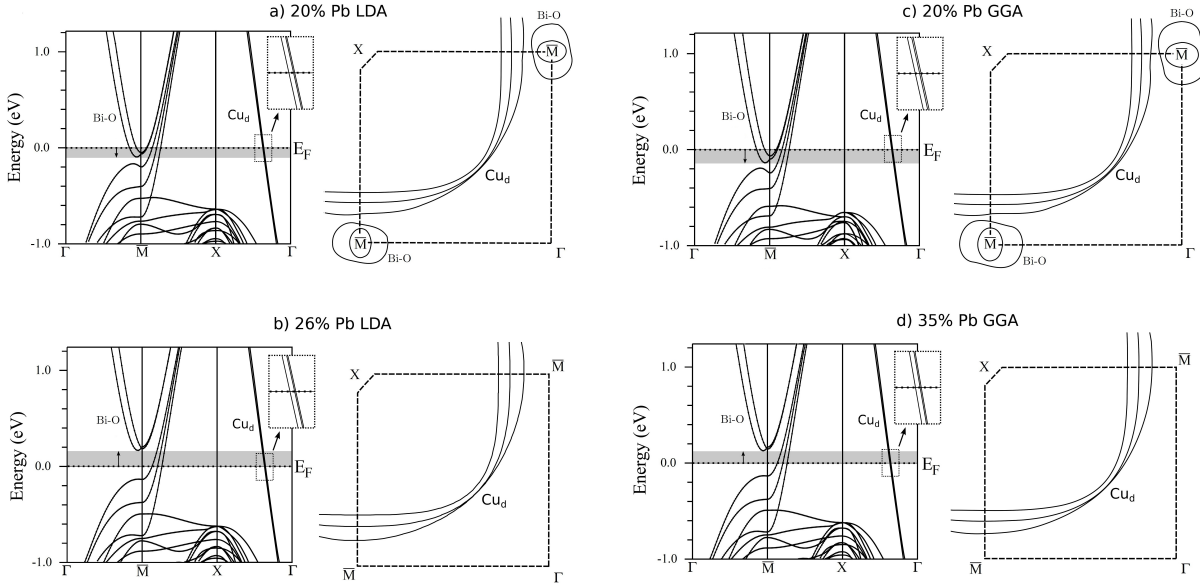


FIG. 2. The band structure and Fermi Surface (at $k_z = 0$) of the $\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ compound. LDA with a) 20% Pb b) 26% Pb. GGA c) 20% Pb d) 35% Pb.

Bi-O pockets from the FS as experiment requires. For Bi2223 the adequate percentage differs when LDA or GGA is used in the calculation. We find that a minimum of 26% Pb is appropriate when LDA is used³⁰ (see Fig. 2b). When GGA is used, then only a minimum of 35% Pb has to be introduced in the sample to make the Bi-O pockets disappear from the FS (see Fig. 2d). In both cases, the Bi-O plane has a slight metallic character. This is due to Bi p_z -O3 p_z -O4 p_z . Experimental results show that in bulk Bi2212 the Bi-O plane is non-metallic³³⁻³⁵. In disagreement with the just-mentioned works, K. Asokan *et al.*³⁶ reported an experiment that supports the conclusion that in both Bi2212 and Bi2223 are metallic. As it seems, more experimental studies in Bi2223 are required to decide whether the Bi-O planes in this compounds are metallic.

The bands associated with the Cu-O plane do not change very much with the doping (see Fig. 2). Three closed surfaces centered around the X point of the IBZ contribute to the FS. Two of them are degenerated in the nodal direction. They are associated to the outer CuO_2 planes (OP). The third one is formed from the inner CuO_2 plane (IP). These results agree very well with experiment¹⁶. Nuclear magnetic resonance experiments^{37,38} show that the hole OP concentration is higher than the IP one. A further effect of the doping (26%, LDA and 35%, GGA) is to enhance the distance in energy between the two degenerate surfaces

mentioned and the third one which is in better agreement with experiment¹⁶.

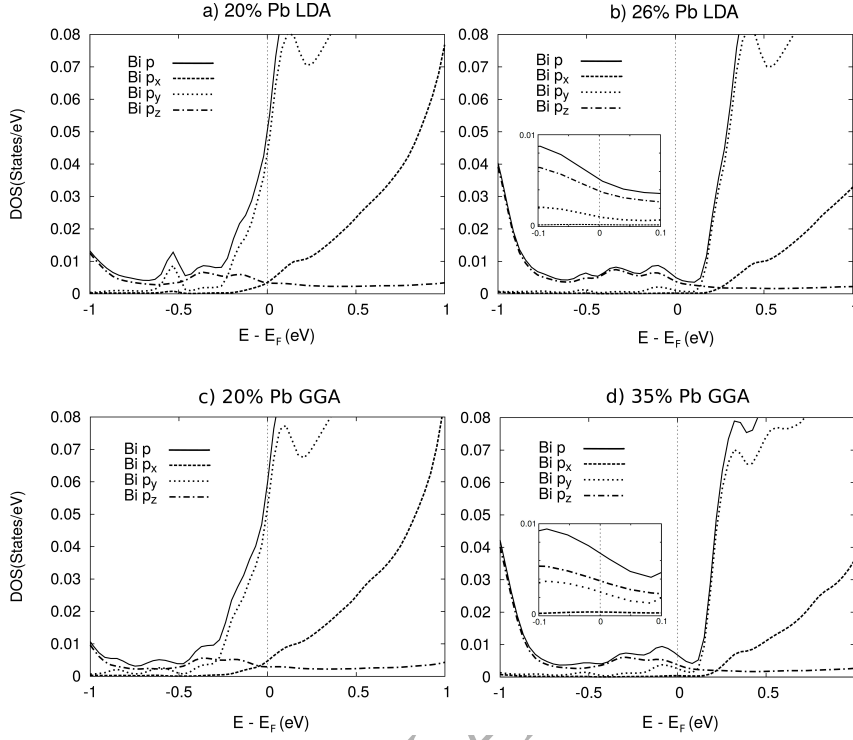


FIG. 3. Projected density of states (PDOS) of Bi atom around the Fermi level for $\text{Bi}_{2-x}\text{Pb}_x\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$. LDA with a) 20% Pb b) 26% Pb. GGA c) 20% Pb d) 35% Pb.

In Fig. 3, we show the projected density of states (PDOS) around the E_F for the Bi atom. In Fig. 3a we show the calculation at 20% doping using LDA. The main contribution to the Bi-PDOS (50.3×10^{-3} states/eV-atom) comes from Bi p-states (86%) mainly from p_y states. The Bi $p_{x,z}$ states have a comparatively small contribution (6.3×10^{-3} states/eV-atom). A peak in the Bi-PDOS appears at -0.51 eV. It is formed by Bi p_y states which are associated to the interaction between the Cu-O and Bi-O planes. The Bi p states are responsible for the Bi-O pockets at FS. When the doping is enhanced to 26% (LDA) the Bi $p_{x,y}$ states shift to higher energies (see Fig. 3b). As a consequence, the contribution of these states at E_F diminishes 1.2×10^{-3} states/eV-atom. The Bi p_z states remain unaffected by the doping. The projected contribution at E_F is 4.0×10^{-3} states/eV-atom. At 26% doping (LDA) the Bi-O pockets do not appear at FS anymore (see Fig. 2b). A slight metallic character remains on the Bi-O planes which is to be mainly (75%) attributed to the Bi p_z . At 26% doping the peak in the PDOS at -0.51 eV disappears which is due to the weaker interaction between

the planes Cu-O and Bi-O³⁰.

GGA needs more doping concentration to make the Bi-O pockets disappear from the FS (Fig. 3c and 3d). At 20% Pb concentration, the contribution of the Bi p states at E_F is 20% higher (60.3×10^{-3} states/eV-atom). It is due mainly (87%) to Bi p_y states. The contribution of the Bi $p_{x,z}$ states is small (7.7×10^{-3} states/eV-atom). The peak at -0.51 eV does not appear in this case. As we show in Fig. 2c, at 20% doping the Bi-O pockets are present at E_F .

Since to avoid the Bi-O pockets at the FS we need 9.0% more Pb doping with GGA than with LDA (see Fig. 3d), the effective atom Pb/Bi will have less electronic charge in the same proportion when VCA is used. So GGA is less effective in breaking the Bi-O and Cu-O planes interaction. Even though the Bi-O pockets disappear from the FS, Bi remains metallic due to small presence of Bi p-states at E_F (6.2×10^{-3} states/eV-atom).

TABLE III. Effects of Pb-doping on the minimum of the Bi-O energy bands change with respect to E_F upon doping, δ_{Bi-O} , the total density of states at E_F , $N(E_F)$, the Fermi level, E_F , and the total energy of the system, E_{total} in Bi2223. $\Delta(\%)$ represents the percentage difference of the values obtained using the same potential.

Pb Doped	δ_{Bi-O} [eV]	$N(E_F)$ [states/eV-cell]	E_F [eV]	E_{total} [eV]
20% LDA	-0.05	2.8143	6.45	-1531807
26% LDA	+0.08	2.4932	6.22	-1528236
Δ_{LDA}	0.13	-0.3211	-0.22	+3571
20% GGA	-0.07	2.9284	6.73	1533047
35% GGA	+0.06	2.6743	6.85	1529476
Δ_{GGA}	0.13	-0.2541	+0.02	+3570

In Table III, we show how the minimum of the Bi-O energy bands change with respect to E_F upon doping, δ_{Bi-O} , the total density of states at E_F , $N(E_F)$, the Fermi energy, E_F , and the total energy of the system, E_{total} . Notice that the disappearance of the Bi-O pockets at the E_F translates in a lower $N(E_F)$ as is to be expected. It is interesting that $N(E_F)$ is lower when LDA is used. Also with GGA, E_F is slightly higher. The minimum of the Bi-O bands (measured with respect to E_F) is inversely proportional to E_F (see shadowed zone

in Fig. 2) and proportional to E_{total} . This means that with more than 20% Pb, the sample is less stable. Therefore as it seems, the strength of the interaction between the Bi-O and Cu-O planes is crucial to the stability of the sample.

TABLE IV. Effect of Pb doping on the ratio of the atom-projected local density of states (LDOS) at E_F to the total density of states at the Fermi level for the atoms Bi, O2, O3, O4, and Cu2 (with both LDA and GGA). All values are multiplied by $\times 10^{-3}$ factor. $\Delta(\%)$ represents the percentage difference of the values obtained using the same potential, taking as reference the concentration that reports the presence of Bi-O pockets in each case. The minus sign means a decrease compared to the reference value.

Pb Doped	Bi/Pb			O3			O4		
	p_x	p_y	p_z	p_x	p_y	p_z	p_x	p_y	p_z
20% LDA	1.24	15.42	1.20	0.76	7.45	2.36	1.66	1.15	2.52
26% LDA	0.09	0.43	1.56	0.32	0.42	2.02	0.32	0.42	2.02
$\Delta_{LDA}(\%)$	-88%	-93%	+30%	-57%	-94%	-15%	-80%	-63%	-20%
20% GGA	1.63	17.97	1.00	0.92	8.50	3.58	2.25	2.13	1.87
35% GGA	0.15	0.85	1.30	0.35	0.70	1.87	0.29	0.29	1.58
$\Delta_{GGA}(\%)$	-89%	-91%	+31%	-62%	-92%	-48%	-87%	-86%	-16%

Pb Doped	Cu2		O2		
	$d_{x^2-y^2}$	d_{z^2}	p_x	p_y	p_z
20% LDA	143.11	5.46	5.61	32.84	0.73
26% LDA	168.16	7.27	6.47	38.31	0.41
$\Delta_{LDA}(\%)$	+18%	+33%	+15%	+17%	-44%
20% GGA	140.53	4.53	5.63	32.90	0.80
35% GGA	161.02	5.88	6.74	38.07	0.33
$\Delta_{GGA}(\%)$	+15%	+30%	+20%	+16%	-59%

Doping with Pb into Bi2223 using VCA has important effects not only in the electronic properties of the Bi-atom but also on the neighboring atoms. In the Table IV, we show the effect that the doping has on the atoms Bi, O2, O3, O4 and Cu2. In each case we show the ratio of the atom-projected local density of states (LDOS) at E_F to the total density of states

at the Fermi level for the atoms Bi, O2, O3, O4, and Cu2 (with both LDA and GGA). As it is seen in Table IV, by increasing the Pb concentration up to avoiding the Bi-O pockets, the contribution of Bi $p_{x,y}$ states decreases, while the Bi p_z states reveal an increase of 30% (LDA) and 31 % (GGA) of its contribution at E_F , compared to 20% Pb in each case. The contribution of p_z states of O3 and O4 atoms are the least affected by the presence of Pb. It is observed that the inclusion of Pb generates an increase in the electronic contribution at E_F of Cu2 d and O2 p states, except O2 p_z states, whose contribution decreases by 44% (LDA) and 59% (GGA). We do not find any noticeable effect on the Sr-atom.

IV. CONCLUSIONS

In this work we present our study of the effects of substituting Bi with Pb in the Bi2223 compound on its structural and electronic properties and compare the results when calculating them with the LDA and GGA approximations. Our calculation was done using the Full-potential linearized augmented plane wave method plus Local orbitals within the Local density approximation using Wien2k code. We used the virtual crystal approximation (VCA) to account for the substitution of Bi for Pb.

We found that GGA better reproduces (up to 0.2% difference with experiment) the lattice parameters while LDA presents higher differences (0.9%). This is due to the presence of alkaline earth metals (Sr, Ca), and transition metals as Cu better described with GGA. The internal coordinates of the Cu2 and O2 are not well described by neither the LDA nor the GGA. The difference with the experiment is between 11% up to 15%. LDA better describes the position of the O3 atom which plays an important role in the electronic properties of Bi2223. In both cases LDA and GGA, it is showed that when the structure is relaxed, the O3 atom enhances its distance to the Cu2 atom and diminishes the one to the Bi/Pb atom, as showed in a previous work without the inclusion of any doping. We further found that the Bi-O pockets disappear from the Fermi Surface (in agreement with the experiment) when Pb doping is introduced. The required doping differs in both LDA (26%) and GGA (35%). This difference is due to the fact that within GGA the interaction between the Bi-O and Cu-O planes requires more energy for it to be broken. They are the cause for the Bi-O pockets to appear at E_F . Once the Bi-O pockets problem is solved, we looked at the character of the Bi-O plane. We found it to be slightly metallic. This is due to Bi p_z -O3 p_z -O4 p_z states.

These bands cross the Fermi level in the direction $\overline{M}$ -X.

A last conclusion regarding the minimum of the Bi-O bands (measured with respect to the Fermi level), which turned out to be proportional to the inverse of the density of states at E_F and proportional to the total energy E_{total} in both, the LDA and the GGA calculations. This means that when the doping is higher than 20% the system is less stable. We conclude that the strength in the Bi-O and Cu-O planes defines to a certain extend the stability of this system.

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