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Different self-consistent electronic structures of $PrBa_2Cu_3O_7$ from LSDA+U calculations

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Based on the density-functional theory and using the full-potential linearized augmented-plane-wave method the electronic structure of $PrBa_2Cu_3O_7$ (Pr123) system was calculated. The rotationally invariant local spin-density approximation plus Hubbard parameter U was employed for Pr(4f) orbitals. One self-consistent solution more stable than the previous solution, which has been proposed by Liechtenstein and Mazin (LM) [Phys. Rev. Lett. **74**, 1000 (1995)], was found. This new solution favors the suggestion that the pure Pr123 samples should be intrinsically superconductor and metal similar to the other $RBa_2Cu_3O_7$ (R=Y or a rare-earth element) samples. Moreover, the results of ^{17}O NMR spectroscopy study of the conventional nonsuperconducting Pr123 samples [Y. H. Ko *et al.*, Physica C **224**, 357 (1994)] were interpreted by means of our new solution. It was argued that the loss of superconductivity in the conventional Pr123 samples should be associated with transition of holes from O2($2p_\sigma$) orbitals to O2($2p_\pi$) orbitals. Altogether, it was proposed that some imperfections can be responsible for this phenomenon. Meanwhile, more pieces of evidence are required to verify this proposal.

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I. INTRODUCTION

Since the early years of discovery of high temperature superconductivity, the most prepared $PrBa_2Cu_3O_7$ (Pr123) samples had shown nonsuperconducting and nonmetallic behaviors in contrast to $RBa_2Cu_3O_7$ (R123) samples.[1] However, Blackstead *et al.*[2] reported superconductivity in Pr123 powders and thin films in 1995. On the other hand Zou *et al.*[3] have also reported bulk superconductivity in Pr123 single crystals in 1998. In addition, bulk superconductivity in polycrystalline Pr123 samples was reported by Araujo-Moreira *et al.*[4] in 2000. There are some experimental evidences which imply that the nonsuperconducting Pr123 samples are not pure samples. For instance, the c-axis lattice constant of nonsuperconducting Pr123 samples reveals a noticeable departure from the c-axis vs R^{3+} ionic radii curve in the R123 superconducting samples.[3] In contrast, the c-axis lattice constant of superconducting Pr123 samples falls in the consistent curve of other superconducting R123 samples.[3,4] In Ref. 4 it has experimentally been shown that using a wrong chemical route, based on oxygen atmosphere, leads to the formation of a superoxide that inhibits the formation of the superconducting phase in the conventional Pr123 samples. By improving the fabrication route,[4] the structural imperfections of Pr123 samples have comprehensively been reduced and the new samples show superconductivity like other R123 samples. Indeed, the recent experiments[3,4] indicate the pure Pr123 is a normal Y123-like oxide superconductor.

Based on the density-functional theory,[5] the electronic structures of Y123 and Pr123 have been calculated in several works.[6–17] The local (spin) density approximation [L(S)DA] (Ref. 18) provides many properties of Y123 such as the structural parameters, phonon frequencies,[8] and Fermi surfaces[9] in surprisingly good agreement with the experiments. However, the L(S)DA is not reliable for the Pr123. For instance, the LSDA calculation implies a Pr valency intermediate between 4+ and 3+ (about 3.6+),[11] which is inconsistent with the experimental value that is near 3+.[19] To overcome the failures of the LSDA, the LSDA plus Hubbard parameter U (LSDA+U) (Ref. 20) has been used for Pr(4f) electrons in Ref. 14 by Liechtenstein and Mazin (LM), in 1995. In this reference, the Pr atom shows almost 3+ valency and one partially empty $pf\sigma^*$ (O-Pr) band crosses Fermi energy. In Ref. 14, it has been argued that this $pf\sigma^*$ band grabs holes from the superconducting $pd\sigma^*$ (O-Cu) bands and it is responsible for suppression of superconductivity in the Pr123. The LM model suggests that the pure Pr123 samples are intrinsically nonsuperconductor. After the observation of superconductivity,[3] Mazin has argued that if this finding is true, the Pr123 is a more novel superconductor than all other cuprate high-T_c materials known: It is the only one where superconducting carriers are not residing in the $pd\sigma^*$ bands.[21] Indeed, the former suggestion (i.e., Pr123 is intrinsically nonsuperconductor) leaves the superconductivity of the recent samples unexplained.[3,4] Moreover, the latter suggestion (i.e., Pr123 is a novel intrinsically superconductor) leaves the nonsuperconductivity of the conventional samples unexplained.

Later, we have used the LSDA+U for Pr(4f) electrons[16,17] and reported that there is no partially empty $pf\sigma^*$ band in our band-structure results in contrast to Ref. 14. It has been argued that perfect Pr123 samples should be metal and superconductor similar to Y123 compound and some impurities should be responsible for the suppression of superconductivity and metallic character in the conventional samples.[16,17] Why do our LSDA+U results differ greatly from the LM results and which one is more compatible with the experimental observations? Here, it was shown that the final self-consistent results in the LSDA+U calculations of Pr123 greatly depend on the starting configuration of occupation number matrix for Pr(4f) orbitals. Two special self-

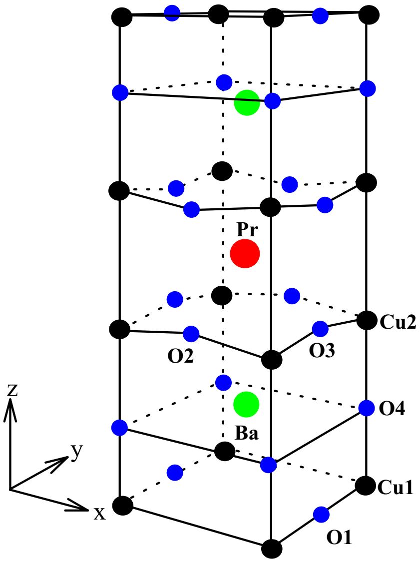

FIG. 1. (Color online) The unit cell of $PrBa_2Cu_3O_7$.

consistent solutions were presented and carefully compared with each other and some experimental observations.

II. COMPUTATIONAL DETAILS

Present calculations were performed by the precise full-potential linearized augmented-plane-wave (FP-LAPW) method.[22] Additional local orbitals (LO) were used for all semicore states.[23] We have used the well-known WIEN2k code for this purpose.[24] The data of the crystalline structure of Pr123 were taken from the neutron-diffraction results.[25] The unit cell of Pr123 and the labeling of various atoms were also shown in Fig. 1. All calculations were performed in ferromagnetic ordering similar to Refs. 10, 11, and 13–17. Atomic sphere radii of 2.80, 2.90, 1.80, and 1.65 a.u. were taken for Pr, Ba, Cu, and O, respectively. Approximately, 1900 LAPW plus 38 LO functions were used as the basis set. Self-consistency was obtained using a set of 16 special k points (same as in Refs. 11, 16, and 17) in the irreducible Brillouin zone (IBZ). It was also tested that calculations with 72 k points yield almost the same results. In all calculations, band states (valence and semicore states) were treated scalar relativistically and core states full relativistically.

Similar to the LM calculation,[14] we have used the rotationally invariant scheme of LSDA+U functional, which has been described in Ref. 20. It can be written as the following:

$$E^{\mathrm{LSDA}+U}[\rho,\vec{m},\{n\}] = E^{\mathrm{LSDA}}[\rho,\vec{m}] + E^{U}[\{n\}] - E^{dc}[\{n\}],$$

where ρ and $\vec{m}$ are the electron and magnetization density, respectively, and $\{n\}$ is the occupation number matrix.[20] $E^{\mathrm{LSDA}}[\rho,\vec{m}]$ is the standard LSDA functional.[18]

$$\begin{aligned} E^{U}[\{n\}] = \frac{1}{2}\sum_{\{m\},\sigma} \{ & \langle mm''|V_{ee}|m'm'''\rangle n^{\sigma}_{mm'} n^{-\sigma}_{m''m'''} \\ & + (\langle mm''|V_{ee}|m'm'''\rangle \\ & - \langle mm''|V_{ee}|m'''m'\rangle) n^{\sigma}_{mm'} n^{\sigma}_{m''m'''} \}, \end{aligned}$$

where V_{ee} are the screened Coulomb interactions among the nl ($4f$) electrons.[20] The "double-counting" term $E^{dc}[\{n\}]$ is an approximation to the electron-electron interaction for the Pr($4f$) orbitals, which has already been contained in $E^{\mathrm{LSDA}}[\rho,\vec{m}]$. There are different versions for this term.[26] In the "fully localized limit" (FLL) [i.e., "self-interaction corrected" (SIC)] approximation, which has been used in both Ref. 14 and the present work, it is defined as

$$E^{dc}[\{n\}] = \frac{1}{2}UN(N-1) - \frac{1}{2}J[N_{\uparrow}(N_{\uparrow}-1) + N_{\downarrow}(N_{\downarrow}-1)],$$

where $N_{\sigma}=\mathrm{Tr}(n^{\sigma}_{mm'})$ and $N=N_{\uparrow}+N_{\downarrow}$. The screened U parameter[20,26] was set to the Pr metal value of 5.8 eV,[27] similar to Ref. 14. At the first step, the value of screened J parameter[20,26] was set to zero. This corresponds to neglect the nonsphericity of the electronic interactions (i.e., $\langle mm'|V_{ee}|m''m'''\rangle = \delta_{mm''}\delta_{m'm'''}U$) and the differences among the interactions in like-spin and unlike-spin channels. (For detailed descriptions see Ref. 26.) At the second step, the usual 0.68 eV value[15] was used for the J. Increasing of the J value from zero to 0.68 eV has not changed the results, qualitatively.

As mentioned before, the final self-consistent results in the LSDA+U calculations of Pr123 greatly depend on the starting configuration of occupation number matrix for Pr($4f$) orbitals. In this paper, two special calculations were reported. In the first calculation, the starting occupation numbers corresponding to Pr($4f_{z(x^2-y^2)}$) and Pr($4f_{z(5z^2-3r^2)}$) were set occupied. With these selections the results of Ref. 14 were reproduced. (In Ref. 14, it has been mentioned that the starting configuration was such that the occupied states corresponded to complex f harmonics with $m=\pm 2$. The Pr($4f_{z(x^2-y^2)}$) orbital is produced with combination of these complex harmonics.) In the second calculation, instead of Pr($4f_{z(x^2-y^2)}$), the starting occupation numbers corresponding to Pr($4f_{y(y^2-3x^2)}$) (combination of complex harmonics with $m=\pm 3$) were set occupied. The reason for this selection is discussed in Sec. III.

III. RESULTS AND DISCUSSION

Electronic density of states (DOS) for both the calculations was shown in Fig. 2. (In all figures $J=0$. Using $J=0.68$ eV does not change the results, qualitatively.) Implementation of U produces the Hubbard splitting between the occupied and empty Pr($4f$) states. The Pr($4f$)-minority spin states are entirely above the Fermi energy for both the calculations. In the first calculation, some Pr($4f$)-majority spin states lie across the Fermi energy, but in the second calculation they do not lie across it. For $J=0$ ($J=0.68$ eV), the wave functions within the Pr sphere contribute spin magnetizations of 1.93 and 1.96 μ_B/Pr (1.93 and 1.98 μ_B/Pr) for the first and second calculations, respectively. These values imply a Pr valency near 3+, which is consistent with experiments.[3,19]

The band structures of the first and second calculations for the majority spin were shown in Fig. 3. The bands 2 and 3 are derived from the two CuO_2 planes and have the

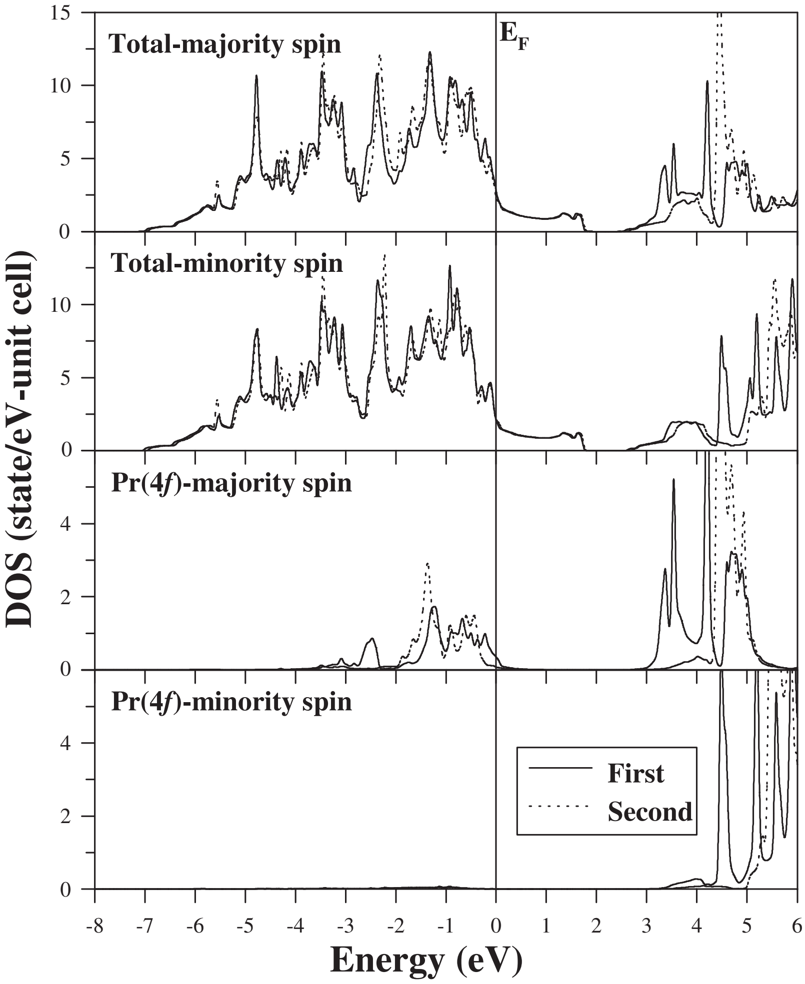

FIG. 2. The electronic DOS for the first calculation (First) and the second calculation (Second).

usual two-dimensional character of $\mathrm{Cu2}(3d_{x^2-y^2})-\mathrm{O2}(2p_x)-\mathrm{O3}(2p_y)$ antibonding. The bands 1 and 4 are corresponding to the $\mathrm{CuO_3}$ chain. The almost empty dispersive band 1 has the character of $\mathrm{Cu1}(3d_{y^2-z^2})-\mathrm{O1}(2p_y)-\mathrm{O4}(2p_z)$ antibonding and the almost filled flat band 4 has the $\mathrm{Cu1}(3d_{yz})-\mathrm{O1}(2p_z)-\mathrm{O4}(2p_y)$ antibonding character. These four partially occupied bands also exist in the band structure of Y123.[6] In comparison with the Y123 band structure,[6] an additional band 5 crosses the Fermi level in Fig. 3(a). As has been described in Ref. 14, band 5 grabs some holes from the superconducting bands (i.e., bands 2 and 3). In order to investigate the bonding nature of this band at the high-symmetry $S=(\pi/a,\pi/b,0)$ point, the corresponding charge density contour plots were presented in Fig. 4. This figure shows that the holes of band 5 mainly have $\mathrm{Pr}(4f_{z(x^2-y^2)})-\mathrm{O2}(2p_y)-\mathrm{O3}(2p_x)$ antibonding character. Figure 3(a) is very similar to the corresponding figure (Fig. 1) of Ref. 14. There are some minor differences which may be related to differences in methods of calculations or computational parameters. For instance, we have used FP-LAPW method but Ref. 14 has used full-potential linear muffin-tin orbital (FP-LMTO) method.

In Fig. 3(b), no band with Pr(4*f*) character crosses the Fermi level. The four partially filled bands 1–4 are coincident with the corresponding bands in Y123 band structure.[6] So, the number of superconducting holes in the $\mathrm{CuO_2}$ planes of the second calculation is equal with the corresponding ones in Y123. Instead of the band 5 of Fig. 3(a), there is another band with completely different character in Fig. 3(b). This band, which was labeled "5" in Fig. 3(b), is completely occupied and lies about 0.39 eV below the Fermi energy at the *S* point. The charge density contour plots of this band at the *S* point shows $\mathrm{Pr}(4f_{y(y^2-3x^2)})-\mathrm{O2}(2p_z)-\mathrm{Cu2}(3d_{xz})$ antibonding character (Fig. 5). The existence of states with $\mathrm{Pr}(4f_{y(y^2-3x^2)})-\mathrm{O}(2p)-\mathrm{Cu}(3d)$ character has also been reported for $\mathrm{Y_{1-x}Pr_xBa_2Cu_3O_7}$ system by embedded cluster model calculation.[28] In that model, a $\mathrm{PrCu_8O_{24}}$ cluster has been located in the potential range of the $\mathrm{YBa_2Cu_3O_7}$ crystal. In contrast to our LSDA+U calculation results, the $\mathrm{Pr}(4f_{y(y^2-3x^2)})-\mathrm{O}(2p)-\mathrm{Cu}(3d)$ states of the cluster calculation lie above the Fermi energy.

Figure 3(b) is similar to the band structure of our previous report;[16] in both, no band with Pr(4*f*) character crosses the Fermi level. In spite of it, there is no $\mathrm{Pr}(4f_{y(y^2-3x^2)})-\mathrm{O2}(2p_z)-\mathrm{Cu2}(3d_{xz})$ hybridization in Ref. 16. In this reference, the starting occupation number matrix has been calculated from the LSDA self-consistent results, which differs greatly from that which was used in the second calculation. We have found that the second calculation of the present report is more stable than the corresponding calculation in our previous work (Ref. 16), and so it is computationally more reliable. In the following paragraph, we will show that

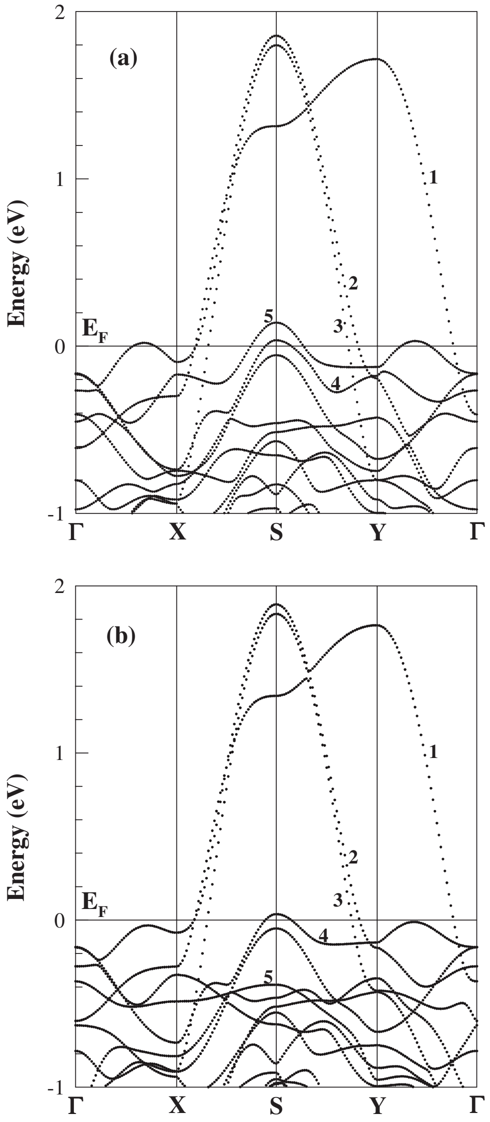

FIG. 3. The band structures of (a) the first and (b) the second calculations for the majority spin.

the band 5 of Fig. 3(b) is very helpful for discussing some important properties of Pr123 samples.

It is worth comparing the total energies for the two solutions. For $J=0$ ($J=0.68$ eV) case, the second self-consistent solution has a total energy about 23 mRy/cell (25 mRy/cell) lower than the first self-consistent solution and so, it is more stable. This result reveals that the LSDA+U approach, which we have used here, does not support the Pr($4f_{z(x^2-y^2)}$) hybridization model. In spite of that, since the LSDA+U does not contain all strong-correlation effects in Pr123,[26] we cannot claim that the Pr($4f_{z(x^2-y^2)}$) hybridization model is not physically true.

Before us, some people have also proposed the existence of Pr($4f_{y(y^2-3x^2)}$)−O2($2p$)−Cu3($3d$) hybridization to discuss the wonderful experimental electric-field gradient (EFG) values of the nonsuperconducting Pr123 samples.[29] The EFG is a traceless symmetric tensor of rank 2, defined as the second derivative of the electrostatic potential (with respect to spatial coordinates) evaluated at the position of the nucleus. The EFG at the oxygen sites of $RBa_2Cu_3O_{7-\delta}$ systems can be measured very accurately by the ^{17}O NMR spectroscopy.[29–31] We have computationally shown in Ref. 17 that, in the diagonal representation, the largest component of EFG tensor (in short EFG) at the O2 (O3) site is almost proportional to the number of superconducting $2p_\sigma$ holes in this site. It can also be deduced experimentally. For instance, it has been known that with reducing chain oxygens (with increasing δ) in $YBa_2Cu_3O_{7-\delta}$ compound, the number of doped $2p_\sigma$ holes at O2 (O3) site is reduced.[33] As was shown in Table I, the EFG value at O2 (O3) site of $YBa_2Cu_3O_{6.6}$ is lower than the corresponding one in $YBa_2Cu_3O_7$, which confirms our proposal.

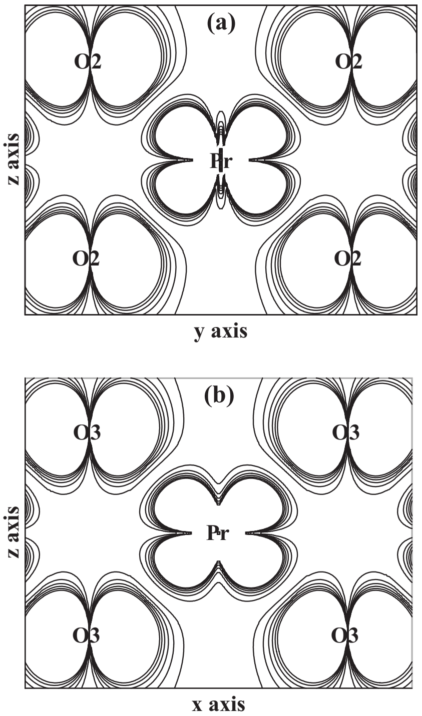

FIG. 4. The charge density contour plots at S point for the band 5 of the first calculation in (a) Pr-O2 (100) plane and (b) Pr-O3 (010) plane. The contours are from 0.001 to 0.011 at intervals of 0.002 eÅ^{-3} on a linear scale.

The experimental amount of EFG at O2 site in (nonsuperconducting) Pr123 is noticeably smaller than the EFG at O2 site in Y123, but the EFG at O3 site in (nonsuperconducting) Pr123 is equal to the EFG at O3 site in Y123 (Table I). At first glance, it may be proposed that the substitution of Pr at Y site reduces the superconducting holes in O2 site, while superconducting holes in O3 site do not noticeably change.[29] Now, let us follow this proposal by means of our second solution. As mentioned before, in the band structure of the second solution [Fig. 3(b)] no band with Pr($4f$) character crosses the Fermi level. The four partially filled bands 1–4 are coincident with the corresponding bands in Y123 band structure (which has been reported in Fig. 1 of Ref. 6). So, the number of $2p_\sigma$ holes in the O2 and O3 sites should be equal with the corresponding ones in Y123. It is in contrast with the above proposal that the substitution of Pr at Y site reduces the O2($2p_\sigma$) superconducting holes. Some indirect observations have shown that there are more than 0.23 Pr on Ba site (Pr_{Ba})/unit cell in nonsuperconducting Pr123

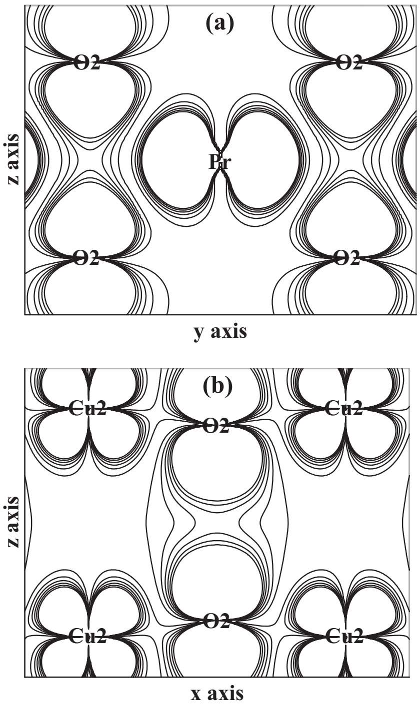

FIG. 5. The charge density contour plots at S point for the band 5 of the second calculation in (a) Pr-O2 (100) plane and (b) Cu2-O2 (010) plane. The contours are from 0.001 to 0.011 at intervals of 0.002 eÅ^{-3} on a linear scale.

samples.[34] In addition, there are some pieces of evidence which indicate the existence of oxygen disorders in these samples.[29,34,35] By these considerations, it can be supposed that the imperfections push up the band 5 [Fig. 3(b)] to cross the Fermi energy in the conventional nonsuperconducting samples. Since this band has O2($2p_\pi$) character and has no O3 character, it should grab the superconducting O2($2p_\sigma$) holes while the O3($2p_\sigma$) holes should not noticeably change. In this condition, it is noticeable that the pushed up band 5 crosses the Fermi energy around the S point [Fig. 3(b)]. Since the band structure is almost flat in the k_z direction of Brillouin zone, the second solution also predicts that the nonsuperconducting hole states mainly lie around the high-symmetry (π/a, π/b, k_z) line.

Altogether, the above arguments can be summarized as follows: (i) The (almost) pure Pr123 samples should be intrinsically superconductor and metal similar to the other R123 samples as has recently been reported in some Pr123 samples.[2–4] (ii) The imperfections cause the superconducting p_σ holes in the O2 sites to be transferred into the nonsuperconducting p_π states in these sites and the superconductivity is suppressed. In this case, the superconducting p_σ holes in the O3 sites should approximately be unchanged. In addition to the ^{17}O NMR spectroscopy,[29] comparison between the maximum entropy method (MEM) charge density of nonsuperconducting Pr123 [Fig. 2(b) in Ref. 36] and that of Y123 samples [Fig. 3(b) in Ref. 36] strongly confirms the latter argument.

TABLE I. The experimental EFG in units of 10^{21} V m^{-2} at oxygen sites of $YBa_2Cu_3O_{6.6}$, $YBa_2Cu_3O_7$, and (nonsuperconducting) $PrBa_2Cu_3O_7$. In the conversion from frequency unit to 10^{21} V m^{-2} units the quadrupole moment $Q=-0.026b$ for ^{17}O (Ref. 32) was used.

	O1	O2	O3	O4
$YBa_2Cu_3O_{6.6}$ [a]		9.4	9.4	11.0
$YBa_2Cu_3O_7$ [b]	17.3	10.5	10.2	11.6
$PrBa_2Cu_3O_7$ [c]		6.9	10.2	11.1

[a] Reference 30.
[b] Reference 31.
[c] Reference 29.

The above claims are mainly based on the LSDA+U calculations and implications of the ^{17}O NMR spectroscopy. As mentioned before, the LSDA+U is only an approximation and it does not contain all strong-correlation effects. In addition, the ^{17}O NMR spectroscopy results may be interpreted completely different from one that we have proposed. So, the present paper cannot claim that the Pr($4f_{z(x^2-y^2)}$) hybridization model is not physically true. However, more pieces of evidence are required to verify or deny the above proposal. In addition, it should also be remarked that the Pr($4f_{z(x^2-y^2)}$) hybridization model is able to explain the different T_c suppression in doped $Pr_xR_{1-x}Ba_2Cu_3O_7$ compounds for different R hosts.[14] However, this important question of whether our proposed model can explain the different T_c suppression or cannot remains unaddressed.

Finally, some notes should be mentioned. (i) We do not claim, in the scope of LSDA+U, our second solution is the most stable case. It is one solution more stable than the LM solution. It should be tested whether there are other solutions more stable than the second solution or not. It is an open question. (ii) In this paper we have used screened U parameter for metallic Pr (Ref. 27) to compare our results with Ref. 14. It is possible that the screened U value in the Pr123 compound differs from that in the Pr metal. (iii) Here, LSDA+U was only used for Pr($4f$) electrons. In Ref. 15, it has been suggested that the U should be used for the Cu($3d$) electrons, too. Figure 1 of Ref. 15 shows that only one band with CuO_3 chain character crosses the Fermi energy, and the other bands are completely empty or completely occupied. Therefore, concentration of holes in the $CuO_2-Pr-CuO_2$ trilayer is zero (i.e., there are no p_σ or p_π holes in the $CuO_2-Pr-CuO_2$ trilayer). It is basically inconsistent with the experimental observations.[29,37,38] It seems the U_{Cu} overestimates the strong-correlation of Cu($3d$) electrons of Pr123 system and produces incorrect results. Thus, we have not used it here.

IV. CONCLUSIONS

Electronic structures of Pr123 system were calculated using the FP-LAPW method. The rotationally invariant LSDA+U was employed for Pr($4f$) orbitals. It was shown that the final self-consistent solution greatly depends on the starting configuration of occupation number matrix for Pr($4f$) orbitals. One self-consistent solution more stable than the LM solution was presented. It predicts superconducting and metallic character of pure Pr123 samples similar to the other R123 samples. Moreover, the results of the ^{17}O NMR spectroscopy were considered together with our new solution. Altogether, this explanation for the suppression of superconductivity in the conventional Pr123 samples was suggested; the imperfections cause the superconducting holes to be transferred into the nonsuperconducting hole states which lie around the high-symmetry $(\pi/a, \pi/b, k_z)$ line of Brillouin zone and so, the superconductivity is suppressed. In this case, the superconducting $2p_\sigma$ holes in the O2 sites of nonsuperconducting Pr123 samples should be depleted and the ones in the O3 sites should be almost unchanged. Since, the LSDA+U does not contain all strong-correlation effects, more pieces of evidence are required to verify the above proposal. It is beyond the scope of the present paper.

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[1] M. Akhavan, Physica B **321**, 265 (2002); M. R. Mohammadizadeh, H. Khosroabadi, and M. Akhavan, *ibid.* **321**, 301 (2002); M. R. Mohammadizadeh and M. Akhavan, Eur. Phys. J. B **33**, 381 (2003); **42**, 321 (2004); M. R. Mohammadizadeh and M. Akhavan, Supercond. Sci. Technol. **16**, 1216 (2003); **16**, 538 (2003); M. R. Mohammadizadeh and M. Akhavan, Physica C **390**, 134 (2003).

[2] H. A. Blackstead, D. B. Chrisey, J. D. Dow, J. S. Horwitz, A. E. Klunzinger, and D. B. Pulling, Phys. Lett. A **207**, 109 (1995); H. A. Blackstead, J. D. Dow, D. B. Chrisey, J. S. Horwitz, M. A. Black, P. J. McGinn, A. E. Klunzinger, and D. B. Pulling, Phys. Rev. B **54**, 6122 (1996).

[3] Z. Zou, J. Ye, K. Oka, and Y. Nishihara, Phys. Rev. Lett. **80**, 1074 (1998); J. Ye, S. Sadewasser, J. S. Schilling, Z. Zou, A. Matsushita, and T. Matsumoto, Physica C **328**, 111 (1999).

[4] F. M. Araujo-Moreira, P. N. Lisboa-Filho, S. M. Zanetti, E. R. Leite, and W. A. Ortiz, Physica B **284-288**, 1033 (2000); F. M. Araujo-Moreira, P. N. Lisboa-Filho, A. J. C. Lanfredi, W. A. Ortiz, S. M. Zanetti, E. R. Leite, A. W. Mombrú, L. Ghivelder, Y. G. Zhao, and V. Venkatesan, J. Magn. Magn. Mater. **226-230**, 283 (2001).

[5] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L. J. Sham, *ibid.* **140**, A1133 (1965).

[6] C. O. Rodriguez, R. Weht, and N. E. Christensen, Physica C **282-287**, 1621 (1997).

[7] H. Khosroabadi, M. R. Mohammadizadeh, and M. Akhavan, Physica C **370**, 85 (2002); Physica B **321**, 360 (2002).

[8] C. Ambrosch-Draxl, H. Auer, R. Kouba, E. Ya. Sherman, P. Knoll, and M. Mayer, Phys. Rev. B **65**, 064501 (2002).

[9] R. Kouba, C. Ambrosch-Draxl, and B. Zangger, Phys. Rev. B **60**, 9321 (1999).

[10] G. Y. Guo and W. M. Temmerman, Phys. Rev. B **41**, 6372 (1990).

[11] D. J. Singh, Phys. Rev. B **50**, 4106 (1994).

[12] C. Ambrosch-Draxl, P. Blaha, and K. Schwarz, J. Phys.: Condens. Matter **6**, 2347 (1994).

[13] M. Biagini, C. Calandra, and S. Ossicini, Phys. Rev. B **52**, 10468 (1995).

[14] A. I. Liechtenstein and I. I. Mazin, Phys. Rev. Lett. **74**, 1000 (1995).

[15] M. C. Qian, W. Y. Hu, Q. Q. Zheng, and H. Q. Lin, J. Appl. Phys. **85**, 4765 (1999).

[16] V. Ghanbarian and M. R. Mohammadizadeh, Phys. Status Solidi C **3**, 3122 (2006).

[17] V. Ghanbarian and M. R. Mohammadizadeh, Eur. Phys. J. B **61**, 309 (2008).

[18] J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992).

[19] G. Hilscher, E. Holland-Moritz, T. Holubar, H.-D. Jostarndt, V. Nekvasil, G. Schaudy, U. Walter, and G. Fillion, Phys. Rev. B **49**, 535 (1994); S. T. Boothroyd, S. M. Doyle, and R. Osborn, Physica C **217**, 425 (1993); K. Nehrke, M. W. Pieper, and T. Wolf, Phys. Rev. B **53**, 229 (1996); K. Nehrke and M. W. Pieper, Phys. Rev. Lett. **76**, 1936 (1996).

[20] A. I. Liechtenstein, V. I. Anisimov, and J. Zaanen, Phys. Rev. B **52**, R5467 (1995).

[21] I. I. Mazin, Phys. Rev. B **60**, 92 (1999).

[22] E. Sjöstedt, L. Nordström, and D. J. Singh, Solid State Commun. **114**, 15 (2000); G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt, and L. Nordström, Phys. Rev. B **64**, 195134 (2001).

[23] D. Singh, Phys. Rev. B **43**, 6388 (1991).

[24] K. Schwarz and P. Blaha, Comput. Mater. Sci. **28**, 259 (2003).

[25] M. Guillaume, P. Allenspach, J. Mesot, B. Roessli, U. Staub, P. Fischer, and A. Furrer, Z. Phys. B: Condens. Matter **90**, 13 (1993).

[26] V. I. Anisimov, F. Aryasetiawan, and A. I. Lichtenstein, J. Phys.: Condens. Matter **9**, 767 (1997), and references therein; M. T. Czyżyk and G. A. Sawatzky, Phys. Rev. B **49**, 14211 (1994).

[27] J. F. Herbst, R. E. Watson, and J. W. Wilkins, Phys. Rev. B **17**, 3089 (1978).

[28] P. Wei, H. W. Ying, and Z. Q. Qi, Physica C **209**, 400 (1993).

[29] Y. H. Ko, H. K. Kweon, H. C. Lee, and N. H. Hur, Physica C **224**, 357 (1994).

[30] Y. Yoshinari, H. Yasuoka, Y. Ueda, K. Koga, and K. Kosuge, J. Phys. Soc. Jpn. **59**, 3698 (1990).

[31] M. Takigawa, P. C. Hammel, R. H. Heffner, Z. Fisk, K. C. Ott, and J. D. Thompson, Phys. Rev. Lett. **63**, 1865 (1989).

[32] M. J. Stevenson and C. H. Townes, Phys. Rev. **107**, 635 (1957).

[33] M. Cyrot and D. Pavuna, *Introduction to Superconductivity and High-T_c Materials* (World Scientific, Singapore, 1992).

[34] H. A. Blackstead, J. D. Dow, I. Felner, and W. B. Yelon, Phys. Rev. B **63**, 094517 (2001).

[35] M. R. Mohammadizadeh and M. Akhavan, Phys. Rev. B **68**, 104516 (2003).

[36] M. Takata, T. Takayama, M. Sakata, S. Sasaki, K. Kodama, and M. Sato, Physica C **263**, 340 (1996).

[37] M. Merz, N. Nücker, E. Pellegrin, P. Schweiss, S. Schuppler, M. Kielwein, M. Knupfer, M. S. Golden, J. Fink, C. T. Chen, V. Chakarian, Y. U. Idzerda, and A. Erb, Phys. Rev. B **55**, 9160 (1997).

[38] M. W. Pieper, F. Wiekhorst, and T. Wolf, Phys. Rev. B **62**, 1392 (2000).