PHYSICAL REVIEW B **89**, 224505 (2014)

Orbital mixture effect on the Fermi-surface–T_c correlation in the cuprate superconductors: Bilayer vs. single layer

Hirofumi Sakakibara,[1,*] Katsuhiro Suzuki,[1] Hidetomo Usui,[2] Satoaki Miyao,[3] Isao Maruyama,[4] Koichi Kusakabe,[3] Ryotaro Arita,[5,6] Hideo Aoki,[7] and Kazuhiko Kuroki[2]

[1]*Department of Engineering Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan*
[2]*Department of Physics, Osaka University, Machikaneyama-Cho, Toyonaka, Osaka 560-0043, Japan*
[3]*Department of Materials Engineering Science, Osaka University, Machikaneyama-Cho, Toyonaka, Osaka 560-8531, Japan*
[4]*Department of Information and Systems Engineering, Fukuoka Institute of Technology, Wajiro-higashi, Higashi-ku, Fukuoka 811-0295, Japan*
[5]*Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan*
[6]*JST, PRESTO, Kawaguchi, Saitama 332-0012, Japan*
[7]*Department of Physics, The University of Tokyo, Hongo, Tokyo 113-0033, Japan*

(Received 11 March 2014; revised manuscript received 22 May 2014; published 9 June 2014)

By constructing $d_{x^2-y^2} - d_{z^2}$ two-orbital models from first principles, we have obtained a systematic correlation between the Fermi surface warping and theoretically evaluated T_c for various bilayer as well as single-layer cuprates. This reveals that a smaller mixture of the d_{z^2} orbital component on the Fermi surface leads simultaneously to larger Fermi-surface warping and higher T_c. The theoretical correlation strikingly resembles a systematic plot for the experimentally observed T_c against the Fermi surface warping due to Pavarini *et al.* [Phys. Rev. Lett. **87**, 047003 (2001)], and the present result unambiguously indicates that the d_{z^2} mixture is one key factor that determines T_c in the cuprates.

DOI: 10.1103/PhysRevB.89.224505 PACS number(s): 74.20.−z, 74.62.Bf, 74.72.−h

I. INTRODUCTION

In a family of superconductors in which the transition temperature T_c varies sensitively according to the lattice structure and/or the constituent elements, it is imperative to extract parameters that are systematically correlated with T_c. For the high-T_c cuprates in particular, Pavarini *et al.* have shown that there is a striking correlation between the experimentally observed T_c and the Fermi-surface warping [see Fig. 1(b)] [1]. Namely, they have obtained single-orbital tight-binding models for various cuprates to estimate the ratio "r" between the nearest and second-nearest-neighbor hoppings, which is a measure of the warping of the Fermi surface. Plotting the experimental T_c against the theoretically evaluated r, they noticed that T_c empirically increases with the Fermi surface warping.

The trend for higher T_c for more degraded nesting is rather puzzling, since, while there have been some approaches for explaining the trend [2–5], fluctuation exchange (FLEX) [6] as well as dynamical cluster approximation studies [6–8] have shown that the Fermi surface warping and T_c should theoretically be *anti*-correlated when the Cu-$d_{x^2-y^2}$ orbital (plus the hybridized oxygen $2p$ orbitals) alone is taken into account in the models. In order to resolve this puzzle, some of the present authors have previously introduced a two-orbital model that explicitly considers the d_{z^2} Wannier orbital on top of the $d_{x^2-y^2}$ [9,10]. In fact, there has been a long history of the study on possible importance of the d_{z^2} orbital and/or the apical oxygen [1,11–25]. In Refs. [9,10], we showed that ΔE, the level offset between $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals, dominates both the warping of the Fermi surface and T_c. It was shown, focusing on the single-layer cuprates, that La_2CuO_4 has, despite a better-nested Fermi surface, a lower T_c than those in $HgBa_2CuO_4$, $Tl_2Ba_2CuO_6$, and $Bi_2Sr_2CuO_6$ due to a strong d_{z^2} orbital mixture on the Fermi surface that degrades T_c. However, among the above mentioned four single-layer cuprates, only La_2CuO_4 has a small ΔE (i.e., a strong d_{z^2} mixture), so that we are still in need of a convincing study to clarify whether ΔE indeed controls T_c systematically in a wider range of cuprates that include the multilayer ones as analyzed in Pavarini's plot [1].

Thus the purpose of the present paper is to examine the systematics, where we extend the analysis to bilayer cuprates as well as those single-layer ones that have relatively lower T_c. This has enabled us to study the correlation between the theoretically estimated T_c and the Fermi-surface warping for a much wider class of existing materials [Fig. 1(a)]. The systematics have turned out to reproduce the experimental trend in T_c, and we shall unambiguously conclude that the d_{z^2} orbital mixture is indeed a key factor that strongly governs the T_c in the cuprates.

II. ORIGIN OF THE MATERIAL DEPENDENCE OF FERMI-SURFACE WARPING

A. Construction of the two-orbital model

Let us start with the construction of the two-orbital model. First-principles electronic structures of the materials are obtained with the VASP package [26], where experimentally determined lattice parameters are adopted. We have used the PBE exchange-correlation functional. We then employ the $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals as projection functions [27] to model the band structure around the Fermi energy. The main band around the Fermi energy contains considerable contributions from the oxygen $2p$ orbitals, so that they are effectively included in the Wannier functions. Similarly,

*sakakibara@presto.phys.sci.osaka-u.ac.jp

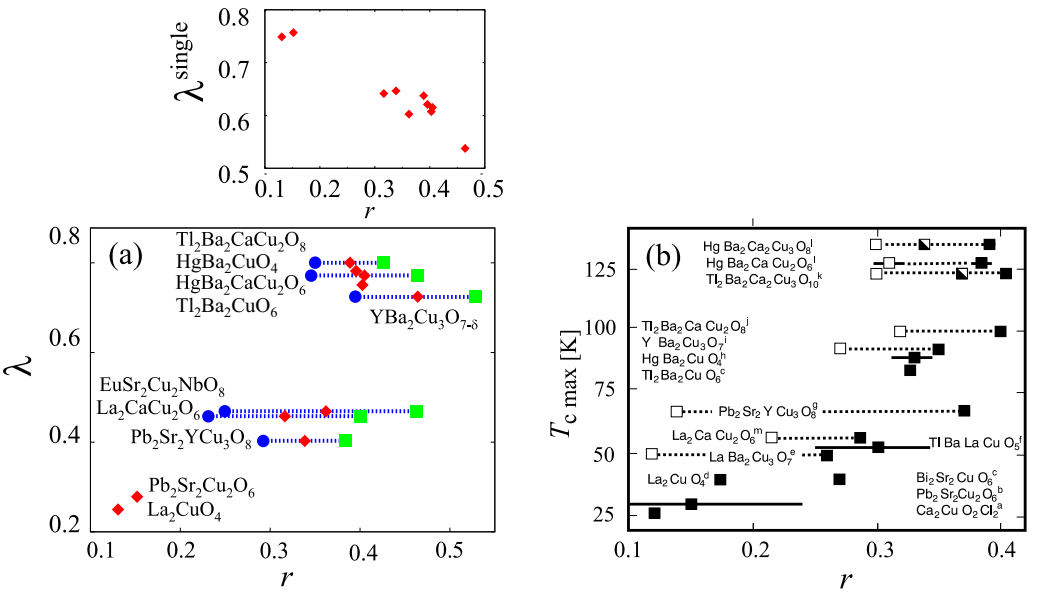

FIG. 1. (Color online) (a) Eigenvalue of the Eliashberg equation λ obtained for the two-orbital model plotted against $r = (|t_2| + |t_3|)/|t_1|$ that dominates the warping of Fermi surfaces. For bilayer cuprates r(diamonds), $r_{\rm inner}$(circles), and $r_{\rm outer}$(squares) are also shown while for single-layer cuprates only r is shown (defined in Sec. II B, see text). Inset: The $\lambda^{\rm single}$ obtained within the single-orbital model for the same materials. There, $r_{\rm inner}$,$r_{\rm outer}$ are not displayed for clarity, and $T = 0.02$ eV is adopted for calculating $\lambda^{\rm single}$. (b) Experimentally observed T_c plotted against $r \sim t'/t$ (taken from Ref. [1]). For multilayer cuprates, open and solid squares at the ends of the dashed line correspond to our $r_{\rm inner}$ and $r_{\rm outer}$, respectively.

the p_z orbital in the apical oxygens is implicitly included in the d_{z^2} Wannier orbital. Namely, we consider two kinds of antibonding state between the d orbitals of copper and p orbitals of oxygen in this model. In the bilayer systems, the total number of Wannier orbitals is four. Let us mention in passing that the present ΔE, the level offset between the two Wannier orbitals, should not be directly compared to the d-d excitation energy observed experimentally in, e.g., the RIXS experiments [28–30], because, while the present ΔE, defined for the Wannier orbitals consisting of Cu-3d and O-2p orbitals, is evaluated within the GGA scheme (with the correlation effects beyond the GGA taken into account in the FLEX procedure), RIXS experiments measure the energy that includes full electron correlation effects.

Figure 2 compares the band dispersion of the two-orbital model for eight cuprates [31]: single-layer (a) La_2CuO_4, (b) $Pb_2Sr_2Cu_2O_6$, and bilayer (c) $La_2CaCu_2O_6$, (d) $Pb_2Sr_2YCu_3O_8$, (e) $EuSr_2NbCu_2O_8$, (f) $YBa_2Cu_3O_{7-\delta}$(YBCO), (g) $HgBa_2CaCu_2O_6$(HBCO) and (h) $Tl_2Ba_2CaCu_2O_8$. The crystal structures are given in Refs. [33–40], respectively. Experimentally, the first five materials are known to have relatively lower T_c (<70 K), while the last three have higher T_c (>90 K) [41]. In Fig. 2, we display the weight of the d_{z^2} Wannier orbital with the thickness of the lines, which shows that there exist significantly strong d_{z^2} mixtures around the flat portions of the bands near the Fermi energy in (a)–(e). By contrast, compounds (f)–(h) have the d_{z^2} orbital components mostly on the bands well below the Fermi energy. In bilayer systems the main band is split into two, where the d_{z^2} component, if any, is seen to primarily reside on the upper band. The band splitting is known to be caused by the interlayer hoppings, which are mediated by orbitals spreading along the c axis such as the 4s and d_{z^2} orbitals [1]. In Fig. 2 we also display the Fermi surfaces at $k_z = 0$, where we can see that in (a)–(e) the (outer) Fermi surfaces are basically concave against the Γ point [$(k_x,k_y) = (0,0)$], while the inner Fermi surfaces (arising from the upper band) that have larger d_{z^2} weights are convex for bilayer systems in (c)–(e).

B. Suppression of the Fermi surface warping by the d_{z^2} orbital mixing

From the above result, we can see that the warping of the inner Fermi surface decreases as the d_{z^2} mixture becomes stronger. In the figure the band filling is fixed at $n = 2.85$, but we have checked that this tendency persists when the band filling is varied. Although this trend has been noticed in our previous studies [10], we can now describe this more systematically and quantitatively for various materials. For this purpose we have first to quantify the degree of warping of the Fermi surface. This is accomplished by constructing a *single*-orbital model so that the main bands intersecting the Fermi level are reproduced with a single Wannier orbital per site. This Wannier orbital mainly consists of the $d_{x^2-y^2}$ orbital, but also has tails with a d_{z^2} orbital character. We can then define the parameter, $r = (|t_2| + |t_3|)/|t_1|$ in terms of the second (t_2) and third (t_3) neighbor hoppings of the single-orbital model, which is a direct measure of the Fermi surface warping [1]. For bilayer materials, r can be defined with hoppings within each layer. Bilayers have two sites per unit cell with outer and inner Fermi surfaces, so that we can also obtain the respective measures of the warping of the outer and inner Fermi surfaces as $r_{\rm outer,inner} = (|t_2 \pm t_{2\perp}| + |t_3 \pm t_{3\perp}|)/|t_1 \pm t_{1\perp}|$, where $t_{i\perp}$ is the interlayer hopping to the sites vertically above (or below)

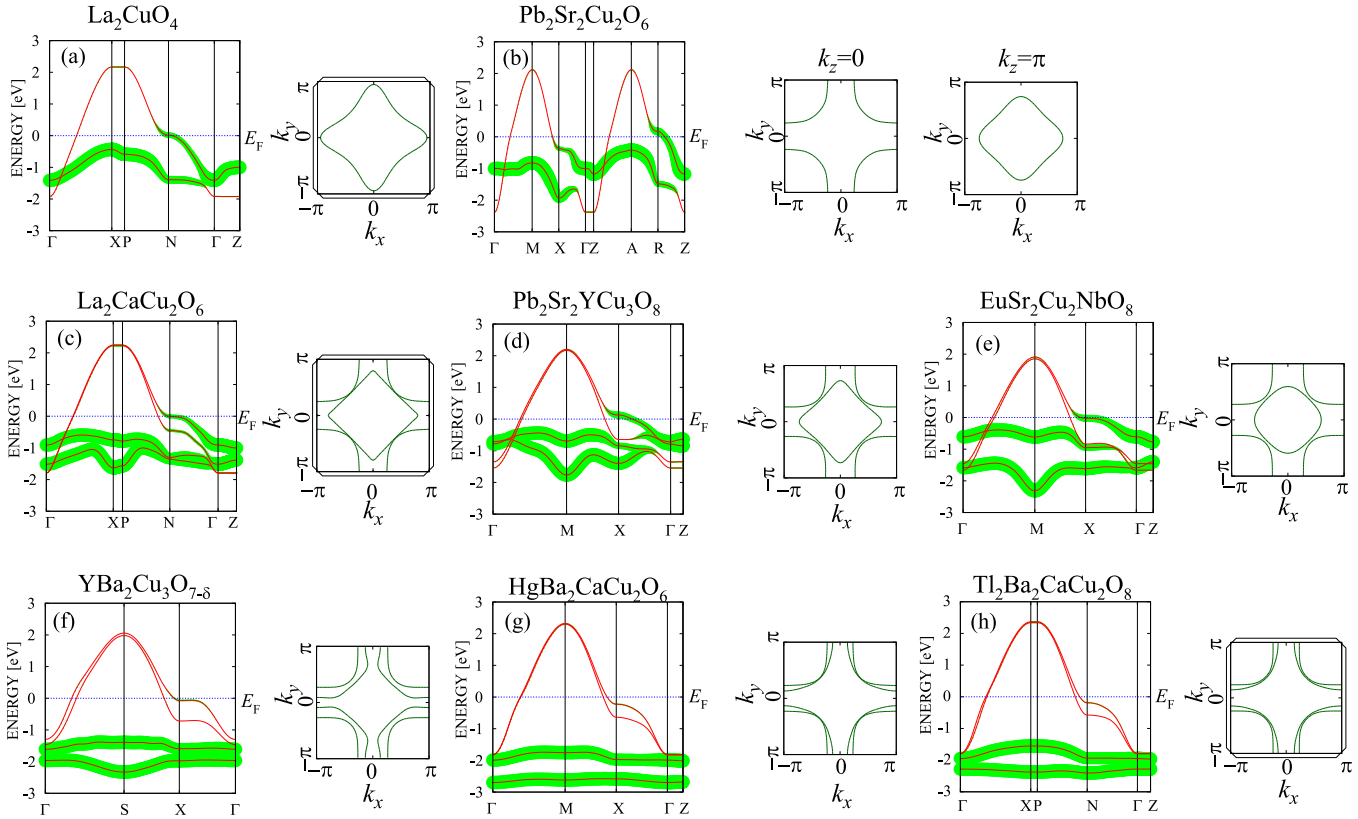

FIG. 2. (Color online) Band structures in the two-orbital model for (a) La_2CuO_4, (b) $Pb_2Sr_2Cu_2O_6$, (c) $La_2CaCu_2O_6$, (d) $Pb_2Sr_2YCu_3O_8$, (e) $EuSr_2NbCu_2O_8$, (f) $YBa_2Cu_3O_{7-\delta}$, (g) $HgBa_2CaCu_2O_6$, and (h) $Tl_2Ba_2CaCu_2O_8$. The thickness of the lines represents the strength of the d_{z^2} orbital character. The insets depict the Fermi surfaces at $k_z = 0$, except in (b), where the Fermi surface at $k_z = \pi$ is also shown to display a relatively strong k_z dispersion. The Fermi energy is set for the total band filling $n = 2.85$ per layer (15 percent hole doping).

the ith neighbor. We stress that r in the single-orbital model includes the effects of both the hoppings within the $d_{x^2-y^2}$ Wannier orbitals and those between the $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals in the two-orbital model.

In Fig. 3(a), we plot r against ΔE for all the bilayer cuprates considered. The result shows that r tends to increase with ΔE, which can be understood as follows [9,10]. In the two-orbital model that explicitly considers the d_{z^2} orbital, the second (and also the third) neighbor hopping takes place via two paths, i.e., (i) directly between $d_{x^2-y^2}$ Wannier orbitals and (ii) indirectly via the d_{z^2} orbital. As ΔE becomes smaller, path (ii) becomes more effective. In the single-orbital model, the two paths both contribute to t_2 and t_3, but they have opposite signs, so that $t_2(t_3)$ and hence r are smaller when the contribution from path (ii) is larger. To be precise, $r_{\rm YBCO}$ is larger than $r_{\rm HBCO}$ despite $\Delta E_{\rm YBCO}$ being smaller than $\Delta E_{\rm HBCO}$. By analyzing the two-orbital model, we find that the ratio $(|t_2| + |t_3|)/|t_1|$ *within the* $d_{x^2-y^2}$ *Wannier orbitals*, i.e., path (i), which we refer to as $r_{x^2-y^2}$ (Ref. [42]), is significantly larger in YBCO, and we are coming back to this point below.

III. MANY-BODY ANALYSIS

We now move on to superconductivity. As shown in our previous studies [9,10], it is imperative to adopt the two-orbital model that explicitly considers the d_{z^2} orbital to have a reliable estimate of T_c. In the two-orbital model we consider intra- and interorbital electron-electron interactions. The intraorbital U is considered to be in the range of 7–10t (where $t \simeq 0.45$ eV is the nearest-neighbor hopping) for the cuprates, so we take the intraorbital $U = 3.0$ eV. The Hund's coupling J and the pair hopping J' are typically $\sim 0.1U$, so we take $J = J' = 0.3$ eV. Here we observe the orbital rotational symmetry which gives the interorbital $U' = U - 2J = 2.4$ eV. We apply FLEX [43,44] to this multiorbital Hubbard model and solve the linearized Eliashberg equation. In multiorbital FLEX, the Green's function and spin and charge susceptibilities are given as matrices [45]. The eigenvalue of the Eliashberg equation λ increases upon lowering the temperature, and reaches unity at $T = T_c$. Therefore λ at a fixed temperature can be used as a qualitative measure for T_c. The temperature is fixed at $k_{\rm B}T = 0.01$ eV in the present calculation. The total band filling (number of electrons /site) is fixed at $n = 2.85$, for which the filling of the main band amounts to 0.85 (15% hole doping). We take a $32 \times 32 \times 4$ k-point mesh for the three-dimensional lattice with 1024 Matsubara frequencies. FLEX takes account of the self-energy correction self-consistently and amends the overestimated tendency toward magnetism in the random-phase approximation. On the other hand, FLEX cannot reproduce the Mott transition that should be present at half filling nor the T_c suppression in the underdoped regime. Therefore, we stick to the optimal doping regime in the present study.

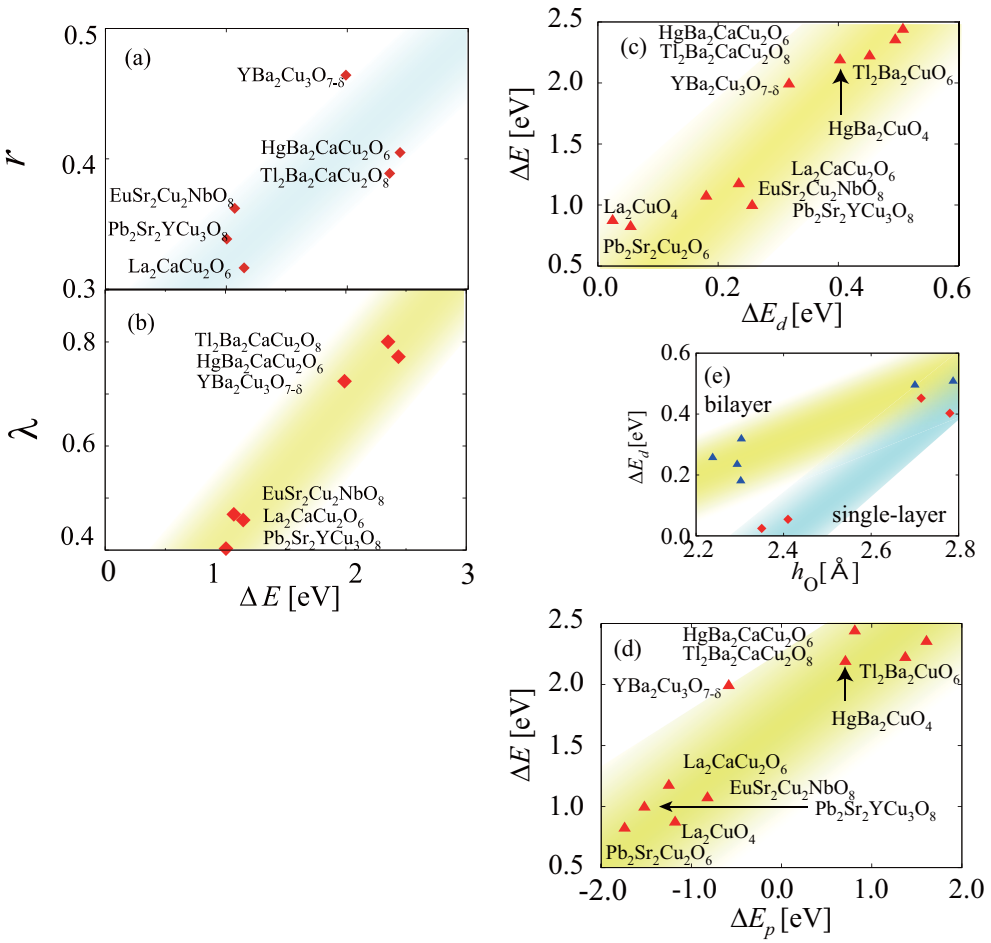

FIG. 3. (Color online) (a) The parameter $r = (|t_2| + |t_3|)/|t_1|$ in the single-orbital model, which is a measure of the Fermi surface warping, plotted against ΔE for the bilayer cuprates. (b) The eigenvalue λ of the Eliashberg equation for d-wave superconductivity is plotted against ΔE for materials (c)–(h) in Fig. 2. (c) ΔE is plotted against ΔE_d. (d) ΔE is plotted against ΔE_p. (e) ΔE_d is plotted against h_O for single-layer (red diamonds) and bilayer (blue triangles) cuprates.

IV. CORRELATION AMONG T_c, FERMI SURFACE, AND LATTICE STRUCTURE

A. Correlation between T_c and the Fermi surface

In Fig. 3(b) we plot λ against ΔE calculated for the five bilayer cuprates. We can see a very well-defined correlation between ΔE and λ. If we combine Figs. 3(a) and 3(b), we can look at the relation between λ (obtained for the two-orbital model) against the measure of the Fermi surface warping r (defined in terms of the single-orbital model) [46], which is precisely Fig. 1(a). Since λ is a measure of T_c, we can immediately notice that the figure strikingly resembles Pavarini's plot [1] for the experimentally observed T_c against r in Fig. 1(b) [49]. This is the key result in the present paper.

For comparison, we show in the inset of Fig. 1(a) the eigenvalue of the Eliashberg equation within the *single-orbital* model, $\lambda^{\rm single}$, for the same materials. Here we take the same value of on-site U as in the two-orbital model, but raise the temperature to $T = 0.02$ eV, since FLEX convergence in the single-orbital model is degraded for small r at lower temperatures. The result for $\lambda^{\rm single}$ exhibits an opposite tendency of decreasing with r, which firmly endorses that the d_{z^2} orbital mixture is indeed a key factor that determines T_c of the cuprates.

Besides the overall trend, we can also note the following two features. First, in our λ-r plot λ is larger for bilayer systems than in single-layer ones, which reflects the difference in ΔE. There may be some interlayer many-body interactions (such as the pair hopping [50]) that can further enhance T_c in the bilayer systems, which is not taken into account here. Another point to note is the comparison between YBCO and HBCO. Despite $r_{\rm YBCO} > r_{\rm HBCO}$, λ obtained here is larger for HBCO, which agrees with the experimental results for T_c. As mentioned above, $r_{x^2-y^2}$ is very large for YBCO, which is the main reason why the single-orbital r is large in this material. Namely, a smaller λ in YBCO is caused by a large $r_{x^2-y^2}$ rather than by a small ΔE, which we have actually checked by varying these quantities in a range covering these materials.

B. Origin of the material dependence of ΔE

Finally, let us pinpoint the origin of the material dependence of ΔE. For this purpose, we now construct a model that explicitly considers all of the Cu-3d and O-2p orbitals by introducing as many number of Wannier orbitals. Namely,

the level offset ΔE_d between Cu-$d_{x^2-y^2}$ and Cu-d_{z^2} and the level offset ΔE_p between in-plane O-p_σ and apical-O-p_z determine the final ΔE as shown in our previous study [10]. The level offsets, $\Delta E_d = E(d_{x^2-y^2}) - E(d_{z^2})$ and $\Delta E_p = E(p_\sigma) - E(p_z)$, are defined as the differences in the onsite energies between the atomiclike orbitals. In Figs. 3(c) and 3(d), we plot ΔE against ΔE_d and ΔE_p.

We are now in a position to discuss how the two level offsets are determined by the lattice structure. The apical oxygen height h_O controls the crystal-field splitting, so that h_O is correlated with ΔE_d (Ref. [10]). In the bilayer materials, however, we can see that ΔE_d tends to be larger than in the single-layer ones despite the small h_O. We can identify this to be coming from the *pyramidal* coordination of the oxygen atoms with one apical oxygen per Cu in the bilayer cuprates, as opposed to the octahedral coordination with two apical oxygens in single-layer cuprates. Thus the effect of the apical oxygen is more or less halved in the bilayer systems, so that the *effective* h_O becomes larger. This in turn makes ΔE_p play a more important role in the material dependence of ΔE and hence T_c. For example, $La_2CaCu_2O_6$ and YBCO have very small values of h_O [in Fig. 3(e)], and consequently they have similar values of ΔE_d. However, YBCO has a much larger ΔE_p (smaller absolute value), which results in a larger ΔE. ΔE_p playing a more important role than ΔE_d is also seen in terms of the Madelung energy difference, ΔV_A, between the apical and in-plane oxygens. T_c is found to be correlated with ΔV_A rather than the apical oxygen height as in a previous study (Ref. [21]), where ΔV_A is in turn correlated with ΔE_p [10]. One way to control h_O is to apply a hydrostatic pressure to decrease it, but this has small effect on T_c, especially for multilayer cuprates because of the reason mentioned above [51].

V. CONCLUDING REMARKS

To summarize, we have revealed a systematic correlation between the Fermi surface warping and the theoretically evaluated T_c by constructing two- and single-orbital models of various bilayer as well as single-layer cuprates. A striking agreement of the theoretical result with Pavarini's plot for experimental T_c's [1] unambiguously indicates that the d_{z^2} mixture is indeed a key factor that determines T_c in the cuprates. The level offset ΔE between $d_{x^2-y^2}$ and d_{z^2} Wannier orbitals mainly depends on two parameters, ΔE_d and ΔE_p, but in multilayer cuprates the latter plays a more important role than the former, so that the apical oxygen height is less important.

Let us recapitulate that the strongly warped Fermi surface is not the *cause* of the high T_c, but a consequence of the r-T_c correlation where the d_{z^2} orbital mixture (i.e., small ΔE) happens to suppress both of the warping (the single-orbital r) and T_c *at the same time*. Conversely, we can exploit this to note that higher-T_c materials can in principle be conceived if we can realize smaller r where r is reduced due to smaller $r_{x^2-y^2}$ (the hopping ratio within the $d_{x^2-y^2}$ Wannier orbitals) rather than due to smaller ΔE. The reason why we have an almost universal r-T_c correlation in actual materials is traced back to r that increases with ΔE [Fig. 3(a)], because $r_{x^2-y^2}$ does not vary widely within the known cuprates. From these observations, we here propose that *designing* materials with small d_{z^2} mixture and strongly reduced $r_{x^2-y^2}$ (which would give a small r) may lead to higher T_c than the known cuprates, provided other conditions are essentially unchanged [42].

ACKNOWLEDGMENTS

H.S. acknowledges Keon Kim and Shinnosuke Sato for discussions on $EuSr_2NbCu_2O_8$. We wish to thank Ole Andersen for permission to quote Fig. 5 of Ref. [1]. The numerical calculations were performed at the Supercomputer Center, ISSP, University of Tokyo. This study has been supported by Grants-in-Aid for Scientific Research from JSPS [Grants No. 23009446 (H.S.), No. 25009605 (K.S.), No. 23340095 (R.A.), No. 24340079 (K. Kuroki), No. 23540408 and No. 26400357 (K. Kusakabe and I.M.)]. R.A. acknowledges financial support from JST-PRESTO.

[1] E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001).
[2] C. T. Shih, T. K. Lee, R. Eder, C. Y. Mou, and Y. C. Chen, Phys. Rev. Lett. **92**, 227002 (2004).
[3] H. Yokoyama, M. Ogata, Y. Tanaka, K. Kobayashi, and H. Tsuchiura, J. Phys. Soc. Jpn. **82**, 014707 (2013).
[4] S. Shinkai, H. Ikeda, and K. Yamada, J. Phys. Soc. Jpn. **75**, 104712 (2006).
[5] T. Moriya and K. Ueda, J. Phys. Soc. Jpn. **63**, 1871 (1994).
[6] For a review, see, e.g., D. J. Scalapino, in *Handbook of High Temperature Superconductivity*, edited by J. R. Schrieffer and J. S. Brooks (Springer, New York, 2007), Chap. 13.
[7] P. R. C. Kent, T. Saha-Dasgupta, O. Jepsen, O. K. Andersen, A. Macridin, T. A. Maier, M. Jarrell, and T. C. Schulthess, Phys. Rev. B **78**, 035132 (2008).
[8] Th. Maier, M. Jarrell, Th. Pruschke, and J. Keller, Phys. Rev. Lett. **85**, 1524 (2000).
[9] H. Sakakibara, H. Usui, K. Kuroki, R. Arita, and H. Aoki, Phys. Rev. Lett. **105**, 057003 (2010).
[10] H. Sakakibara, H. Usui, K. Kuroki, R. Arita, and H. Aoki, Phys. Rev. B **85**, 064501 (2012).
[11] C. Weber, K. Haule, and G. Kotliar, Phys. Rev. B **82**, 125107 (2010).
[12] C. Weber, C. Yee, K. Haule, and G. Kotliar, Europhys. Lett. **100**, 37001 (2012).
[13] T. Takimoto, T. Hotta, and K. Ueda, Phys. Rev. B **69**, 104504 (2004).
[14] A. J. Freeman and J. Yu, Physica B **150**, 50 (1988).
[15] X. Wang, H. T. Dang, and A. J. Millis, Phys. Rev. B **84**, 014530 (2011).
[16] L. Hozoi, L. Siurakshina, P. Fulde, and J. van den Brink, Sci. Rep. **1**, 65 (2011).
[17] S. Uebelacker and C. Honerkamp, Phys. Rev. B **85**, 155122 (2012).

[18] M. Mori, G. Khaliullin, T. Tohyama, and S. Maekawa, Phys. Rev. Lett. **101**, 247003 (2008).

[19] H. Kamimura and M. Eto, J. Phys. Soc. Jpn. **59**, 3053 (1990); M. Eto and H. Kamimura, *ibid.* **60**, 2311 (1991).

[20] K. Shiraishi, A. Oshiyama, N. Shima, T. Nakayama, and H. Kamimura, Solid State Commun. **66**, 629 (1988).

[21] Y. Ohta, T. Tohyama, and S. Maekawa, Phys. Rev. B **43**, 2968 (1991).

[22] S. Maekawa, J. Inoue, and T. Tohyama, in *The Physics and Chemistry of Oxide Superconductors*, edited by Y. Iye and H. Yasuoka (Springer-Verlag, Berlin, 1992), pp. 105–115.

[23] O. K. Andersen, A. I. Liechtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids **56**, 1573 (1995).

[24] L. F. Feiner, J. H. Jefferson, and R. Raimondi, Phys. Rev. Lett. **76**, 4939 (1996).

[25] L. Hozoi and M. S. Laad, Phys. Rev. Lett. **99**, 256404 (2007).

[26] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993); G. Kresse and J. Furthmüller, *ibid.* **54**, 11169 (1996); [http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html]. Here we adopt the GGA-PBEsol exchange correlation functional introduced by J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. **100**, 136406 (2008), and the wave functions are expanded with plane waves up to a cutoff energy of 550 eV. $10^3 k$-point meshes are used.

[27] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997); I. Souza, N. Marzari, and D. Vanderbilt, *ibid.* **65**, 035109 (2001); The Wannier functions are generated by the code developed by A. A. Mostofi, J. R. Yates, N. Marzari, I. Souza, and D. Vanderbilt (http://www.wannier.org/).

[28] M. M. Sala, V. Bisogni, C. Aruta, G. Balestrino, H. Berger, N. B. Brookes, G. M. de Luca, D. Di. Castro, M. Grioni, M. Guarise, P. G. Medaglia, F. Miletto Granozio, M. Minola, P. Perna, M. Radovic, M. Salluzzo, T. Schmitt, K. J. Zhou, L. Braicovich, and G. Ghiringhelli, New J. Phys. **13**, 043026 (2011).

[29] M. Le Tacon, M. Minola, D. C. Peets, M. Moretti Sala, S. Blanco-Canosa, V. Hinkov, R. Liang, D. A. Bonn, W. N. Hardy, C. T. Lin, T. Schmitt, L. Braicovich, G. Ghiringhelli, and B. Keimer, Phys. Rev. B **88**, 020501 (2013).

[30] J. Schlappa, K. Wohlfeld, K. J. Zhou, M. Mourigal, M. W. Haverkort, V. N. Strocov, L. Hozoi, C. Monney, S. Nishimoto, S. Singh, A. Revcolevschi, J.-S. Caux, L. Patthey, H. M. Ronnow, J. van den Brink, and T. Schmitt, Nature (London) **485**, 82 (2012).

[31] Here, the f orbitals in the Eu atom are treated as a core potential, and chain states in material (f) are neglected. The material (e) has some variation in the chemical composition of the Nb site (Nb→Fe, Ga, Al, Co, or Mo), and the situation is likely to be similar in most of them Ref. [32].

[32] J. Shimoyama, K. Otzschi, T. Hinouchi, and K. Kishio, Physica C **341**, 563 (2000); Y. Morita, H. Yamauchi, and M. Karppinen, Solid State Commun. **127**, 493 (2003); J. T. Vaughey, J. P. Thiel, E. F. Hasty, A. Groenke, Charlotte L. Stern, K. R. Poeppelmeier, B. Dabrowski, D. G. Hinks, and A. W. Mitchell, Chem. Mater. **3**, 935 (1991); A. Ono, Jpn. J. Appl. Phys. **36**, 849 (1997); I. Felner and E. Galstyan, Phys. Rev. B **69**, 024512 (2004).

[33] J. D. Jorgensen, H.-B. Schuttler, D. G. Hinks, D. W. Capone, K. Zhang, M. B. Brodsky, and D. J. Scalapino, Phys. Rev. Lett. **58**, 1024 (1987).

[34] H. W. Zandbergen, W. T. Fu, J. M. van Ruitenbeek, L. J. de Jongh, G. van Tendeloo, and S. Amelinckx, Physica C **159**, 81 (1989).

[35] R. J. Cava, A. Santoro, J. J. Krajewski, R. M. Fleming J. V. Waszczak, W. F. Peck, Jr., and P. Marsh, Physica C **172**, 138 (1990).

[36] M. A. Subramainan, J. Gopalakrishan, C. C. Torardi, P. L. Gai, E. D. Boyes, T. R. Askew, R. B. Flippen, W. E. Farneth, and A. W. Sleight, Physica C **157**, 124 (1989).

[37] The crystal structure is given in C. Greaves and P. R. Slater, IEEE Trans. Mag. **27**, 1174 (1991). Superconductivity with $T_c = 40$ K has recently been observed in K. Kim, M. Kato, T. Noji, and Y. Koike, Physica C **492**, 165 (2013).

[38] M. A. Beneo, L. Soderholm, D. W. Capone, II, D. G. Hinks, J. D. Jorgensen, J. D. Grace, Ivan K. Schuller, C. U. Segre, and K. Zhang, Appl. Phys. Lett. **51**, 57 (1987).

[39] B. A. Hunter, J. D. Jorgensen, J. L. Wagner, P. G. Radaelli, D. G. Hinks, H. Shaked, and R. L. Hitterman, and R. B. Von Dreele, Physica C **221**, 1 (1994).

[40] M. A. Subramanian, J. C. Calabrese, C. C. Torardi, J. Gopalakrishnan, T. R. Askew, R. B. Fluppen, K. J. Morrisey, Y. Chowdhry, and A. W. Sleight, Nature (London) **332**, 420 (1988).

[41] H. Eisaki, N. Kaneko, D. L. Feng, A. Damascelli, P. K. Mang, K. M. Shen, Z.-X. Shen, and M. Greven, Phys. Rev. B **69**, 064512 (2004).

[42] H. Sakakibara, K. Suzuki, H. Usui, K. Kuroki, R. Arita, D. J. Scalapino, and H. Aoki, Phys. Rev. B **86**, 134520 (2012).

[43] N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).

[44] T. Dahm and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995).

[45] K. Yada and H. Kontani, J. Phys. Soc. Jpn. **74**, 2161 (2005).

[46] We have also calculated λ for Hg- and Tl- single-layer cuprates. The structure is taken from Refs. [47,48], respectively.

[47] J. L. Wagner, P. G. Radaelli, D. G. Hinks, J. D. Jorgensen, J. F. Mitchell, B. Dabrowski, G. S. Knapp, and M. A. Beno, Physica C **210**, 447 (1993).

[48] C. C. Torardi, M. A. Subramanian, J. C. Calabrese, J. Gopalakrishnan, E. M. McCarron, K. J. Morrissey, T. R. Askew, R. B. Flippen, U. Chowdhry, and A. W. Sleight, Phys. Rev. B **38**, 225 (1988).

[49] Strictly speaking, there are discrepancies in the evaluated r in some materials, which may be due to the difference in the methods for obtaining r.

[50] A. recent theoretical study shows that the interlayer pair hoppings give some enhancement of T_c in Hg multilayer cuprates: K. Nishiguchi, K. Kuroki, R. Arita, T. Oka, and H. Aoki, Phys. Rev. B **88**, 014509 (2013).

[51] H. Sakakibara, K. Suzuki, H. Usui, K. Kuroki, R. Arita, D. J. Scalapino, and H. Aoki, J. Phys.: Conf. Ser. **454**, 012021 (2013).