

Electronic mechanism of critical temperature variation in $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$

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We have performed systematic studies of the trend of the critical temperature T_c due to both Madelung site potential difference between in-plane oxygen and copper sites ΔV_M and interlayer effect in the optimally doped 123 superconductors $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$. ΔV_M is found to decrease with the increase of the trivalent rare-earth ionic radius $r_{R^{3+}}$. This change enhances the next-nearest-neighbor hopping integral t' , which results in the experimentally observed increase of T_c with $r_{R^{3+}}$. The coherent interlayer single-particle hopping t_\perp has a more profound effect than t' on the nearly linear trend of T_c as a function of $r_{R^{3+}}$. These results reveal the importance of the electronic origin of the rare-earth ionic size effect on T_c in this family.

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I. INTRODUCTION

Ever since the discovery of the high-critical-temperature (high- T_c) superconductivity on cuprate ceramics, a satisfactory theory of this singular phenomenon has not been completed. Nevertheless, several features have been shown to play a key role in the appearance of superconductivity in these materials. These are a layered crystal structure, a strong antiferromagnetic coupling between neighbor Cu^{2+} ions to form two-dimensional magnetic layers, a peculiar electronic structure, and appropriate doping of the so-called “parent compounds,” typically La_2CuO_4 or $\text{YBa}_2\text{Cu}_3\text{O}_6$. It is widely accepted that the stoichiometric proximity between the superconducting and insulating phases and the interaction of carriers with magnetic degrees of freedom are essential for the existence of high- T_c superconductivity. Inspired by the pioneering ideas of Torrance and Metzger¹ about the relevance of the Madelung potential in determining the insulating, semiconductor, or metallic character of a large family of oxides, researchers^{2,3} have been intensively studying whether charge transfer within the plane is via the long-range Madelung site potentials V_M . However, if the essential physics of the cuprates within the CuO_2 layers is common to all superconducting compounds, then the origin of their widely differing values of the maximum T_c must originate outside of the CuO_2 layers. The long-range nature of the Madelung site potential difference between in-plane oxygen and copper sites, ΔV_M , has the advantage of incorporating the influence of interplanar interactions, which should play a considerable role in the determination of T_c . Therefore, ΔV_M might have the capacity to incorporate interlayer effect. However, this is still an open question.

The typical 123 family of optimally doped bilayer compounds, $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ ($\delta \sim 0$), is a good candidate for investigating this topic. Since the compositions in this study are at optimal doping, the dependence of charge transfer between the chain and plane is removed. $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ is the first high- T_c superconductor whose T_c is above the boiling tem-

perature of liquid nitrogen (77 K). Substitution of Y with rare-earth elements leads to a systematic variation of T_c among the optimally doped $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ series. That is, the maximum T_c modestly increases with increasing the trivalent rare-earth ionic radius ($r_{R^{3+}}$).^{4,5} Optimally doped $\text{NdBa}_2\text{Cu}_3\text{O}_{7-\delta}$ has a T_c as high as 96 K.⁵ Understanding this ionic size effect in these materials is very important not only because it can shed light on a possible method to increase T_c at the ambient condition through the application of chemical pressure by element substitution, but also because it may provide an important clue in determining the possible mechanism responsible for the superconductivity in high- T_c cuprates. Moreover, there is growing interest in $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ for industrial applications. For example, in many bulk forms and multilayer applications, Y is replaced by Nd, Sm, or other rare-earth elements.^{6,7} Although a nice trend of the maximum T_c in $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductors has been revealed previously,^{4,5} detailed studies at the microscopic scale are missing due to the complexity of both the geometry and electronic structures.

In this paper, we investigate the variation of ΔV_M among the nearly optimally doped $R\text{Ba}_2\text{Cu}_3\text{O}_{7-\delta}$ compounds. We find that ΔV_M systematically increases with an increase of the trivalent rare-earth ionic radius. This systematic increase results in an enhancement of the next-nearest-neighbor hopping integral t' , accordingly. We therefore obtain a modest increase of T_c with the rare-earth ionic radius in this series on the basis of a d -wave BCS formalism by using a three-dimensional dispersion relation. The experimentally observed several Kelvin increase of T_c can be well reproduced when we considered the interlayer single-particle hopping. Our results suggest that the rare-earth ionic size effect is an electronic origin.

II. MADELUNG SITE POTENTIALS

Since the parent materials of high- T_c cuprate superconductors can be considered as charge-transfer insulators, ionic

bonding makes a large contribution to the lattice energy. It suggests that the methods of conventional oxides can be applied to study atomistic phenomena in cuprates. The cuprates turn into superconductors at a proper doping level and temperature. However, the charge carrier density is very low compared with that of conventional metals. In addition, the charge carriers are confined within copper-oxygen planes. Consequently, the screening effect is not so strong as that of conventional metals. In fact, many previous theoretical investigations are based on such an ionic picture, generating lots of valuable information.⁸

Considering that T_c varies with doping level, we should choose structures at optimal-doped composition to explore the intrinsic trend among $RBa_2Cu_3O_{7-\delta}$. Fortunately, a systematic low-temperature neutron diffraction study of the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds has been done by Guillaume *et al.*⁹ Our calculations are based on these structural data. In ionic crystals, the Madelung site potential at a given site is defined as the electrostatic potential due to charge monopoles, after the charge monopole located at that site has been removed—i.e., the potential due to all other monopoles in the system. The other points remain fixed for the sake of the calculation. The present calculations were done using the Ewald method.¹⁰ In the formulation of Tosi the formulas are¹¹

$$\begin{aligned} \phi(\vec{r}'_p) &= \frac{1}{\pi v} \sum_h ' S(\vec{h}) \vec{k}_h^{-2} \exp(-\pi^2 \eta^2 \vec{k}_h^2 + 2\pi i \vec{k}_h \vec{r}'_p) \\ &+ \sum_l ' \sum_p \zeta_p \frac{1 - F\left(\frac{|\vec{r}'_p - \vec{r}_l - \vec{r}_p|}{\eta}\right)}{|\vec{r}'_p - \vec{r}_l - \vec{r}_p|} - \frac{2\zeta'_p}{\eta\pi^{1/2}}, \\ S(\vec{h}) &= \sum_p \zeta_p \exp(-2\pi i \vec{k}_h \vec{r}_p), \\ F(m) &= 2\pi^{-1/2} \int_0^m \exp(-m^2) dm, \\ m &= \frac{|\vec{r}'_p - \vec{r}_l - \vec{r}_p|}{\eta}. \end{aligned} \quad (1)$$

The symbols have the following meaning: \vec{r}'_p and ζ'_p , position vector and charge of the point at which the potential will be calculated; \vec{r}_p and ζ_p , position vector and charge of other ions in the unit cell; $\vec{k}_h = h_1 \vec{a}^* + h_2 \vec{b}^* + h_3 \vec{c}^*$ is in the reciprocal space; $\vec{r}_l = l_1 \vec{a} + l_2 \vec{b} + l_3 \vec{c}$ is in the coordination space; \sum'_h runs over integers values of h_1, h_2, h_3 except the zero point; \sum_p runs over all positions; \sum'_l runs over integers values of l_1, l_2, l_3 except the zero point; η is the half-width of the Gaussian function; v is the volume of the unit cell.

A number of investigators have made use of the ionic crystal model as a starting point for the description of the electronic structure of cuprate superconductors, since their insulating parent materials can be regarded as ionic crystal to good accuracy. The Madelung potential at each lattice site can provide important information on the structural and electronic properties of this ionic system. In particular, the dif-

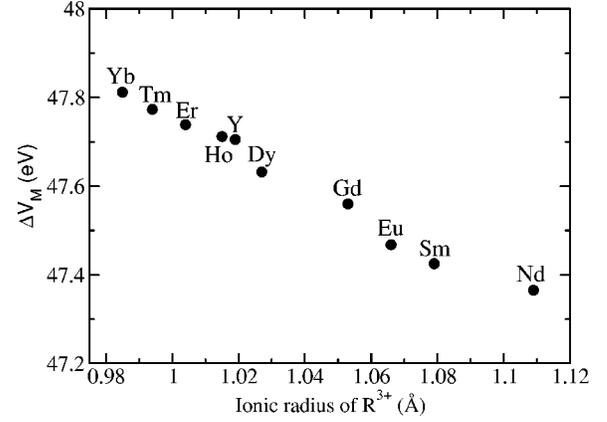


FIG. 1. Rare-earth ionic radius ($r_{R^{3+}}$) dependence of the Madelung site potentials between in-plane oxygen and copper, ΔV_M , for the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds.

ference in the Madelung site potentials between in-plane oxygen and copper,¹

$$\Delta V_M = V_M(\text{O}_{\text{plane}}) - V_M(\text{Cu}_{\text{plane}}), \quad (2)$$

has been proven to play an essential role in the characterization of the electronic structure.

Based on the neutron diffraction data of the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$,⁹ we have calculated the difference of Madelung site potentials ΔV_M . Figure 1 shows the calculated ΔV_M as a function of the rare-earth ionic radius $r_{R^{3+}}$. The rare-earth ionic radii were taken from the work of Shannon.¹² ΔV_M was observed to decrease with increasing $r_{R^{3+}}$. Considering the experimental fact that T_c modestly increases with increasing $r_{R^{3+}}$,^{4,5} our present results suggest that there is a nearly inverse linear relation between ΔV_M and T_c . This inverse linear relation has also observed previously in many hole-doped copper oxides.³ Actually, ΔV_M is more like a specific parameter which includes the contribution from both the apical oxygen and CuO_2 plane.

Studies of charge distribution^{13,14} have revealed that the optimal density of hole carriers n_H^{opt} decreases with increasing $r_{R^{3+}}$ in the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$. This implies that both the difference of the Madelung site potentials and the hole carrier density reflect an essentially equivalent physical content. Therefore, at optimal doping, these two interesting quantities provide an effective measure of the intrinsic variation of the maximum value of T_c . That is, superconducting cuprates with larger T_c tend to have a smaller n_H^{opt} or ΔV_M . This tendency has been found to be well held in typical monolayer cuprates.¹⁵

III. NEXT-NEAREST-NEIGHBORING HOPPING INTEGRAL

In the following we consider the modification of the next-nearest-neighboring hopping integral t' to gain better understanding of the striking correlation between ΔV_M and T_c . It is well established that the hole dispersion for the t - t' - J model is approximately given by^{16,17}

$$\varepsilon_k = (J + 2t') \cos k_x \cos k_y + \frac{J}{4} (\cos 2k_x + \cos 2k_y). \quad (3)$$

The importance of t' has been emphasized by Lee¹⁸ based on an idea that at low doping the t' term causes a different physics as compared with that of the original t - J model, since a hole can propagate on the same sublattice without disturbing spins. The sign of t' in the resulting t - t' - J model changes between the hole and electron doping systems: $t > 0$ and $t' < 0$ for the hole-doped system and $t < 0$ and $t' > 0$ for the electron-doped system. The sign difference originates from the fact that the d^9 state has a positive charge, while the d^{10} has a negative one as compared with the d^9 state. Thus the location of the saddle points is largely determined by the intrasublattice hopping parameter t' rather than by t and/or J . The same holds for the flatness of the dispersion near the saddle points and thus for the width of the van Hove singularity.

The hopping parameter t' can be determined from the three- or more-band Hubbard model.¹⁷ When the Cu-O hopping integral t_{pd} (between $3d_{x^2-y^2}$ and p_σ orbitals) is much less than both the Cu-Cu Coulomb repulsion U_d at O site and Cu-O energy-level splitting Δ , the dependence of t' on the initial parameters in the lowest order of t_{pd}/Δ can be written as¹⁹

$$t' = 0.09 \frac{t_{pd}^2}{\Delta - 1.45t_{pp}} - 0.124t_{pp}, \quad (4)$$

for a hole-doped system. Here t_{pp} is the transfer integral between the nearest-neighbor oxygen p_σ orbitals.

The Cu-O energy-level (on O p_σ and Cu $3d_{x^2-y^2}$ orbitals) splitting Δ is given by³

$$\Delta = \frac{\Delta V_M}{\epsilon(\infty)} + \Delta_0. \quad (5)$$

Here we have taken into account the electrostatic potential changes due to the polarization of surrounding ions. Since the polarization is characterized by the dielectric factor at optical frequencies $\epsilon(\infty)$, representing the nonlocal charge relaxation at infinite frequencies caused by core polarization of to background ions. The Madelung site potential is approximated as $\Delta V_M/\epsilon(\infty)$. In addition, at the atomic limit three more quantities are needed to consider hole transfer from Cu^{2+} to O^{2-} : the second electron affinity of the O^{2-} ion, the third ionization energy of the Cu^{3+} ion, and the Coulombic interaction between the introduced electron and hole. For simplicity, they are combined into one parameter Δ_0 . ΔV_M turns the large negative Δ_0 into the small level separation Δ of positive sign. Δ coincides with charge-transfer gap if there are no hopping interactions. Following Tohyama and Maekawa,²⁰ we chose the compound-independent parameters $\epsilon(\infty) = 3.3$ and $\Delta_0 = -10.88$ eV, which can give overall agreement with the observed values of the charge-transfer gap.

The hopping parameter t' can be directly estimated by using Eqs. (4) and (5). Recent studies^{15,21} suggest that the appearance of apical oxygen outside the CuO_2 planes affects superconductivity mainly via t' . We therefore need to include the effects of the Cu $d_{3z^2-r^2}$ orbital and O p_z orbital at the

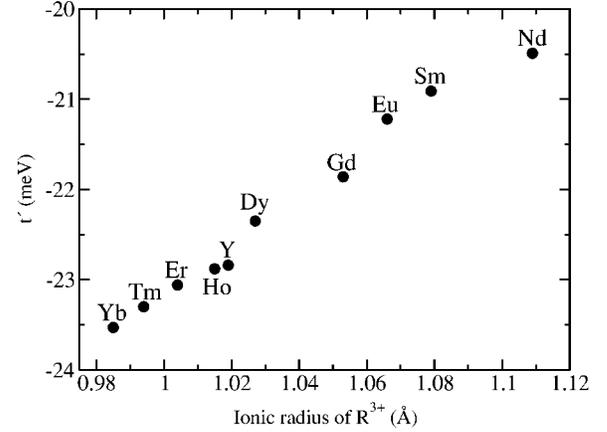


FIG. 2. Rare-earth ionic radius ($r_{R^{3+}}$) dependence of the next-nearest-neighbor hopping integral t' for the nearly optimally doped $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$ compounds.

apex of the pyramid with respect to the hopping integral among those orbitals and O p_σ orbitals in the Cu-O plane. The apical oxygen affects the hopping integral due to new hopping processes via the hybridized states. This effect is assumed to be mainly reflected by the energy levels splitting Δ rather than other parameters such as t_{pd} and t_{pp} , though they may contribute to the slight change of the hopping parameters in general.

We took $t_{pd} = 1.3$ eV and $t_{pp} = 0.65$ eV, which were estimated by the analysis of the photoelectron spectroscopy.²² We then obtained the t' values using the above-determined parameters. The results are summarized in Fig. 2. As can be seen, the hopping integral t' is enhanced with increasing the rare-earth ionic radius in the nearly optimally doped $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$ compounds. This systematic enhancement is mainly due to the state hybridizing between O: p_z and Cu: $d_{3z^2-r^2}$ orbitals.²³ It has been found³ that the superexchange interaction J does not depend significantly on the compounds. Experiments and calculations give a $J = 0.128$ eV for cuprates.²⁴ Thus, the coefficient $(J + 2t')$ of the $\cos k_x \cos k_y$ term in Eq. (3) also increases with the radius of the trivalent rare-earth ion. The results confirm the previous observations^{15,21} that a larger t' or $J + 2t'$ is in favor of a higher T_c . Note that the optimal density of hole carriers n_H^{opt} systematically decreases with increasing t' when $J + 2t' > 0$,¹⁵ the present results shown in Fig. 2 indicate a modest reduction of n_H^{opt} with the increase in $r_{R^{3+}}$ for the optimally doped $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$. This is again self-consistent with the reported $r_{R^{3+}}$ dependence of n_H^{opt} in this system.^{13,14}

IV. CRITICAL TEMPERATURE VARIATION

Since we have established the systematic evolution of the hole dispersion in the $\text{RBa}_2\text{Cu}_3\text{O}_{7-\delta}$ series, we are able to understand the experimentally observed variation of T_c in this series based on the developed theoretical model for the anisotropic bilayer superconductors.²⁵ Neglecting the anisotropy of interactions in both the ab direction and c direction, we obtain the T_c equation for a given chemical potential μ (Ref. 25):

$$1 = \frac{1}{2N} \sum_k V g^2(k) (W_k^+ + W_k^-), \quad (6)$$

with $W_k^\pm = |\xi_k^\pm - \mu|^{-1} \tanh[|\xi_k^\pm - \mu|/(2T_c)]$, where $g(k) = (\cos k_x - \cos k_y)/2$ and $\xi_k^\pm = \varepsilon_k \pm t_\perp g^2(k)$, N is the number of k vectors, V is the in-plane pairing interaction, and t_\perp is the coherent interlayer single-particle hopping integral. The constraint condition for the hole carrier density n_H in conjunction with μ is given by

$$n_H = \frac{1}{2} - \frac{1}{4N} \sum_k [(\xi_k^+ - \mu)W_k^+ + (\xi_k^- - \mu)W_k^-]. \quad (7)$$

Recent angle-resolved photoemission spectroscopy²⁶ and transport^{27,28} measurements indicate the validity of this kind of d -wave BCS formalism in describing the superconducting state of high- T_c superconductors.

In order to elucidate the effect of ΔV_M and t' on T_c , we first neglect the interlayer effect by putting $t_\perp = 0$ into Eqs. (6) and (7). Once having the knowledge of the hole dispersion ε_k , one can calculate the hole density dependence of T_c for different values of V . Thus, t' and V are only two parameters entered into Eqs. (6) and (7) to determine T_c . The basic experimental fact is that the maximum T_c increases but the optimal hole density n_H^{opt} decreases with increasing the trivalent rare-earth ionic radius in the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds. Therefore, the change of t' and/or V must reflect this experimental fact. We have examined which parameter is most probably responsible for the systematic change of both T_c and n_H^{opt} . We found that although T_c can monotonically increase with increasing V , n_H^{opt} scarcely changes with V . However, assuming V to be compound independent but t' a dominant parameter, we obtained not only a systematic increase of T_c but also a monotonic decrease of n_H^{opt} , which is in agreement with the experiments.^{4,5,13,14} This strongly indicates that t' is a dominant parameter for the ionic size effect, although V may vary slightly among the $RBa_2Cu_3O_{7-\delta}$ series. It is therefore reasonable to assume V as a compound-independent parameter in this system. Furthermore, antiferromagnetic van Hove scenario has been proposed to account for many unusual normal state and superconducting properties of high- T_c cuprates.²⁹ According to this scenario, the interaction V is proportional to the superexchange interaction J . A constant J chosen based on the theoretical analysis and experiments^{3,24} is a good indicator of a compound-independent V for the cuprates. On the other hand, all cuprates, although being different, have an important common feature—namely, containing the same basis structural unit, the CuO_2 plane. The driving force of superconductivity is believed to come mainly from the almost same CuO_2 plane; the interlayer interaction V is expected not to be different among the cuprates. The choice of such a constant V has been recently found to be suitable in describing the variation of T_c among the hole-doped cuprates.¹⁵ Thus, the assumption of a compound-independent V is physically reasonable in the present analysis.

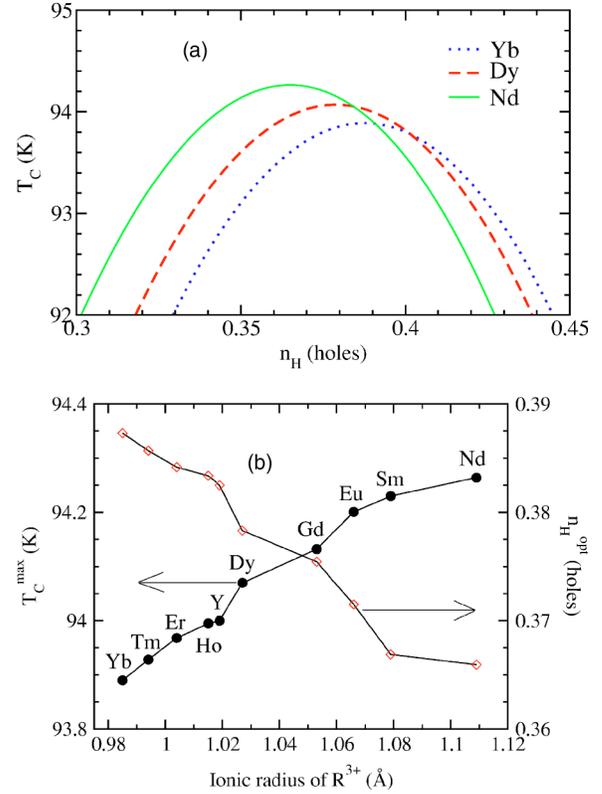


FIG. 3. (Color online) (a) Calculated critical temperature T_c versus hole carrier density n_H for selected $RBa_2Cu_3O_{7-\delta}$ ($R = Yb, Dy, Nd$) around optimal doping. (b) Rare-earth ionic radius ($r_{R^{3+}}$) dependence of the maximum T_c and optimal density n_H^{opt} for the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds.

A value of V can be deduced from the experimental value of $T_c = 94$ K for optimally doped $YBa_2Cu_3O_{7-\delta}$. Substituting the different hole dispersion relation into Eqs. (6) and (7), we obtain the relevant parabolic relation between T_c and n_H for various compounds. In Fig. 3(a), we plot the calculated T_c versus n_H curves for some selected $RBa_2Cu_3O_{7-\delta}$ around optimal doping level by changing the rare-earth ion from smaller Yb through Dy to larger Nd. As clearly seen, with the increase in $r_{R^{3+}}$, the maximum T_c shifts to the high value at the expense of the reduction of the optimal density of hole carriers n_H^{opt} . Figure 3(b) shows the $r_{R^{3+}}$ dependence of both the maximum T_c and n_H^{opt} for various optimally doped materials. Note that T_c modestly increases with increasing $r_{R^{3+}}$. The theoretical results are consistent with the experiments,^{4,5} though the change of T_c is not significant. The obtained systematic reduction of n_H^{opt} with the rare-earth ionic radius also agrees well with the previous reports.^{13,14} It is therefore indicated that the observed rare-earth ionic size effect on T_c in the optimally doped $RBa_2Cu_3O_{7-\delta}$ is in reality due to the modification of the hole dispersion through changing t' .

A direct modification of the substitution of the trivalent rare-earth ion is the distance between the adjacent nearest CuO_2 planes within a unit cell (d_{CuO_2}). Neutron data⁹ show a 7.2% increase of d_{CuO_2} from $YBa_2Cu_3O_7$ to $NdBa_2Cu_3O_7$. The interlayer coupling is then expected to play an important role in the variation of T_c in these materials. The increased

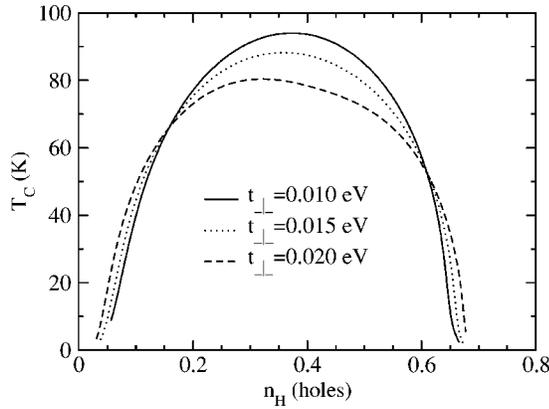


FIG. 4. Calculated critical temperature T_c versus hole carrier density n_H for $t_{\perp}=0.010, 0.015,$ and 0.020 eV, respectively. V was chosen to give a maximum T_c of 94 K for a compound with $t_{\perp}=0.010$ eV.

d_{CuO_2} with trivalent rare-earth ionic radius would lead to the decrease of the interlayer single-particle hopping integral t_{\perp} . Optical measurements indicate a value of t_{\perp} in the range of 0.003 and 0.040 eV for $YBa_2Cu_3O_{7-\delta}$.³⁰ We have examined how T_c varies with the interlayer parameter t_{\perp} . Figure 4 shows that T_c is suppressed by increasing t_{\perp} around the optimal doping. It is clear that, at optimal doping, the increasing interlayer distance d_{CuO_2} with $r_{R^{3+}}$ would result in the enhancement of T_c^{max} due to the reduction of t_{\perp} .

Assuming that $t_{\perp} \propto d_{CuO_2}^{-2}$, we would estimate the evolution of T_c with the interlayer effect. Taking the optimally doped $YBa_2Cu_3O_{7-\delta}$ as a reference material, we have $t_{\perp} = t_{\perp}^Y (d_{CuO_2}^Y / d_{CuO_2})^2$. Using the experimentally observed d_{CuO_2} from neutron diffraction,⁹ we can calculate the systematic change of T_c for various compounds once giving a value of t_{\perp}^Y . Figure 5 shows the rare-earth ionic radius dependence of T_c^{max} in the optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds for $t_{\perp}^Y=0.010$ and 0.020 eV, respectively. In both cases, V was taken to yield a maximum T_c of 94 K for $YBa_2Cu_3O_{7-\delta}$. We also plot the relevant d_{CuO_2} evolution with the rare-earth ionic radius in the inset of Fig. 5. We noticed that the enhanced interlayer single-particle hopping greatly enlarges the difference of T_c^{max} from $YbBa_2Cu_3O_7$ to $NdBa_2Cu_3O_7$. When $t_{\perp}=0.020$ eV, the calculated T_c^{max} of 92.7 and 96.5 K for $YbBa_2Cu_3O_7$ to $NdBa_2Cu_3O_7$, respectively, are in good agreement with the experimental values of 92.5 and 96.0 K.⁵ The experimental observed several Kelvin increase of T_c^{max} with the rare-earth ionic radius^{4,5} is therefore well reproduced by considering the interlayer effect. This further follows that the rare-earth ionic size effect in $RBa_2Cu_3O_{7-\delta}$ compounds is an electronic origin.

V. CONCLUSIONS

We have carried out systematic studies of the critical temperature T_c variation originating from the Madelung site po-

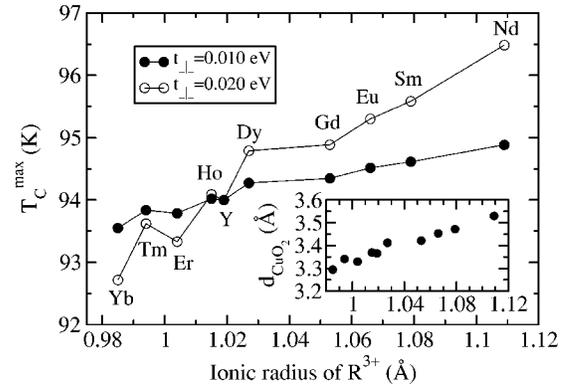


FIG. 5. Rare-earth ionic radius ($r_{R^{3+}}$) dependence of the maximum critical temperature T_c calculated by using $t_{\perp}^Y=0.010$ and 0.020 eV, respectively. The inset shows the $r_{R^{3+}}$ dependence of the distance between the adjacent nearest CuO_2 planes, d_{CuO_2} , for the nearly optimally doped $RBa_2Cu_3O_{7-\delta}$ compounds.

tential difference between in-plane oxygen and copper sites, ΔV_M , and from the interlayer effect for the family of the optimally doped $RBa_2Cu_3O_{7-\delta}$ cuprates. It turns out that the apical oxygens notably modify the O: p -hole-band structure, which leads to the systematic reduction of ΔV_M with an increase of the trivalent rare-earth ionic radius. This change enhances the next-nearest-neighbor hopping integral. T_c is in turn enhanced due to the shortened apical O in-plane Cu distance with increasing the rare-earth ionic radius. This trend is consistent with the experiments, although the magnitude of the variation of the maximum T_c due to the change of t_{\perp} is not significant. Note that there exist significant effects of the adjacent nearest CuO_2 separation on interlayer coupling. We found that the interlayer single-particle hopping integral is the dominant factor responsible for the trend of the maximum T_c in the optimally doped $RBa_2Cu_3O_{7-\delta}$ cuprates. This suggests that the Madelung potential studies give the correct physics in a qualitative picture. To reach quantitative agreement, the interlayer effect has to be included. Our approach has another more important impact in that it permits a fast prediction of the effect of a given structural modification in the T_c for searching new superconducting oxides. For example, it is a promising direction to increase T_c through enlarging the adjacent nearest CuO_2 separation which could be realized by carefully doping larger trivalent ion at the Y site.

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- ¹J. B. Torrance and R. M. Metzger, Phys. Rev. Lett. **63**, 1515 (1989).
- ²Y. Ohta, T. Tohyama, and S. Maekawa, Phys. Rev. Lett. **66**, 1228 (1991).
- ³Y. Ohta, T. Tohyama, and S. Maekawa, Phys. Rev. B **43**, 2968 (1991).
- ⁴J. G. Lin, C. Y. Huang, Y. Y. Xue, C. W. Chu, X. W. Cao, and J. C. Ho, Phys. Rev. B **51**, 12 900 (1995).
- ⁵G. V. M. Williams and J. L. Tallon, Physica C **258**, 47 (1996).
- ⁶A. Hu, N. Sakai, and M. Murakami, Appl. Phys. Lett. **78**, 2539 (2001).
- ⁷A. Hu, M. Murakami, and H. Zhou, Appl. Phys. Lett. **83**, 1788 (2003).
- ⁸See S. L. Chaplot, Phys. Rev. B **37**, 7435 (1988); R. C. Baetzold, *ibid.* **38**, 11 304 (1988); S. Valkealahti and D. O. Welch, Physica C **162**, 540 (1989); N. F. Wright and W. H. Butler, Phys. Rev. B **42**, 4219 (1990).
- ⁹M. Guillaume, P. Allenspach, W. Henggeler, J. Mesot, B. Roessli, U. Staub, P. Fischer, A. Furrer, and V. Trounov, J. Phys.: Condens. Matter **39**, 7963 (1994).
- ¹⁰P. P. Ewald, Ann. Phys. (Leipzig) **64**, 253 (1921).
- ¹¹M. P. Tosi, Solid State Phys. **16**, 1 (1964).
- ¹²R. D. Shannon, Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr. **32**, 751 (1976).
- ¹³X. J. Chen, J. Sha, Z. A. Xu, Z. K. Jiao, and Q. R. Zhang, Physica C **282–287**, 797 (1997).
- ¹⁴S. V. Samoylenkov, O. Yu. Gorbenko, and A. R. Kaul, Physica C **278**, 49 (1997).
- ¹⁵X. J. Chen and H. Q. Lin, Phys. Rev. B **69**, 104518 (2004).
- ¹⁶J. Bata, A. M. Olés, and J. Zaanen, Phys. Rev. B **52**, 4597 (1995).
- ¹⁷V. I. Belinicher, A. L. Chernyshev, and V. A. Shubin, Phys. Rev. B **54**, 14 914 (1996).
- ¹⁸P. A. Lee, Phys. Rev. Lett. **63**, 680 (1989).
- ¹⁹V. I. Belinicher, A. L. Chernyshev, and V. A. Shubin, Phys. Rev. B **53**, 335 (1996).
- ²⁰T. Tohyama and S. Maekawa, J. Phys. Soc. Jpn. **65**, 667 (1996).
- ²¹E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, Phys. Rev. Lett. **87**, 047003 (2001).
- ²²H. Eskes, G. A. Sawatzky, and L. F. Feiner, Physica C **160**, 424 (1989).
- ²³H. Matsukawa and H. Fukuyama, J. Phys. Soc. Jpn. **59**, 1723 (1990).
- ²⁴M. S. Hybertsen, E. B. Stechel, M. Schluter, and D. R. Jennison, Phys. Rev. B **41**, 11 068 (1990).
- ²⁵X. J. Chen, H. Q. Lin, W. G. Yin, C. D. Gong, and H.-U. Habermeyer, Phys. Rev. B **64**, 212501 (2001).
- ²⁶H. Matsui, T. Sato, T. Takahashi, S.-C. Wang, H.-B. Yang, H. Ding, T. Fujii, T. Watanabe, and A. Matsuda, Phys. Rev. Lett. **90**, 217002 (2003).
- ²⁷Yu. I. Latyshev, T. Yamashita, L. N. Bulaevskii, M. J. Graf, A. V. Balatsky, and M. P. Maley, Phys. Rev. Lett. **82**, 5345 (1999).
- ²⁸C. Proust, E. Boaknin, R. W. Hill, L. Taillefer, and A. P. Mackenzie, Phys. Rev. Lett. **89**, 147003 (2002).
- ²⁹E. Dagotto, A. Nazarenko, and A. Moreo, Phys. Rev. Lett. **74**, 310 (1995).
- ³⁰S. L. Cooper and K. E. Gray, in *Physical Properties of High Temperature Superconductors IV*, edited by D. M. Ginsberg (World Scientific, Singapore, 1994).