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A tight-binding description of high-temperature superconductors

Brent A Richert and Roland E Allen

Center for Theoretical Physics, Department of Physics, Texas A&M University,
College Station, Texas 77843, USA

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Abstract. A single tight-binding model, with transferable parameters, provides a good description of the electronic structures of all currently known high-temperature superconductors, in the sense that results in the local density approximation are satisfactorily reproduced. Using this model, one can study the effects of atomic substitutions, vacancies, and structural modifications.

In earlier work [1], we calculated the energy bands, the local densities of states, and the atomic valences of $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ in the one-electron approximation, using a semi-empirical tight-binding model with p and s orbitals included for the O atoms and d and s orbitals for all the metal atoms. We now apply this same model to the Bi cuprates [2–6], the Tl cuprates [7–13], and the bismuthates [14–18]. In addition to the parameters previously fitted [1] to La_2CuO_4 , we need the s, p, and d energies for Bi and Pb, and the $sp\sigma$, $pp\sigma$, and $pp\pi$ inter-atomic matrix elements [19, 20]. (In [1], no $pp\sigma$ or $pp\pi$ interactions were needed, and the results were insensitive to the value $\eta_{sp\sigma} = 0.9$ used in that work.) To obtain these new parameters, we have fitted the calculations of Mattheiss and Hamann [21] for BaBiO_3 and BaPbO_3 . The resulting atomic parameters are listed in table 1; the inter-atomic parameters are $\eta_{sp\sigma} = 1.4$, $\eta_{pp\sigma} = 1.5$, and $\eta_{pp\pi} = -0.6$.

Using the crystal structure and atomic positions determined by Tarascon and co-workers [22], we first consider the $T_c \approx 85$ K material $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$. Other workers [6, 23] have identified structural displacements of the atoms from their ideal locations in, e.g., the BiO bilayers; however, we neglect these modifications in order to compare with other calculations. The one-electron band structure for this material has been calculated by several groups, all obtaining similar results [24–28]. It is found to be predominantly two-dimensional, with little dispersion in the direction perpendicular to the copper–oxygen planes. Two Cu(d)–O(p) anti-bonding bands are found to cross the Fermi energy from below, while two Bi p bands dip below E_F near the Brillouin zone boundary at the symmetry point D in the [100] direction. In order to fit these results with our tight-binding model, we have included the second-neighbour Bi–Bi interactions [24], using the same inter-atomic parameters η as for nearest neighbours, but neglecting d–d interactions. We regard these Bi–Bi interactions as justified by the large covalent radius of Bi and the relatively small lattice parameter $a = 3.81$ Å [22], even though only nearest-neighbour interactions were needed for the earlier materials [1]. (To be precise,

Table 1. Atomic tight-binding parameters for Bi and Tl superconductors.

	ϵ_s (eV)	ϵ_p (eV)	ϵ_d (eV)	r_d (Å)
Hg	-11.6	-7.2	-17.0	1.0
Tl	-14.8	-8.3	-23.0	1.0
Pb ^a	-18.0	-9.4	-29.0	1.0
Bi ^b	-21.2	-10.5	-35.0	1.0
K	-4.2	—	-3.2	1.2
Ca	-5.4	—	-3.2	1.2
Sr	-5.0	—	-6.8	1.6
Ba	-4.5	—	-6.6	1.6
Cu ^c	-12.0	—	-14.0	0.95
O	-29.0	-14.0	—	—

^a Parameters fitted to BaPbO₃ [21].

^b Parameters fitted to BaBiO₃ [21].

^c Parameters fitted to La₂CuO₄ [1].

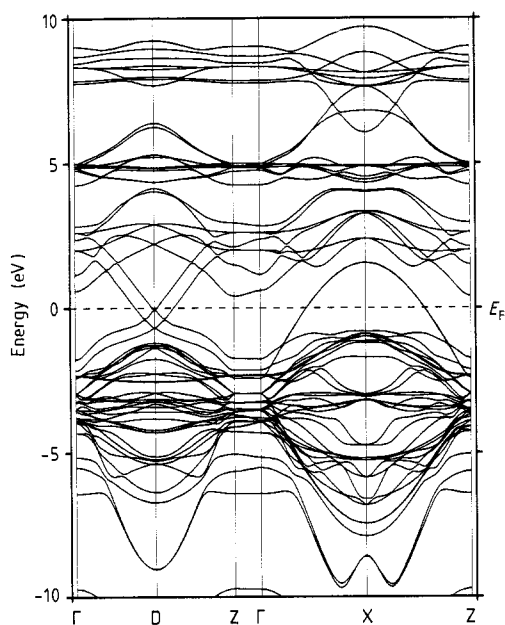


Figure 1. Electronic energy bands for the BCT crystal structure of Bi₂CaSr₂Cu₂O₈. The zero of energy has been shifted to the Fermi energy E_F . Two Cu(d)–O(p) anti-bonding bands cross E_F along the GX symmetry line. Two Bi p bands disperse to the Fermi energy, with one band dipping below E_F near the Brillouin zone boundary at the symmetry point D in the [100] direction.

we include interactions between the large atoms Bi and Pb when the atomic separation is less than 3.9 Å.) We ignore the long-range structural modulation [22], which should have only a minor effect on the electronic properties. The electronic energy bands, local densities of states, Fermi energy E_F , and atomic valences of all materials are calculated as in [1].

The energy bands of Bi₂CaSr₂Cu₂O₈ along the symmetry lines of the Brillouin zone for the BCT crystal structure [29] are shown in figure 1, with the zero of energy shifted to E_F . We note that the bands show relatively little dispersion along ΓZ , perpendicular to the copper–oxygen planes, and are dominated by anti-bonding bands of Cu(d)–O(p) crossing the Fermi energy along GX, just as for La_{1.85}Sr_{0.15}CuO₄ and YBa₂Cu₃O₇ [1]. The new features of this band structure are the two Bi p bands which disperse down to

Table 2. Valences Δn for (a) Bi–Ca–Sr–Cu–O systems and (b) $\text{BaPb}_{0.75}\text{Bi}_{0.25}\text{O}_3$ and $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$.

(a)	Bi	Pb	Ca	Sr ^a	Cu ^a	O(1) ^a	O(2) ^a	O(3) ^a
$\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$	1.80	—	1.51	1.09	0.84	−1.09	−1.14	−1.18
$\text{BiPbCaSr}_2\text{Cu}_2\text{O}_8$	1.79	1.23	1.51	1.09	1.01	−1.03	−1.14	−1.17
$\text{Bi}_2\text{Sr}_2\text{CuO}_6$	1.83	—	—	1.15	0.87	−1.05	−1.18	−1.20

(b)	Ba	K	Bi	Pb	O
$\text{BaPb}_{0.75}\text{Bi}_{0.25}\text{O}_3$	1.49	—	2.29	1.29	−1.01
$\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$	1.62	0.62	1.80	—	−1.01

^a Averaged over sites in the unit cell for $\text{BiPbCaSr}_2\text{Cu}_2\text{O}_8$.

the Fermi energy, with one band crossing below E_F to about -0.7 eV at D. As in the other calculations [24–28], these p bands form occupied electron pockets near the Brillouin zone boundary. Distortion in the BiO layers [6, 23], neglected here and in previous theoretical treatments, may affect the occupation of these bands.

The atomic valences Δn are presented in table 2. In our notation, O(1) is the oxygen site within the CuO_2 planes, O(2) is in the SrO region separating the Cu and Bi layers, and O(3) is in the BiO layer. The valences for Cu and O(1) are similar to those found previously for the copper-oxygen plane regions in $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ [1].

Photoemission studies [30–35] of the phase $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$ confirm the basic occupied electronic states predicted by the earlier one-electron calculations [24–28] and this work (with some discrepancies in detail). In particular, the photoemission feature observed at a binding energy of 10–11 eV [14–17] corresponds to the occupied Bi s bands of the calculations. Angle-resolved resonant photoemission studies [36] indicate an energy band dispersion of 0.2 to 0.5 eV near the Fermi energy along the ΓX symmetry line in $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$. Also, inverse photoemission measurements [37] of $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$ reveal unoccupied states similar to those of the calculated bands.

We now consider the effect of periodic substitution of Pb for one Bi atom within the crystal structure of $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$. We neglect local strains and changes in the lattice constants resulting from substitution, but the fact that Bi and Pb have nearly equal covalent radii indicates that such changes should be small. The Fermi energy is found to shift by -0.19 eV; the calculated valences are given in table 2.

We next consider the material $\text{Bi}_2\text{Sr}_2\text{CuO}_6$, with $T_c = 6$ K [38]. We find a single Cu(d)–O(p) band crossing E_F along ΓX , with Bi p bands again dipping below the Fermi energy at D. The valences shown in table 2 are similar to those of $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$.

Let us now turn to the bismuthates $\text{BaPb}_{1-y}\text{Bi}_y\text{O}_3$, with $T_c = 13$ K [14], and $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$, with $T_c = 30$ – 34 K [15–18]. The doping is treated in the virtual-crystal approximation. Our energy bands in figure 2 for $\text{BaPb}_{0.75}\text{Bi}_{0.25}\text{O}_3$ agree well with the previous calculation [21] for this superconductor, with both calculations using a model cubic structure with $a_0 = 4.29$ Å. For $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$, we use the cubic structure of Cava and co-workers [16], with $a_0 = 4.293$ Å. Our energy bands in figure 3 are in good agreement with the calculation [39] for $\text{Ba}_{0.5}\text{K}_{0.5}\text{BiO}_3$. (We omit the very core-like Ba p states.) The valences for these bismuth oxide superconductors are again listed in table 2.

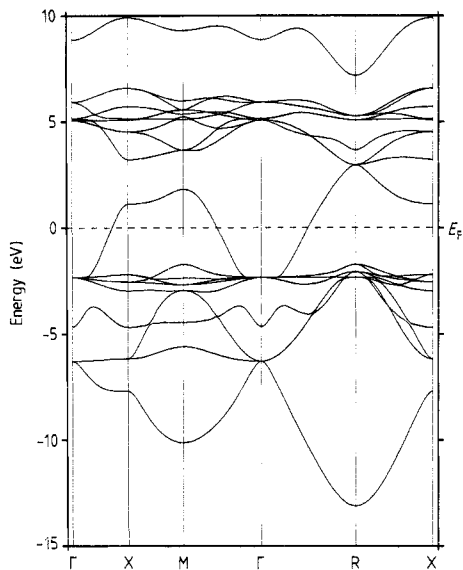


Figure 2. Energy bands for cubic $\text{BaPb}_{0.75}\text{Bi}_{0.25}\text{O}_3$.

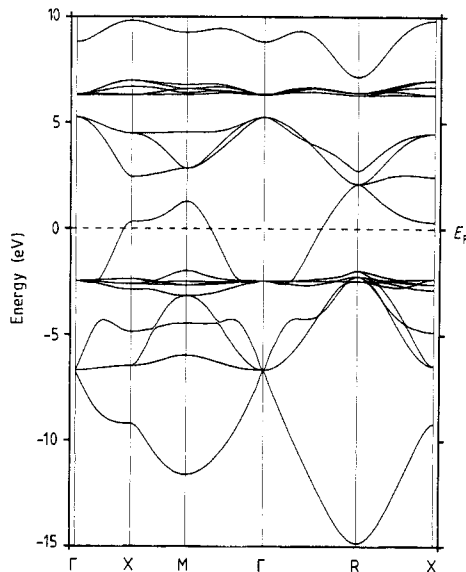


Figure 3. Energy bands for cubic $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$. The Bi(s)-O(p) anti-bonding bands provide the conduction states.

Photoemission studies by Ruckman and co-workers [40] of $\text{Ba}_{0.6}\text{K}_{0.4}\text{BiO}_3$ show occupied states similar to those of the calculated bands, with oxygen p states dominating the structure near the Fermi energy. Using both photoemission and inverse photoemission, Weaver and co-workers [41] find occupied and unoccupied states that are in good agreement with those calculated here.

Let us now consider Tl cuprates [7–13]. (The atomic positions for $\text{TlCa}_3\text{Ba}_2\text{Cu}_4\text{O}_{11}$ were extrapolated from those of the analogous three-layer copper oxide superconductor [42].) The atomic parameters are given in table 1. We have included the valence p orbitals for Tl, Hg, and Pb, since these orbitals are required for a proper treatment of charge transfer in the M–O layers, where M represents one of these metal atoms. We extrapolate the energies ε_s , ε_p , and ε_d for Tl and Hg from the Bi and Pb energies determined above for the Bi-containing superconductors. For Tl atoms (and for Pb or Hg replacing Tl), we include the same second-neighbour interactions as were required for Bi.

Our calculated bands for $\text{Tl}_2\text{Ba}_2\text{CuO}_6$ are shown in figure 4. We note again the pd σ anti-bonding state of Cu(d)–O(p) near the Fermi energy. The Tl–Tl in-plane interactions cause the Tl p bands to disperse by about 3 eV from Γ to D along the [100] direction. These bands do not dip below the Fermi energy as do the Bi p bands in $\text{Bi}_2\text{CaSr}_2\text{Cu}_2\text{O}_8$, but the Tl(s)–O(p) hybrid states do cross below E_F to about -0.5 eV at Γ , forming occupied electron pockets. The valences for $\text{Tl}_2\text{Ba}_2\text{CuO}_6$ are shown in table 3. Our notation for the atomic sites places oxygen site O(1) within the CuO_2 plane, site O(2) in the BaO region separating the Cu and Tl layers, and site O(3) in the TlO layer. In the present model, the total density of states at the Fermi energy $\rho(E_F)$ is 2.0 states $\text{eV}^{-1}/\text{cell}$. Our calculated valences for $\text{Tl}_2\text{CaBa}_2\text{Cu}_2\text{O}_8$ [43–45] are also given in table 3; for this material, $\rho(E_F) = 2.7$ states $\text{eV}^{-1}/\text{cell}$.

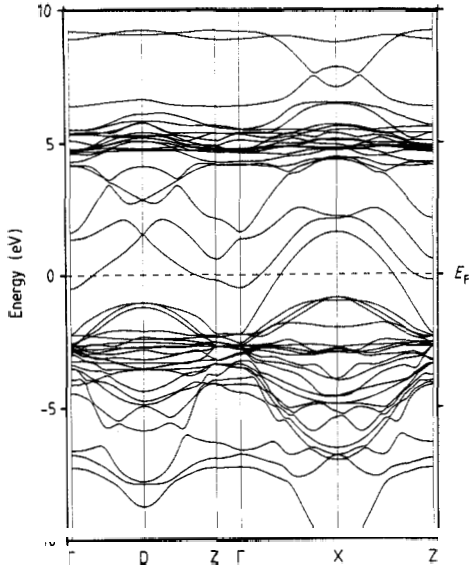


Figure 4. Electronic energy bands for BCT $\text{Tl}_2\text{Ba}_2\text{CuO}_6$. A $\text{Tl}(s)\text{--O}(p)$ band dips below E_F , making both the CuO_2 planes and TlO layers metallic.

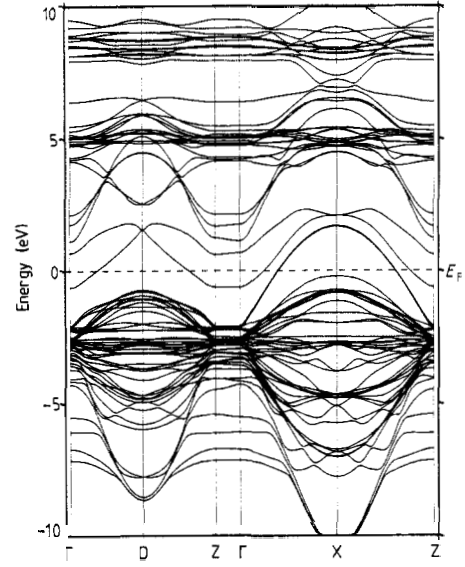


Figure 5. Electronic energy bands for BCT $\text{Tl}_2\text{Ca}_2\text{Ba}_2\text{Cu}_3\text{O}_{10}$.

Table 3. Valences Δn for (a) Tl-containing superconductors and (b) $\text{TlM}\text{CaBa}_2\text{Cu}_2\text{O}_8$.

(a)	Tl	Ca ^a	Ba	Cu ^b	Cu(2)	O(1)	O(2)	O(3)	O(4)
$\text{Tl}_2\text{Ba}_2\text{CuO}_6$	1.05	—	1.36	0.89	—	-1.10	-1.04	-0.72	—
$\text{Tl}_2\text{CaBa}_2\text{Cu}_2\text{O}_8$	1.05	1.45	1.37	0.86	—	-1.13	-1.03	-0.71	—
$\text{Tl}_2\text{Ca}_2\text{Ba}_2\text{Cu}_3\text{O}_{10}$	1.06	1.45	1.38	0.54	1.02	-1.27	-1.09	-1.08	-0.65
$\text{TlCa}_3\text{Ba}_2\text{Cu}_4\text{O}_{11}$	1.07	1.45	1.36	0.90	1.07	-1.12	-1.06	-1.10	-1.17
(b)	Tl	M	Ca	Ba ^c	Cu ^c	O(1) ^c	O(2) ^c	O(3) ^c	
M=Hg	1.02	0.50	1.45	1.38	1.14	-1.03	-1.10	-0.83	
M=Pb	1.06	1.46	1.45	1.37	0.66	-1.21	-0.98	-0.62	

^a Averaged over central Ca(1) and outer Ca(2) sites for $\text{TlCa}_3\text{Ba}_2\text{Cu}_4\text{O}_{11}$.

^b Central Cu(1) site for $\text{Tl}_2\text{Ca}_2\text{Ba}_2\text{Cu}_3\text{O}_{10}$ and $\text{TlCa}_3\text{Ba}_2\text{Cu}_4\text{O}_{11}$.

^c Averaged over sites in the unit cell.

The electronic energy bands of $\text{Tl}_2\text{Ca}_2\text{Ba}_2\text{Cu}_3\text{O}_{10}$ are shown in figure 5. This 125 K superconductor has three anti-bonding $\text{Cu}(d)\text{--O}(p)$ states which cross E_F , corresponding to the triple layer of CuO_2 planes stacked with Ca ions. Small electron pockets are again formed by $\text{Tl}(s)\text{--O}(p)$ anti-bonding states which dip below E_F to -0.6 eV at the symmetry points Γ and Z . The atomic valences in table 3 show that Cu(2), in the outer CuO_2 planes adjacent to the BaO layers, has a higher valence than those of the other Tl materials. However, the central copper site Cu(1) shows a decreased number

of holes, with a valence of only 0.54. The notation for the oxygen atoms places O(1) in the central CuO_2 planes, O(2) in the outer CuO_2 planes, O(3) in the BaO layer, and O(4) in the TlO layer. The calculated $\rho(E_F)$ is 5.3 states $\text{eV}^{-1}/\text{cell}$.

The single-Tl-layer superconductor $\text{TlCa}_3\text{Ba}_2\text{Cu}_4\text{O}_{11}$ contains four CuO_2 layers separated by Ca ions. The results of the valence calculation for this material in table 3 show that the inner CuO_2 layers have fewer holes than the outer layers.

Let us now consider the modification of the electronic structure when Tl is partially replaced by Hg or Pb, focusing on the representative material $\text{Tl}_2\text{CaBa}_2\text{Cu}_2\text{O}_8$. We perform a single periodic substitution for Tl within the BCT structure. The added hole of Hg is found to lower E_F by 0.23 eV, and in the present model there is an increase in $\rho(E_F)$ to 4.2 states $\text{eV}^{-1}/\text{cell}$. As can be seen in table 3 there is a small increase in the valence of both Cu and O(1) in the charge-carrying CuO_2 planes, indicating that hole carriers are added in the superconducting region. A similar calculation for Pb replacing Tl shows the Fermi energy to be raised, by 0.19 eV. The valences of table 3 for $\text{TlPbCaBa}_2\text{Cu}_2\text{O}_8$ indicate that doping with Pb significantly decreases the valences of the Cu and O(1) sites in the CuO_2 planes. The density of states at the Fermi energy is also lowered: $\rho(E_F) = 1.9$ states $\text{eV}^{-1}/\text{cell}$, in the present model. The most obvious effect of doping with Hg or Pb in $\text{TlMCaBa}_2\text{Cu}_2\text{O}_8$ is thus the shift of the Fermi energy, with Hg creating holes and Pb destroying them as one expects.

Acknowledgments

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