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Scaling of the transition temperature of hole-doped cuprate superconductors with the charge-transfer energy

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Abstract – We use first-principles calculations to extract two essential microscopic parameters, the charge-transfer energy and the inter-cell oxygen-oxygen hopping, which correlate with the maximum superconducting transition temperature $T_{c,max}$ across the cuprates. We explore the superconducting state in the three-band model of the copper-oxygen planes using cluster Dynamical Mean-Field Theory. We find that the variation in the charge-transfer energy largely accounts for the empirical trend in $T_{c,max}$, resolving a long-standing contradiction with theoretical calculations.

Introduction. – Despite an immense body of theoretical and experimental work, we have limited microscopic insights of which materials-specific parameters govern the trends in the maximum transition temperature $T_{c,max}$ across the copper oxide superconductors. Structurally, all the cuprate families have in common CuO$_2$ planes which support superconductivity. They are described by the chemical formula $X_n$S$_{n-1}$(CuO$_2$)$_n$, where n CuO$_2$ planes are interleaved with $n-1$ spacer layers S to form a multi-layer. These multi-layers are then stacked along the c-axis, separated by a different spacer layer X. Empirically, it is known that $T_{c,max}$ is strongly materials-dependent, ranging from 40 K in La$_2$CuO$_4$ to 138 K in HgBa$_2$Ca$_2$Cu$_3$O$_8$. Additionally, $T_{c,max}$ can be tuned both as a function of doping and the number n of CuO$_2$ planes.

Studies linking the known empirical trends to microscopics have generally established that the properties of the apical atoms (O, F or Cl, depending on the cuprate family) are the relevant materials-dependent parameters. However, conclusions vary regarding their effects on electronic properties, especially in multi-layer cuprates where not all CuO$_2$ have apical atoms. Early theoretical work by Ohta, et al., found correlations between $T_c$ and the Madelung potential of the apical oxygen, arguing that the apical potential controls the stability of the Zhang-Rice singlets [1]. They conclude that $d_{apical}^{Cu-O}$, the distance between the Cu and apical O, is uncorrelated with superconductivity. In a more recent DFT study, Pavarini et al., argue that $d_{apical}^{Cu-O}$ tunes between the single-layer cuprate families, affecting the electronic structure primarily via the one-electron part of the Hamiltonian [2]. Moving the apical oxygens away from the copper oxide plane allows stronger coupling of in-plane O 2p orbitals to the Cu 4s, enhancing the strength of longer ranged hoppings. This effect is characterized by the increase of a range parameter $r \sim t'/t$, describing the relative strength of the next-nearest-neighbor hopping $t'$ to nearest-neighbor hopping $t$ in a one-band model. They find that materials with larger $r$ have larger $T_{c,max}$. Many-body corrections to $t'$ were included by Yin et al. [3].

The development of cluster Dynamical Mean-Field Theory (c-DMFT) combined with first-principles calculations [4,5] has advanced our qualitative and quantitative understanding of the cuprates [6,7]. A satisfactory description of these materials at intermediate energy scales has been achieved, and the consensus is that the cuprates lie in the regime of intermediate correlation strength [8-10] near the Zaanen-Sawatzky-Allen (ZSA) boundary [11]. However, all numerical studies [12-14] contradict the empirical trend of $T_{c,max}$ with the range parameter $r$.

In this paper, we address the origin of the variation of the experimental $T_{c,max}$ across the cuprates using recent advances in electronic structure methods. We carry out first-principles calculations of the hole-doped cuprates, extract chemical parameters by downfolding to the 3-band
The three-band Hamiltonian we treat with c-DMFT is as follows:

$$H = \sum_{i\alpha j\beta \sigma} \epsilon_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^\dagger \hat{c}_{j\beta\sigma} + \sum_{i\alpha \sigma} \epsilon_{i\alpha\sigma} n_{i\alpha\sigma} + U_{dd} \sum_{i\sigma} n_{id\uparrow} n_{id\downarrow},$$  \hspace{1cm} (1)
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Fig. 3: Correlations of $T_{c,max}$ in the copper oxides with the microscopic parameters of the three-band model Hamiltonian with (a) the charge-transfer energy $\epsilon_d - \epsilon_p$, (b) the next-nearest neighbor oxygen-oxygen hopping $t_{pp'}$, and (c) the effective one-band range parameter $r \sim t'/t$. The trend of the dependence of the one-band range parameter agrees with ref. [2].

where $i,j$ run over the in-plane CuO$_2$ unit cells, $\alpha, \beta$ label the orbitals $p_x, p_y$ and $d_{x^2-y^2}$, and $\sigma$ is the electron spin. The hoppings $t_{ij}^{\alpha\beta}$ and onsite energies $\epsilon_{\alpha}$ are those sketched in fig. 1, except for the $d$-orbital onsite energy, where we subtract out a doping- and material-independent double-counting correction $E_{dc}$ to account for correlations included in both LDA and DMFT. The atomic double-counting correction [22], which is very successful for all-electron DFT+DMFT [17], cannot be used because the Wannier functions of the three-band model significantly depart from the atomic wave functions. To determine $E_{dc}$ for the Wannier representation, we match the low-energy Matsubara Green’s function of the three-band model to the corresponding quantity in the $ab$ initio all-electron calculation (see supplementary material [18]). A good match was attained for $E_{dc} = 3.12$ eV for a $d_{x^2-y^2}$ on-site Coulomb repulsion of $U_{dd} = 8$ eV.

To test our method, we use the extracted parameters for the canonical cuprate LSCO and explore the $T = 0$ phase diagram as a function of doping. Our results, shown in fig. 4, are qualitatively similar to experiment. The calculations stabilize antiferromagnetism for low dopings $x < 0.05$, which gives way to a dome of $d$-wave superconductivity. The static order parameter $\Delta = \langle c_1 c_2 \rangle_{\tau=0}$, where 1 and 2 are nearest neighbor sites on the impurity plaquette, reaches a maximum $\Delta_{max}$ near $x \sim 0.13$. We take the magnitude of $\Delta_{max}$ as a proxy for the maximum superconducting temperature $T_{c,max}$. The zero-frequency limit of the anomalous self-energy $\Sigma^{an}(\omega = 0)$ is an additional indicator of superconductivity, which our results show qualitatively follows the magnitude of the order parameter.

We argue that although two independent low-energy parameters correlate with the experimental $T_{c,max}$, it is the charge-transfer energy that controls the variation in $\Delta_{max}$, and thus $T_{c,max}$, across the cuprate families. To address this issue, we take the most correlated cuprate, LSCO, and compute $\Delta_{max}$ as we either i) decrease $\epsilon_d - \epsilon_p$ or ii) increase $t_{pp'}$. Figure 5(a) shows that reducing the correlation strength for fixed $t_{pp'}$ enhances the order parameter $\Delta$, in agreement with the empirical trend in fig. 3(a). However, fig. 5(b) shows that increasing $t_{pp'}$ across the physical parameter regime hardly modifies $\Delta_{max}$, in contrast with the empirical trend in fig. 3(b). Further increasing $t_{pp'}$ to larger, unphysical values strongly suppresses $T_{c,max}$. Thus, our calculations support the hypothesis that a larger
Conclusions. – We have used electronic structure methods to identify the dependence of $T_{c_{\text{max}}}$ on two fundamental parameters: the charge-transfer energy $\epsilon_d - \epsilon_p$ and inter-cell oxygen-oxygen hopping $t_{pp'}$. We find that the position of the apical oxygen tunes both parameters, but the strength of superconductivity, $\Delta_{\text{max}}$, is mainly sensitive to $\epsilon_d - \epsilon_p$. We expect future refinements to explain the remaining variability in $T_{c_{\text{max}}}$. Our work provides a natural interpretation of experiments where epitaxial compression in LSCO resulted in an enhancement of $T_c$ [25]. Epitaxy increases $\epsilon_{\text{Cu}-\text{O}}$ and thus reduces $\epsilon_d - \epsilon_p$. Furthermore, our result provides microscopic insight into the multi-layer cuprates, such as Bi-2223: in addition to layer-dependent doping [26], the smaller value of the charge-transfer energy in the outer layers may explain the enhancement of superconductivity in the outer layers. It has been suggested theoretically and demonstrated experimentally [27] that proximity to a metallic layer reduces the charge-transfer energy. Using this principle in heterostructure design should result in even higher transition temperatures.

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