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LA-UR--88-2549

DE88 016228

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SUBMITTED TO Proceedings of the Adriatico Research Conference on the
Theoretical Understanding of High Temperature Superconductivity,
July 26-29, 1988, Trieste, Italy

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EXCITONIC SUPERCONDUCTIVITY IN COPPER OXIDES

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ABSTRACT: We discuss the possibility of excitonic superconductivity in high T_c copper oxides. The Hamiltonian describing CuO_2 planes supports both antiferromagnetism and low-lying $\text{Cu} \rightarrow \text{O}$ intra and interband charge fluctuations. One crosses from one regime to another as the number of holes per unit cell increases. The high T_c superconductivity takes place at hole concentrations most favorable for *intra*band charge transfer excitations. The dynamic polarizability of the environment surrounding CuO_2 planes plays an important role in enhancing T_c .

The discovery of high temperature superconducting copper oxides [1], [2] has generated intense theoretical activity [3]. Many theories of high temperature superconductivity rely on the close relationship between superconductivity and magnetic properties of CuO_2 planes. Although these materials exhibit antiferromagnetism at stoichiometry and half-filling of CuO_2 planes, it is not at all clear that magnetism helps superconductivity at some finite doping. Here we discuss a novel mechanism for high temperature superconductivity which is excitonic in nature, arises in the effective Hamiltonian appropriate for Cu-O systems, and is intimately related to the specific crystal structure and chemistry of the new materials. We find antiferromagnetism at half-filling in accordance with experiments but the instrumental role in enhancing T_c is played by charge fluctuations which become important for finite doping. The superconducting instability takes place on CuO_2 planes but the dynamic polarizability of the surrounding medium is essential in further raising T_c . The mechanism admits an important role for phonons in La (2-1-4) superconductors, but it is particularly effective in the plane-chain-plane (PCP) structure of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (1-2-3), where the high polarizability of Cu-O chains dramatically enhances the superconducting instability inherent to the CuO_2 planes. We suggest that similar enhancement takes place in newly discovered Bi (4-3-3-4) and Tl (2-1-2-2) based materials with Bi-O and Tl-O layers serving as a highly polarizable medium. This points to a direction to follow in the search for new, higher T_c materials, with CuO_2 planes embedded in a highly polarizable environment as a basic building block.

We first consider a single CuO_2 plane. The simplest Hamiltonian that takes into

account both Cu and O sites can be written

$$H = \epsilon_d \sum_i d_i^\dagger d_i + \epsilon_p \sum_j p_j^\dagger p_j - \sum_{\langle i,j \rangle} t_{i,j} d_i^\dagger p_j + h.c. + \\ + U_d \sum_i n_{d,i} n_{d,i} + U_p \sum_j n_{p,j} n_{p,j} + V \sum_{\langle i,j \rangle} n_{d,i} n_{p,j} \quad , \quad (1)$$

where $t_{i,j}$ is the hopping matrix element between Cu $d_{x^2-y^2}$ and O $p_{x,y}$ orbitals, ϵ_d and ϵ_p are respective local energy levels, $U_d(U_p)$ is the onsite Coulomb repulsion and V is the nearest-neighbor Coulomb repulsion between Cu and O sites. One expects that (1) reflects the essential physics of the problem. If we ignore U_d, U_p, V the resulting band structure consists of bonding (B) and antibonding (AB) Cu-O bands along with a flat nonbonding (NB) oxygen band [4], [5]. At stoichiometry in La_2CuO_4 and $\text{YBa}_2\text{Cu}_3\text{O}_6$ the 2D AB band is $\frac{1}{2}$ -filled and these materials should be metals. On the contrary, experimentally both exhibit antiferromagnetism [6], [7], indicating the importance of correlations. To understand the effect of correlations in (1) we will first use weak coupling theory which enables explicit evaluation of relevant quantities. We find that the physics in the superconducting regime is dominated by low lying charge transfer excitations. Since oxide superconductors appear to be more in the intermediate coupling regime, our result should be interpreted in a qualitative sense. However, quantum chemistry calculations for finite clusters (below) also demonstrate the importance of charge transfer excitations. We therefore expect that overall features of our theory persist in the intermediate coupling regime. Since *both* spin and charge fluctuations can be soft, Hamiltonian (1) differs qualitatively from the Hubbard Hamiltonian, where charge fluctuations are suppressed.

We first consider the case when the AB band in the CuO_2 plane is $\frac{1}{2}$ -filled. After projecting the Hamiltonian (1) onto the AB band we obtain the following effective Hamiltonian:

$$H_{AB}^{\text{eff}} = \sum_{\vec{k}, \sigma} \xi_{\vec{k}} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} + \\ + \sum_{\vec{k}, \vec{k}', \vec{q}, \sigma, \sigma'} [U + 2V \cos(q_x a) X_{\vec{k}+\vec{q}} X_{\vec{k}} + 2V \cos(q_y a) Y_{\vec{k}+\vec{q}} Y_{\vec{k}}] c_{\vec{k}', -\vec{q}, \sigma'}^\dagger c_{\vec{k}+\vec{q}, \sigma}^\dagger c_{\vec{k}, \sigma} c_{\vec{k}', \sigma'} \quad , \quad (2)$$

where a is Cu-O separation, $\xi_{\vec{k}} = \frac{1}{2}(\epsilon_d + \epsilon_p) - \mu + \frac{1}{2}[(\epsilon_d - \epsilon_p)^2 + 16t^2(\sin^2 k_x a + \sin^2 k_y a)^2]^{\frac{1}{2}}$, $U = U_d \cos^4 \theta + U_p \sin^4 \theta$, $V = V \cos^2 \theta \sin^2 \theta$, with $\cos^2 \theta = \frac{1}{2} + \frac{1}{2}[1 + \frac{16t^2}{(\epsilon_d - \epsilon_p)^2}]^{-\frac{1}{2}}$, r being the average of the Cu-O hybridization over the Fermi surface. The coherence factors $X_{\vec{k}}, Y_{\vec{k}}$ are defined as:

$$X_{\vec{k}} = \frac{\sin k_x a}{(\sin^2 k_x a + \sin^2 k_y a)^{\frac{1}{2}}} \quad , \quad Y_{\vec{k}} = X_{\vec{k}}(x \rightarrow y) \quad ,$$

and $c_{\vec{k},\sigma}$ is the annihilation operator in the AB band.

In weak coupling, we can study collective modes of the system by considering the equation for the response function $\chi_{\sigma,\sigma'}(\vec{q},\omega)$ arising from the sum of ring and ladder diagrams:

$$\chi_{\sigma,\sigma'}(\vec{q},\omega) = \chi_0(\vec{q},\omega) + \delta_{\sigma,\sigma'}\chi_0(\vec{q},\omega)I(\vec{q})\text{Tr}\chi(\vec{q},\omega) - \chi_0(\vec{q},\omega)J(\vec{q})\chi_{\sigma,\sigma'}(\vec{q},\omega) \quad , \quad (3)$$

where $\chi_0(\vec{q},\omega)$ is the Lindhard function in the AB band and we have restricted our attention to the interband response. The direct interaction $I(\vec{q})$ and exchange interaction $J(\vec{q})$ follow from (2):

$$I(\vec{q}) = U + 2V \cos(q_x a)\alpha_x(\vec{q}) + 2V \cos(q_y a)\alpha_y(\vec{q}) \quad , \quad (4)$$

$$J(\vec{q}) = U + 2V \sum_{i=1}^2 [|\beta_x^i(\vec{q})|^2 + |\beta_y^i(\vec{q})|^2] \quad . \quad (5)$$

In the above equations we have used the following definitions:

$$\alpha_x(\vec{q}) \equiv \chi^{-1}(\vec{q},\omega=0) \sum_{\vec{k}} K_0(\vec{k},\vec{q}) X_{\vec{k}+\vec{q}} X_{\vec{k}} \quad ,$$

$$\beta_x^i(\vec{q}) \equiv \chi^{-1}(\vec{q},\omega=0) \sum_{\vec{q}} K_0(\vec{k},\vec{q}) X_{\vec{k}+\vec{q}} \gamma_x^i(\vec{k}) \quad ,$$

where $\gamma_x^1 = \cos k_x a$, $\gamma_x^2 = \sin k_x a$. $K_0(\vec{k},\vec{q})$ is defined by $\chi_0(\vec{q},\omega=0) \equiv \sum_{\vec{k}} K_0(\vec{k},\vec{q})$. The definitions of quantities with subscript y are obvious.

At half-filling the Fermi surface has perfect nesting and there will be a tendency to open a gap on the Fermi surface. An instability can occur in both the charge and spin density channels and the resulting CDW and SDW will have periodicity determined by the nesting vectors $\vec{Q}_0 = (\frac{\pi}{2a}, \pm \frac{\pi}{2a})$. One can show by solving (3) that the relative stability of a CDW or SDW depends on the sign of $I(\vec{q})$: First note that $\chi_0(\vec{Q}_0,\omega=0) \propto -\frac{1}{\hbar} \ell n^2(\frac{D}{T})$, where $D \sim 2t$. From (3) follows $\ell n^2(\frac{D}{T_{SDW}(CDW)}) = \lambda_{SDW}^{-1}$, where $\lambda_{SDW} \propto J(\vec{Q}_0) > 0$ and $\lambda_{CDW} \propto J(\vec{Q}_0) - 2I(\vec{Q}_0)$, $T_{SDW}(CDW)$ being the transition temperature of spin (charge) density wave. Obviously, for positive $I(\vec{Q}_0)$ $T_{SDW} > T_{CDW}$, while for negative $I(\vec{Q}_0)$ the situation is reversed. Since $I(\vec{Q}_0) = U > 0$ the ground state in weak coupling is SDW, irrespective of the relative size of U and V . This SDW reflects the qualitative features of the observed antiferromagnetic state [6], [7]. Thus, the *intra*band particle hole excitations arising in (1) account for the antiferromagnetism of these compounds. This point should be emphasized since the *inter*band charge transfer mechanism proposed earlier [8] has difficulty explaining magnetic properties.

However, away from half filling, when holes are added to the system either by doping or by varying oxygen content, the situation may change qualitatively. This is best

appreciated by considering $\chi_0(\vec{q}, \omega = 0)$. As x holes are added to the AB band, the maximum of $\chi_0(\vec{q}, \omega = 0)$ moves from $\vec{Q}_0$ to some $\vec{Q}(x)$, such that $|\vec{Q}(x)| < |\vec{Q}_0|$ and $2V\alpha_x(\vec{Q}(x))\cos Q_x(x)a + 2V\alpha_y(\vec{Q}(x))\cos Q_y(x)a$ becomes progressively more negative (Note that $\alpha_{x,y}(\vec{Q}(x)) < 0$). This is evident from Figure 1 where we plot $\chi_0(\vec{q}, \omega = 0)$ as function of hole count. The maximum occurs for $\vec{Q}(x) = (\pm Q, \pm Q)$ where $Q \simeq \frac{\pi}{2t} - \frac{\mu'}{t}$, for $\epsilon \ll t$ and $\mu' \equiv 2t - \mu$. The relation between x and μ is $x \simeq (\frac{\mu'}{2t})\ell n(\frac{2t}{\mu'})$. For V large enough it is possible to attain a situation where:

$$I(Q_y(x)) = V(x) + 2V(x)\alpha_x(\vec{Q}(x))\cos Q_x(x)a + 2V(x)\alpha_y(\vec{Q}(x))\cos Q_y(x)a < 0 \quad , \quad (6)$$

for some concentration of holes $x > x_c$, x_c being defined by $I(\vec{Q}(x_c)) = 0$. This signals the preference for CDW formation. The real, static CDW deformation does not occur, however, since away from half-filling the nesting features are diminished, as obvious from Figure 1. We then have *low-lying*, finite wavevector ($\vec{Q}(x)$), temperature independent, collective charge excitations in the CuO_2 plane, which will strongly influence the effective electron interactions. For some region of doping $0 < x_c \leq x \leq x_{c1} < 1$, which can be calculated from (3), the frequency of these short wavelength charge fluctuations $\omega_{CF}(\vec{Q}(x))$ will be lower than the corresponding spin fluctuation frequency $\omega_{SF}(\vec{Q}(x))$, and they can be utilized to build an attractive retarded interaction which can lead to superconductivity. Such a region will occur only for $\epsilon \equiv \epsilon_d - \epsilon_p \leq t$ and for $V > \frac{1}{4}U$. Figure 2 shows explicit results for the frequencies of collective modes illustrating this crossover. $\omega_{SF}(\vec{Q}(x)), \omega_{CF}(\vec{Q}(x))$ are plotted as functions of x , up to $x \sim 0.3$, where the approximate form of (3) for $x \ll 1$ becomes inaccurate. The continuing lines represent the trend in the frequencies for larger x , in particular, the upturn in ω_{CF} is caused by a decrease of V as one empties the AB band. The overall behavior of collective modes is qualitatively depicted in Figure 3a. Our *intra-band* charge excitation is distinct from the local charge transfer exciton proposed in [8], although the underlying theme, relying on the low energy cost for $\text{Cu} \leftrightarrow \text{O}$ charge transfer (see below), is similar.

We now discuss superconductivity. Following the Eliashberg formalism outlined in [9] we define the matrix element of the pairing interaction,

$$\lambda_{CF(SF)}(\vec{k}, \vec{k}') = -2\alpha_{CF(SF)}^2 \int_0^\infty d\omega \frac{F(\vec{k}, \vec{k}'; \omega)}{\omega} \quad , \quad (7)$$

where $\alpha_{CF(SF)}$ is the electron-charge fluctuation (spin fluctuation) vertex, and $F(\vec{k}, \vec{k}'; \omega)$ is given by $-\frac{1}{4}\text{Im}\chi^{CF(SF)}(\vec{k}, \vec{k}'; \omega)$, where $\chi^{CF(SF)}(\vec{k}, \vec{k}'; \omega)$ is obtained from (3). In (7) $\vec{k}$ and $\vec{k}'$ are constrained to lie on the Fermi surface. We have used the solution of Eq. (4) to evaluate (7) in various orbital states as a function of model parameters. Here we

Figure 1: The intraband susceptibility $\chi_0(\vec{q}, \omega = 0)$ for different fillings of the AB band. We plot χ_0 along $\vec{q} = (Q, Q)$, as the maximum occurs along this symmetry direction. We have taken $\epsilon \ll t$. The numbers labeling the lines refer to the value of $\frac{\mu'}{2t}$, $\mu' = 0$ corresponding to half-filling. Q is given in units of a^{-1} while χ_0 is in arbitrary units.

Figure 2: The doping dependence of ω_{SF} and ω_{CF} plotted in units of μ' . We have set $U_p = 0$, and $\epsilon \ll t$. For $x > 0.1$ ω_{CF} is larger than μ' and has been cut off by μ' . The absolute size of U_d and V is determined by requiring antiferromagnetism for $x = 0.05$.

Figure 3: a) The generic x -dependence of ω_{SF} and ω_{CF} for CuO_2 plane. The region of $\omega_{CF} < \omega_{SF}$ occurs for sufficiently large V/U as explained in text. $\tilde{\omega}_{CF}$ refers to the interband charge excitations which may lead to the CDW (charge disproportionation) distortion at high doping. b) The qualitative ground state phase diagram as a function of x . Different regions are discussed in text. CDW phase is most likely for $\epsilon = 0$.

only outline results, for a lack of space. In Figure 3b we show the typical results for the ground state of the CuO_2 plane as a function of x . We have set $\epsilon = 0$. SC I is a d-wave superconductivity, produced by low-lying spin fluctuations. In this region T_c is *low*, due to self-energy corrections and dynamic pair-breaking. For $x > x_c$, the superconductivity crosses over to the s-wave type (SC II), where charge fluctuations dominate and T_c can be *high* since the above limitations are absent for an isotropic superconducting state. It is very important to note that phonons enhance T_c in SC II phase (they basically have no effect in SC I). Since T_c calculations are notoriously unreliable one should interpret our results as representing qualitative trend produced by doping the AB band. Finally, for large doping, the AB-NB *interband* charge fluctuations can lead to a CDW phase, a charge disproportionated state with a “frozen-in” $\text{Cu} \leftrightarrow \text{O}$ charge transfer and lattice distortion. In the shaded regions there is a competition between different ground state symmetries and it is possible that the system is a metal at $T = 0$. This phase diagram is very suggestive of a similarity between high T_c oxides and the “old” Ba-Pb-Bi-O superconductor [10], [11]. The newly discovered K-Ba-Bi-O superconductor is also likely to belong to the same class. This behavior is also in qualitative agreement with recent data on the 2-1-4 material which indicate that T_c saturates at 40K for x between 0.15 and 0.25 and then drops quickly to zero at $x \sim 0.30$ [12].

Why is T_c so much higher in 1-2-3 and new Bi and Tl systems than in 2-1-4? We conjecture that the dynamic polarizability of the environment of CuO_2 planes is crucial for elevating T_c . As an illustration, we consider $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ specifically. Consider a single Cu-O chain along the y-axis (see Fig. 4 for the plane-chain-plane (PCP) structure of 1-2-3). We can use the same Hamiltonian (1) where now the relevant atomic orbitals are Cu $d_{y^2-x^2}$ and O $p_{y,x}$. In 1D there is perfect nesting at any band filling. The ensuing instability is driven by deformation of wavevector $Q_y = 2k_F^c$. Just as in the plane, as holes are added to the AB band, Q_y decreases from $\frac{\pi}{2a}$ ($\frac{1}{2}$ -filled) to 0 (AB band empty), and $I(Q_y)$ can become negative, leading to strong charge fluctuations. The actual CDW instability is prevented by hopping, $t_\perp$, between chains and planes, by quantum fluctuations, and by disorder. The reduced dimensionality, however, is likely to make chains more polarizable than planes. In this way we use the high polarizability of a 1D system at wavevector $2k_F^c$ to further enhance the intrinsic polarizability of the Cu-O bond (see below). The high polarizability of the chains will affect the electron-electron interactions on neighboring planes, via an effective chain plane Coulomb coupling, W . This effective interaction for electrons on planes is given by $n_c W^2 \text{Tr} \chi^{\text{chain}}(q_y, \omega)$, where n_c is the linear density of chains. Importantly, this interaction is the *same* for two electrons on adjacent CuO_2 planes or on a single plane.

Consequently, while this part of the attraction is unchanged, the direct Coulomb repulsion will be *significantly reduced* if the electrons are on adjacent planes. This could lead to an appreciable enhancement in T_c for *interplane* over intraplane pairing. Of course, in addition to the chain-induced attraction there is an attractive interaction due to the planes themselves, as discussed before. If the chain-induced attraction dominates, an interesting possibility of *interplane* Cooper pairing arises in the PCP structure of $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$.

In reality the situation in $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ is more complicated. In addition to the linear Cu-O chain, there are bridging oxygens (O(4)), which control the plane-chain coupling, W . The presence of these oxygens induces additional transverse polarization of the chains, favoring intraplane pairing. This mode is a part of an *interband* response, not included in (3). Consider the cluster in Figure 4a. The upper and lower Cu have the coordination of the planes (Cu_p), while the central atom is a unit of the chain (Cu_c). The orbitals of particular interest are the $d_{x^2-y^2}$ orbitals on the Cu_p , the $d_{y^2-z^2}$ orbital on Cu_c , and the p_z orbitals on the bridging O(4) oxygens. Note that the bridging O p_z orbitals have the wrong symmetry to interact directly with $d_{x^2-y^2}$, but can interact with the $d_{y^2-z^2}$ orbital. These three atomic orbitals on the chain combine to give B, NB, and AB molecular orbitals (Figs. 4b, 4c, 4d). The NB orbital will develop into a narrow O p_π band along the chain axis involving O p_z orbitals, while the AB orbital develops into the Cu $d_{y^2-z^2}$ band considered above. Our *ab initio* quantum chemistry calculations [13] on the cluster in Figure 4a suggest that the interband charge transfer mode, in which an electron moves between the NB O p_π orbital and the AB Cu $d_{y^2-z^2}$ band, occurs at low energy, ω_t , of the order of a few 0.1 eV (Singlet and triplet excitons differ by only ~ 0.1 eV). Our best calculations to date suggest that the ground state of the Cu_3O_{12} cluster model for $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ involves an "empty" Cu $d_{y^2-z^2}$ orbital and a pair of electrons in the O p_π NB orbital ($\text{Cu}^{3+}\text{-O}^{2-}$). The state in which the electron is excited from the NB orbital to $d_{y^2-z^2}$ ($\text{Cu}^{2+}\text{-O}^{1-}$) lies a few 0.1 eV above the ground state. Which of these two states has lower energy depends on the nature of correlations included in the configuration interaction. The common denominator in all our calculations, however, is the presence of low-lying charge transfer excitations. By contrast, in cluster models of $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ the lowest charge transfer excitations occur at energy $\sim 2\text{-}3$ eV.

If the above clusters are ordered in chains, there will be strong plane-chain Coulomb coupling, since both the intraband and interband excitations lead to rearrangement of the charge distribution on the bridging oxygens. The strength of the pairing interaction should scale approximately as $\frac{1}{r_1^2}$, where r_1 is the Cu(2)-O(4) distance. With both types of charge transfer excitations included, the retarded attraction will be somewhat stronger with

the electrons on the same plane. Nevertheless, the beauty of the $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ sandwich structure is that the bridging oxygens can couple two distinct planes, and we expect that the system will still take advantage of interplane pairing, thereby defeating in large part the direct Coulomb repulsion. The most favorable situation for interplane pairing will occur in orthorhombic $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ with highly ordered chains, where the longitudinal intraband exciton is likely to be dominant.

Figure 4: a) A Cu_3O_{12} cluster model of the PCP-like structure. b), c) and d) denote the B, NB and AB combinations, respectively. The phase of an atomic orbital is denoted by color. The Cu $d_{x^2-y^2}$ orbitals in the planes are pictured for the readers orientation; they do not interact with the O p_z orbitals.

We emphasize that many related chain complexes have strong CDW (charge disproportionation) tendencies, which are further strengthened by coupling to the lattice. Therefore, it is realistic to expect that the physics of Cu-O chains in $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$, with electron-phonon interactions and out-of-chain (plane) O polarizations included, is dominated by their proximity to a CDW.

Several experiments support our picture. In $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ doped with Co, T_c decreases quickly with the increase of the $\text{Cu}(2)\text{-O}(4)$ bond length [14]. This distance controls W and is even shorter in Bi and Tl superconductors. T_c in $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ depends sensitively on the O content on chains and the nature of $\text{Cu}(1)$ substitutions [15] (It is sufficient for our mechanism that chains maintain their integrity over several lattice spacings.). On the

other hand, to date there has been no positive identification of charge fluctuations in optical experiments. However, a number of recent reflectivity data indicate a broad resonance at ~ 0.2 eV, consistent with an interband excitation.

We have discussed here a novel charge fluctuation mechanism which enhances the transition temperature in oxide superconductors. This mechanism is particularly effective in the PCP structure of 1-2-3 compounds. The fact that T_c decreases from 1-2-3 to 2-1-4 to Ba-Pb-Bi-O structures, points to a relation of superconductivity to effective dimensionality. This is expected in our model, since the effectiveness of our intraband exciton is thereby reduced. At the same time, the role of phonons should increase progressively, leading to a more pronounced isotope effect. The "60 K plateau" observed in $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ upon reducing O content may indicate a crossover from inter to intraplane pairing or the crossover from the regime in which the intraplane pairing is controlled by a linear chain exciton to one where the transverse exciton dominates. Clearly, our proposal suggests several new experimental directions: an EELS finite $\vec{q}$ search for intraband chain excitons; resonant Raman scattering to probe the Cu(1)-O(4) bond stretch; and identifying singlet and triplet local chain excitons in 1-2-3. Finally, our idea of raising T_c by embedding CuO_2 planes in a highly polarizable medium would be strongly supported by a direct observation of low-lying charge fluctuations in Cu-O chains and Bi(Tl)-O layers. The interplane pairing in $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$ is an intriguing possibility and would dramatically confirm the essential role of the interplane medium. We believe that efforts in synthesizing new materials should focus on increasing the polarizability of the surrounding medium and its coupling to CuO_2 planes.

This research has been performed under the auspices of the US DOE.

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