A DFT investigation of pressure effects in the infinite-layer ACuO$_2$ cuprate superconductor for A={Mg, Ca, Sr, Ba}

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We use density functional theory to investigate external-pressure and “internal-pressure” effects in the infinite-layer cuprate ACuO$_2$ for A={Mg, Ca, Sr, Ba}, where internal-pressure is induced by ion-size substitution. Here we refer to the chemical-pressure from altering ion-size as ‘internal-pressure’ and mechanically applied pressure as ‘external-pressure’. Isovalent ion-substitution can thus be utilized to alter the structural and electronic properties of a material, and this can be achieved in a systematic manner where the ion-size progressively changes, as in the rare-earth series R={Lu, ..., La}, or column II ions A={Mg,Ca,Sr,Ba,Ra}. For example, in the R(Ba$_{2-x}$Sr$_x$)Cu$_3$O$_7$ family of cuprate high-temperature superconductors the lattice and structural parameters systematically change with ion-size, demonstrating internal-pressure effects. 

Concurrently, as the ion-size is increased, the maximum superconducting transition temperature, $T_{c\text{max}}$, increases from 70 K for YSr$_2$Cu$_3$O$_7$-$\delta$ to 100 K for LaBa$_2$Cu$_3$O$_7$. 

Recently we showed from two-magnon Raman scattering that the anti-ferromagnetic exchange energy, $J$, systematically decreases across this series from 150 meV to 94 meV. In contrast, in the co-substituted system (La$_{1-x}$Ca$_x$)(Ba$_{1.75-x}$La$_{0.25+x}$)Cu$_3$O$_y$ internal-pressure appears to decrease $T_{c\text{max}}$. These internal-pressure effects on $T_{c\text{max}}$ can be compared with the universal increase of $T_{c\text{max}}$ under external pressure that is observed in the cuprates with a concurrent increase in $T_c$. This presents a paradox in cuprate physics and to understand the salient difference between internal- and external-pressure we have proposed that the cuprate’s polarizability plays a key role. Another consideration is pressure-induced modification of the Fermi-surface and associated electronic density of states (DOS) at the Fermi-energy. Specifically, can this lead to significant variations in $T_c$ (or the superconducting energy gap $\Delta_0$) and can it account for the disparate effects of internal- and external-pressure on $T_c$? We have conducted the present study to investigate this possibility.

Here we seek to elucidate how the electronic properties evolve with internal pressure using density functional theory (DFT) calculations in the model infinite-layer cuprate ACuO$_2$ where internal-pressure is implemented by altering the A-site ion from Mg to Ba. We then compare these results with the simulated effect of external pressure. ACuO$_2$ was chosen because it has the simplest realisable chemical structure that still displays essential aspects of cuprate physics. It has a P4/mmm tetragonal unit-cell with the Cu ion at (0,0,0), O at (a/2,a/2,0) and (0,a/2,0) and A at (a/2,a/2,c/2). The undoped material is insulating due to strong electronic correlations. Superconductivity is observed with $T_{c\text{max}} = 110$ K for hole-doping (due to A vacancies) or $T_{c\text{max}} = 42$ K under electron-doping (by R substitution for A) of the CuO$_2$ layer.

DFT has been used extensively to study the electronic properties of the cuprates. Early calculations accurately reproduced phonon spectra and intensities observable by Raman spectroscopy. More recently Pavarini et al and Sakakibara used DFT methods to identify electronic parameters that might play a role in governing $T_{c\text{max}}$. As a ‘model’ cuprate there have been numerous DFT studies on CaCuO$_2$. These studies found that the experimental lattice parameters were reproduced to within a few percent. The calculated band-structure had similar features to other cuprates, such as the charge-transfer band-gap. Other than a shift in the Fermi-Energy, $E_F$, this band-structure changed little with hole-doping, $p$, up to 10% - a so-called rigid band shift. In the DOS there is a van-Hove-singularity feature $\sim$ 1 eV below $E_F$ and its position is pressure dependent. In addition, various methods have been employed to try to reproduce strong-correlation features of the undoped cuprates, such as the charge-transfer band-gap and the anti-ferromagnetic order on the CuO$_2$ plane. There have also been several reported DFT studies of SrCuO$_2$. Pure SrCuO$_2$ forms 1D chains whilst...
the electron-doped Sr$_{0.9}$R$_{0.1}$CuO$_2$ forms the P4/mmm tetragonal structure.$^{13}$

In distinction to these previous studies, we present here a comparative study of the ACuO$_2$ to investigate internal- and external-pressure effects on the electronic properties in this family of cuprate materials.

II. COMPUTATIONAL DETAILS

The DFT calculations were performed using the Vienna Ab-Initio Simulation Package (VASP) with Projector Augmented Wave (PAW) pseudopotentials from the VASP5.2 library.$^{22,23}$ We used the GGA-PW91 Generalised Gradient Approximation scheme developed by Perdew et al.$^{24,25}$ to derive the form of the exchange-correlation potential and kinetic energy in the single-electron Hamiltonian.

To calculate the equilibrium structural parameters for ACuO$_2$, we determined the 'free-energy' (following the nomenclature used in VASP), $F$, for fixed unit-cell volume, $V$, with a 16 × 16 × 16 k-space, Γ-centred mesh. For each $V$, the ion positions and lattice parameters were first relaxed, using a conjugate-gradient algorithm$^{20}$ in VASP, and this was followed by an accurate calculation of $F$ with fixed ion positions and lattice parameters. The results of this procedure are shown in Fig. 1. The lattice parameters with the lowest free-energy are: $a = b = \{3.779, 3.880, 3.962, 4.019\}$ Å and $c = \{2.907, 3.201, 3.467, 3.888\}$ Å for A=Mg, Ca, Sr and Ba respectively. These correspond to unit-cell volumes of $V = \{40.48, 48.19, 54.85, 61.55\}$ Å$^3$. We do not observe any buckling of the CuO$_2$ layers as expected on symmetry grounds. For calculations of the electronic dispersion we use structures with the lowest $F$ and a 24 × 24 × 24 k-space mesh. Band-structure calculations involve a non-self-consistent calculation using a high-quality self-consistently calculated charge-density as an input.

The grey shaded regions in Fig. 1 indicate experimentally determined structural parameters at room-temperature where they are available.$^{12,13,37,38}$ To our knowledge there are no reports that MgCuO$_2$ has been synthesized. Neither has the synthesis of pure bulk BaCuO$_2$ been reported, suggesting this compound is also unstable. For example de Caro et al.$^{35}$ report up to 30% vacancies on the Cu site with lattice parameters $c \approx 4.2$ Å and $a = 3.906$ Å assumed from lattice matching to the SrTiO$_3$ substrate. Here we find a reversed $c/a$ ratio compared with these experimental results. Superlattices of intercalated Ba-, and Ca- infinite layer compounds have been reported to be superconducting.$^{12,35}$ Although even numbers of Ba- unit-cells are required.$^{35}$ Note that the ion-size dependent $c/a$ lattice-parameter ratio indicates anisotropic stress under ion-substitution so that the internal-pressure effect is not hydrostatic.

To calculate the bulk moduli, $B_0$, we fit the data presented in Fig. 1 to the Murnaghan equation of state$^{2}$ (in SI units):

$$F(V) = F_0 + \frac{B_0 V}{B'_0 (B_0 - 1)} \left[ B'_0 (1 - V_0/V) + (V/V_0)^{B'_0} - 1 \right]$$

(1)

where $B'_0 = -\partial B_0 / \partial P |_T$ is generally taken to be constant. The fits are shown as blue lines in Fig. 1 from which we find $B_0 = 98, 106, 111$ and 127 GPa for A = Ba, Sr, Ca and Mg respectively. As expected, these materials become more compressible as the ion-size increases. By comparison Qin et al.$^{40}$ experimentally determine the bulk moduli of CaCuO$_2$ to be 96 GPa for $P < 6$ GPa and 186 GPa for $P > 6$ GPa, where $P$ denotes (external) pressure. (For comparison with other cuprates, $B_0 = 123$ GPa for YBa$_2$Cu$_3$O$_7$ and 78 GPa for YBa$_2$Cu$_3$O$_{6.33}$).

We thus find reasonable agreement between our calculated stable structural parameters and experimental results.

To simulate external pressure we used relaxed structures at fixed $V$ where $F$ is not at the minimum. For example, CaCuO$_2$ with a unit-cell volume of $V = 45.6$ Å$^3$ corresponds to an external pressure of $P = 9.6$ GPa when using the experimental bulk modulus of 186 GPa (Ref. 40) and has the ratio $c/a = 0.813$, as shown in Fig. 1.

III. RESULTS - ELECTRONIC STRUCTURE

In this paper we are primarily interested in the internal-pressure induced modification of the electronic dispersion, $\epsilon (k)$, close to $E_F$ ($\epsilon (k) = 0$) and how this compares with that caused by external pressure.
In Fig. 2 we show the band-structure along the path \( \Gamma-X-M-\Gamma \) with \( k_z = 0 \) for ACuO\(_2\) at \( P = 0 \). Between \( k = (k_x, k_y) = (0, \pi) \) and \( k = (\pi, \pi) \) there is a strongly dispersive band crossing \( E_F \) close to \( k = (\pi/4, \pi) \) and \( k = (\pi/2, \pi/2) \). This band, shown colored, is associated with states in the CuO\(_2\) plane and is the only band that contributes to the DOS within 0.45 eV of \( E_F \). Between –1 eV and –0.5 eV there are several other bands that move closer to \( E_F \) as the A-site ion-size increases (and as \( V \) concurrently increases).

It is well known that the undoped cuprates, including CaCuO\(_2\), have a charge transfer gap of approximately 2 eV\(^{10,12}\), in contrast to these calculations which imply undoped ACuO\(_2\) is metallic. In fact, this is to be expected from GGA calculations on the undoped system because they do not account for the strong-correlation physics of the undoped cuprates. This deficiency could be addressed by the use of LSDA+U calculations to correct the band gap by the introduction of a Coulomb repulsion term. However, this would cause some difficulties in comparison of ion-size effects, since \( U \) itself should be ion-size dependent due to the effect of ionic polarizability\(^{13}\) on screening\(^{13,15}\).

However, the dispersion reflects the rigidly shifted band structure observed using angle-resolved photoemission spectroscopy (ARPES) at finite doping where the strong-correlations are screened out by angle carriers. Further, the saddle-point vHs is known to reside below \( E_F \) and is crossed in the overdoped region leading to a change in the Fermi-surface topology\(^{10,17}\). So these calculations do reveal the features of the dispersion that are known to exist when correlations are suppressed and it is therefore plausible that the systematic changes with ion-size shown here reflect real band-structure evolution.

The calculated band structure also reveals that the dimensionality of the dispersion is affected by internal- and external-pressure. To illustrate this, in Fig. 3 we plot Fermi-contours (\( \epsilon(k) = 0 \)) in the \((k_x, k_y)\) plane for various \( k_z \) momenta. The \( k_z \) dispersion is smaller for larger A ion-size because these decouple the CuO\(_2\) layers resulting in the more 2-dimensional-like Fermi-surface. When A=Ba there is little change in the Fermi-contours for different \( k_z \). Only when this \( k_z \) dispersion is considered is the Luttinger sum rule satisfied for these undoped materials.

In Fig. 4 we show the total DOS as a function of internal-pressure (i.e. as the A-site ion-size progressively increases). Starting at \( E = -1.5 \) eV, there is a peak in the DOS that progressively moves closer to \( E_F \) as the internal-pressure increases. The multiple bands in this energy region and the significant \( k_z \) dispersion (particularly for the materials with small unit-cell volume, \( V \)) complicate the interpretation of this feature. There is a secondary peak in the DOS between –1 eV for MgCuO\(_2\) and –0.5 eV for BaCuO\(_2\) that derives in part from the saddle-point in the dispersion of the colored band in Fig. 2. In materials with smaller \( V \) this peak is significantly broadened by the large \( k_z \) dispersion.

However, the states directly relevant to superconductivity lie within \( \approx 0.5 \) eV of \( E_F \). This region of the DOS is shown in the inset to Fig. 4 and shows that the DOS at \( E_F \) is similar, but with a slight increase in the DOS from those ACuO\(_2\) with smaller \( V \) to those with larger \( V \). The band contributing to the DOS in this region, shown colored in Fig. 2, can be interpolated using the tight-binding expression;

![Figure 2](image1.png)

**FIG. 2.** (Color online) The ACuO\(_2\) band structure for each \( A \) along the path \( \Gamma-X-M-\Gamma \) with \( k_z = 0 \).

![Figure 3](image2.png)

**FIG. 3.** (Color online) Fermi-contours (\( \epsilon(k) = 0 \)) at each \( k \) calculated for each ACuO\(_2\).
FIG. 4. (Color online) The calculated density of states (DOS) for ACuO₂ illustrating a shift in weight closer to $E_F$ as the A ion-size increases. The DOS is normalised such that each band contains 1 state.

$$\epsilon(k) = c_0 + \frac{1}{2} c_1 \cos(k_x) + \cos(k_y)$$

$$+ c_2 \cos(k_x) \cos(k_y)$$

$$+ \frac{1}{2} c_3 \cos(2k_x) + \cos(2k_y)$$

$$+ c_\perp \cos(k_z/2) [\cos(k_x) - \cos(k_y)]^2$$

The $c_\perp \cos(k_z/2) [\cos(k_x) - \cos(k_y)]^2$ term in Eq. 2 accounts for the $k_z$ dispersion illustrated in Fig. 3. The tight-binding coefficients, $c_i$, extracted from fitting the DFT-derived dispersion, $\epsilon(k)_{\text{DFT}}$, are plotted in Fig. 6. Closed (open) symbols are for internal- (external-) pressure effects and show that the dispersion, $\epsilon(k)$, alters with internal- and external-pressure in a similar fashion. The error for each tight-binding fit, defined as $N^{-2} \sum_k \sqrt{\epsilon(k)_{\text{DFT}} - \epsilon(k)_{\text{fit}}}^2$ where $N$ is the number of data points, are shown in the lower panel. Typical errors are $\approx 1.75$ eV with larger volumes better described by the tight-binding dispersion of Eq. 2. Eq. 2 best describes the band close to $E_F$ and deviates most from the DFT values around the top and bottom of the band. Parameterizing the dispersion thus is justified if one’s interest is restricted to within $\sim 0.5$ eV of the $E_F$, as is indeed the case for our calculations of the superconducting energy gap (described below). Importantly, this allows us to sample the dispersion over a much finer k-space mesh of $3000 \times 3000 \times 100$ points (which is not practically possible using VASP alone) for calculations of the DOS and the superconducting energy gap.

The nearest-neighbor hopping term, $c_1$, shows the largest pressure-induced variation, increasing from $-1.9$ to $-1.5$ eV from the smallest to largest $V$. Concurrently, the next-nearest-neighbor term, $c_2$, increases from $0.05$ to $0.07$ eV resulting in the more ‘rounded’ Fermi-contours of BaCuO₂ seen in Fig. 6. We describe later in the paper how these pressure-induced changes in Fermi-surface shape relate to the superconducting energy gap. $c_\perp$ vanishes as $V$ increases reflecting the weaker $c$-axis coupling between CuO₂ planes at larger $V$ and a more 2-dimensional-like Fermi-surface.

The DOS calculated from the parameterized dispersion, $\epsilon(k)_{\text{fit}}$, is shown in Fig. 7. Full solid lines represent internal-pressure effects (ACuO₂ with A indicated in the legend) and dashed lines represent external-pressure effects (CaCuO₂ with the effective pressure indicated in the legend). Fig. 7 reveals similar features to the DOS calculated with VASP where materials with larger $V$ have higher DOS at $E_F$. Fig. 8 also shows the vHs at $E \approx -0.5$ eV originating from the saddle-point in the band around $(k_x, k_y) = (0, \pi)$ (and symmetry related points). The vHs is significantly broadened by the $k_z$ dispersion for materials with smaller $V$.

IV. DISCUSSION

What bearing might these internal- and external-pressure induced changes in the dispersion and DOS have on superconductivity in these systems? To approach this question we solve the self-consistent BCS gap-equation [1118] to obtain the superconducting energy gap, $\Delta_0$: 
\[ \Delta(k) = -\frac{1}{2} \sum_{k'} \frac{v_{kk'} \Delta(k')}{\sqrt{\epsilon(k')^2 + \Delta(k')^2}} \]  

Here \( v_{kk'} \) is the pairing potential of the form \( v_{kk'} = v_{kk} \delta(k - k) \) where \( \delta(k) = \cos(k_x) - \cos(k_y) \) to reflect \( d \)-wave symmetry, and the \( d \)-wave superconducting gap is given by \( \Delta(k) = \frac{i}{2} \Delta_0 \delta(k) \). Note that in the absence of competing order parameters, such as the pseudogap, one can expect that \( T_c \) is proportional to \( \Delta_0 \). We take \( \epsilon(k) \) from the tight-binding fits, \( \epsilon(k)_{\text{fit}} \), discussed above.

We solve Eq. 3 self-consistently assuming a pressure and ion-size independent \( v = 350 \text{ meV} \) and summing over states \( \epsilon(k) \) within \( \pm 150 \text{ meV} \) of \( E_F \). The resulting \( \Delta_0 \) values are plotted as a function of unit-cell volume in Fig. 7. Closed symbols represent unit-cell volume changes induced by internal-pressure, while the open symbols represent volume changes induced by external-pressure. There is a 30-fold increase in the magnitude of \( \Delta_0 \) for SrCuO\(_2\) and BaCuO\(_2\) (filled squares at \( V = 55 \) and 61.5 Å\(^3\) respectively) are at odds with the general trend in \( \Delta_0 \) and with CaCuO\(_2\) at equivalent \( V \) (open squares). Recall that the tight-binding parameters determining \( \epsilon(k) \) alter under internal- and external-pressure in a similar fashion so that one might expect similar \( \Delta_0 \) from Eq. 4. Furthermore, the DOS at the Fermi-level, \( N(E_F) \), scales only with \( V \) and so, in light of the weak-coupling BCS result for \( d \)-wave superconductivity:

\[ \Delta_0 = 4.28 k_B T_c = 4 \hbar \omega_B \exp \left( \frac{-1}{N(E_F)^{1/2}} \right) \]  

the distinct \( \Delta_0 \) magnitudes for SrCuO\(_2\) and BaCuO\(_2\) are especially surprising. In this equation \( \hbar \omega_B \) the pairing-boson energy scale. However, one can understand these distinct \( \Delta_0 \) as resulting from the difference in the average pairing potential close to the anti-nodes, where \( v_{kk} \) is largest. This is in turn due to the detailed shape of the Fermi-surface. By way of illustration we plot \( v_{kk} \) corresponding to the points where the Fermi contours touch
FIG. 8. (Color online) $\epsilon_{kk}$ corresponding to the points where the Fermi contours touch the zone boundary at $(k_x, k_y) = (\pi, k_{Fz})$ as a function of $k_{Fz}$. The Fermi-surface of BaCuO$_2$ spans regions of lower pairing potential than SrCuO$_2$ which results in the comparatively small $\Delta_0$ in Fig. 7.

the zone boundary at $(k_x, k_y) = (\pi, k_{Fz})$ as a function of $k_{Fz}$ (we append the subscript $F$ to denote a value of $k$ at the Fermi-energy). Combined, Fig. 3 and Fig. 8 show that the Fermi-surface of BaCuO$_2$ spans regions of lower pairing-potential than SrCuO$_2$ which results in the comparatively small $\Delta_0$. This result highlights how sensitive $\Delta_0$ can be to the precise shape of the Fermi-surface.

While Fig. 7 shows that $\Delta_0$ correlates with $V$ independently of how the pressure is applied, because of the near linear relationship between $V$, $c_1$ and $c_2$ (see Fig. 5), the same correlation between $\Delta_0$ and the composite parameter $-c_2/c_1$ or $(-c_2+c_1)/c_1$ holds. The ratio $\alpha' = \alpha/\alpha' \equiv -c_2/c_1$ is the Fermi-surface-shape parameter which Pavarini et al. showed correlates with $T_c^{max}$ across a wide range of cuprates, and this is consistent with the correlation between $-c_2/c_1$ and $\Delta_0$ which we find here.

From this study we draw two main conclusions; firstly it is plausible that internal- and external-pressure can have a significant effect on the superconducting properties via changes in $\epsilon(k)$. Secondly, the effect is essentially the same for both internal- and external-pressure. The second conclusion from this study must be contrasted with the disparate effects of internal- and external-pressure on $T_c$ observed experimentally, for example in the RBa$_2$Cu$_3$O$_{7-\delta}$ (Ref. 3–5, and 7) and (La$_{1-x}$Ca$_x$)(Ba$_{1.75-x}$La$_{0.25+x}$)Cu$_3$O$_y$ (Ref. 8 systems. This work suggests that the pressure-induced modification of $\epsilon(k)$ alone is insufficient to account for the observed pressure-induced variation in $T_c^{max}$, especially if the pairing potential, $V$, and pairing-boson energy-scale are independent of pressure, as we have assumed in the calculation of $\Delta_0$. Clearly there is a delicate interplay between the structural, electronic and superconducting properties in the cuprates and a deeper understanding of this is necessary to understand the dramatic material specificity of $T_c$. Internal- and external-pressure effects offer a powerful approach to study the effect of systematic changes in crystallographic and electronic structure on high-temperature superconductivity both experimentally and theoretically.

In summary, we used DFT to investigate internal-pressure, as induced by ion-size substitution, and external-pressure effects in the infinite-layer cuprate ACuO$_2$. The two key results are that these pressure effects can have a significant effect on the superconducting energy gap, as determined from the self-consistent BCS gap equation, via modifications to the electronic dispersion. Secondly, pressure alters the dispersion independently of how it is applied so that the superconducting energy gap correlates just with the unit-cell volume. This can be contrasted with the experimentally observed disparate effects of internal- and external-pressure on $T_c$ which suggests that a pressure-induced modification of $\epsilon(k)$ alone is insufficient to account for these effects.

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