


**Experiment title:**

High resolution study of phonon anomaly in the new high Tc superconductors oxychlorides

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HS-3461

**Beamline:**

ID28

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18

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**Report:**

Doping the  $\text{Ca}_2\text{CuO}_2\text{Cl}_2$  oxychloride systems creates a new family of HTcS superconductor with Tc up to 43 K in the case of  $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$  with a nominal vacancy doping of  $x=0.20$  [1, 2]. These compounds are interesting since they share  $\text{CuO}_2$  planes with the well known copper-oxides HTcS. Therefore they represent an ideal test bench for the physics governing the high Tc superconductivity that is commonly believed to depend only on the  $\text{CuO}_2$  planes, independently from the details of the

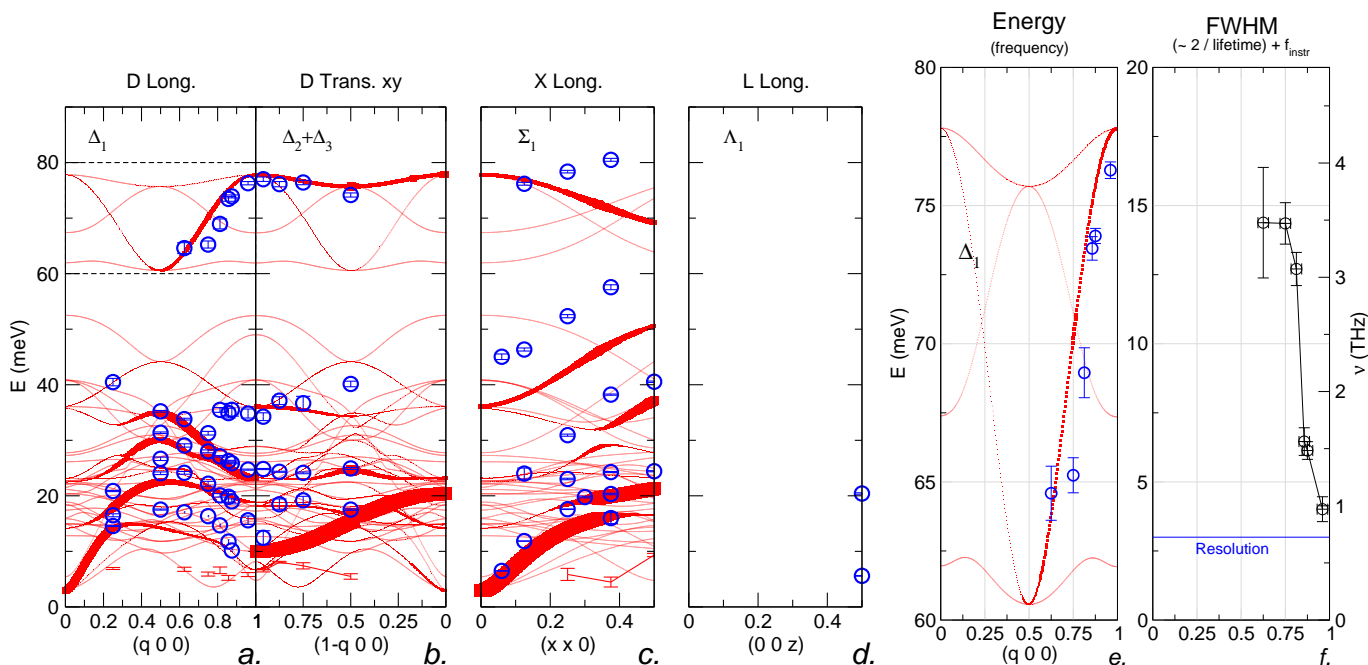


Fig. A.  $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$  phonon dispersion (blue hollow circles) and lifetime (black lines) measured by *ixs* on id28 and calculated frequencies by LDSA (red square). The experimental frequencies are the results of fit with instrumental function of the measured intensities. The red square symbols size is proportional to the calculated dynamical structure factor. Panel a. to d.: Measured and calculated dispersion along the main symmetry dispersion. For the direction  $(q, 0, 0)$  we have the propagation vector parallel (a.) and perpendicular (b.) to the  $\mathbf{Q}$  direction. This correspond to predominantly longitudinal (c.) or in-plane perpendicular (d.) polarisation.  $\Sigma$  (panel c) and  $\Lambda$  (panel d) dispersion are in longitudinal configuration. Panel e. and f.: Cu-O Bond stretching dispersion (e., zoom from panel a.) and lifetime (f.).

oxides blocks between them. Moreover, oxychloride systems present a peculiar feature that is particularly interesting for a comparison with cuprates. They show charge inhomogeneities that have been observed in a “checker-board” state in  $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$  [3], as distinct from the “stripe” structures observed in cuprates. Oxychlorides present an ideal system to study phonon dispersion, particularly the one of the copper-oxygen bond stretching mode, both by means of *inelastic x-ray scattering* (ixs) spectroscopy, and *ab-initio* calculations. First, because they are composed only of low Z atoms as compared to cuprates, thus having much less photo-electron absorption and being easier to model. Moreover, they have a simple 1-layer structure with small disorder, which reduces the number of modes to be measured and calculated.

The results for an under-doped sample of  $\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$  ( $T_c \approx 33$  K,  $x \approx 0.15$ , see Ref. [2]) are shown in Fig. A. Panel a and b shows the dispersion results for the  $\mathbf{q} = (q, 0, 0)$  symmetry  $\Delta$  direction in longitudinal configuration (meaning  $\mathbf{Q} \parallel \mathbf{q}$ , panel a) and in almost transverse *in-plane* configuration (meaning  $\mathbf{Q} \perp \mathbf{q}$ , panel b). Panel c and d shows the dispersion results for the  $\mathbf{q} = (q, q, 0)$  symmetry  $\Sigma$  and  $\mathbf{q} = (0, 0, q)$   $\Lambda$  directions, both in longitudinal configuration. The dispersion of the Cu-O bond-stretching (BS) (or half-breathing) mode is blown up in panel e, and its experimental full width half maximum in panel f.

For most of the dispersion, the experimental results are in good agreement with the calculations. Note that low energy and small  $q$  do not match because the calculated dispersion are obtained using a small  $2 \times 2$   $k$  grid. More detailed dispersion simulation are under way. In particular, we obtain a good agreement between calculated and measured frequencies for the Cu-O BS mode, as already reported for LASCULO [4] and YBCO [5]. However, a small deviation around  $q \approx 0.25$ , in correspondence with a large width increase may point out to an additional effect as discussed in Ref. [6, 7] (see also report of experiment HS-3460). A comparison with the dispersion and width for other cuprates is shown in Fig. B (from Ref. [7]). Calculations of the width for this particular mode are under way. A larger disagreement between measured and calculated frequencies is observed for the “full breathing” longitudinal mode along  $(q, q, 0)$ , which appears to harden considerably in the experiment, compared to the calculation. It would be interesting to check the experimental dispersion along that direction in the anti-ferromagnetic (AF), undoped  $\text{Ca}_2\text{CuO}_2\text{Cl}_2$  compound.

Finally, we note that the calculated Cu-BS or “half breathing” mode calculated in the AF undoped compound (not shown) and in the doped, superconducting one (Fig. A) softens in a quite similar way. This result differs from the cuprate case, where the softening seems to appear mainly on doping, but we do not have measurements on the AF undoped system to experimentally confirm this theoretical result.

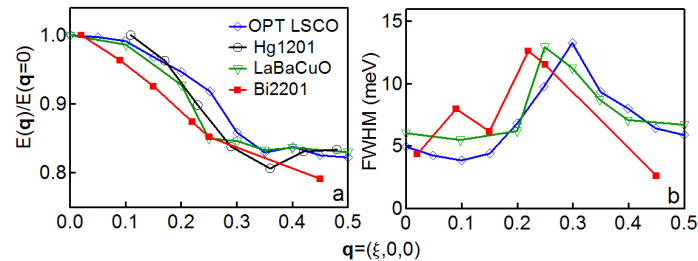


Fig. B. (From Ref. [7]) Panel (a) shows the dispersion of the BS mode for various optimally  $p$ -doped single layer cuprates in comparison with the Bi2201 data presented here. The frequencies are normalised to their value at  $\xi = 0$ . The optimally doped LSCO and LaBaCuO are from [6] and the Hg1201 are from [8]. Panel (b) shows the FWHM when available.

## References

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