

High temperature superconducting oxychlorides: a light element model for cuprates.

Blair Lebert^{1,2}, Matteo d'Astuto¹, Masaki Azuma³, Ikuya Yamada⁴

¹*IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France*

²*Synchrotron SOLEIL, Gif-sur-Yvette, France*

³*Materials and Structures Laboratory, TITech, Yokohama, Japan*

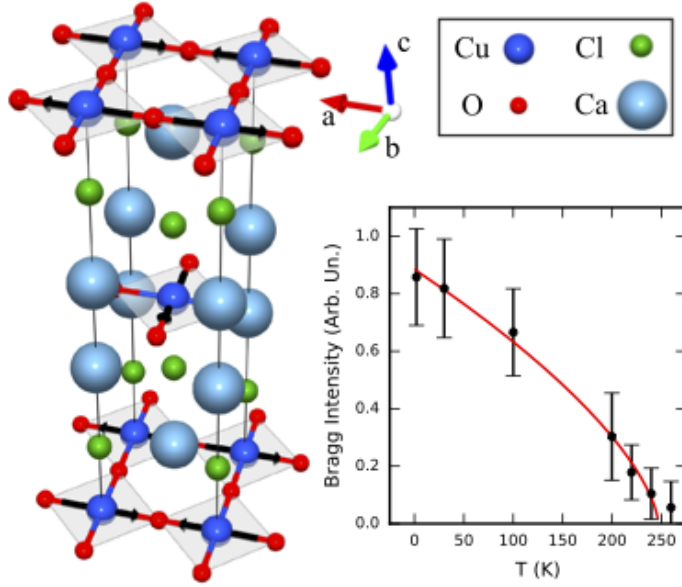
⁴*Nanoscience and Nanotechnology Research Center (N2RC), Osaka, Japan*

The copper oxychloride cuprate $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine [1]. It also shows a remarkable phase diagram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of stripes (or CDW) by near-field spectro-microscopy [2].

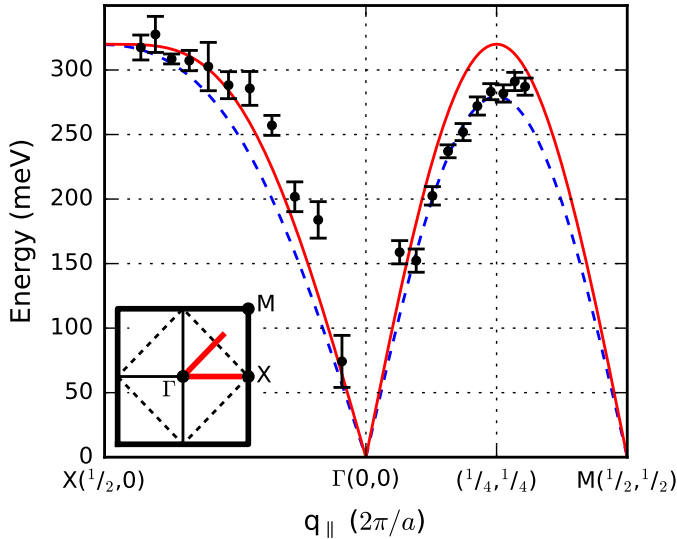
Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo [3], are now feasible for the first time in the HTSCs. This makes CCOC a model system to gain insight into the 30-year-old mystery of HTSCs by bridging the gap between theory and experiment. But relatively little is known about CCOC (for a cuprate) from an experimental point of view.

We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular to the (para)magnon dispersion [4], using recent development in RIXS [5], as well as to the phonon dispersion [6]. We are also looking for a bulk signature of the charge modulation (stripes) from X-ray resonant scattering close to the 1/8 doping.

[1] Z. Hiroi, N. Kobayashi, M. Takano, *Nature* 371, 139 (1994); Y. Kohsaka et al. *JACS* 124, 12275 (2002); [2] T. Hanaguri et al. *Nature* 430, 1001 (2004); K. Fujita et al. *PNAS* 111, E3026-E3032 (2014); [3] K. Foyevtsova et al., *Phys. Rev. X* 4, 031003 (2014); L. K. Wagner, *Phys. Rev. B* 92, 161116(R) (2015); [4] B. Lebert et al., arXiv:1610.08383 / hal-01388544; B. Lebert et al., ESRF experiment HC-2702 (2016), article in preparation; [5] M. P. M. Dean, *Journal of Magnetism and Magnetic Materials* 15, 3 (2015); [6] M. d'Astuto et al. *PRB* 88, 014522 (2013); B. Lebert et al., article in preparation (2017).



(top left) Tetragonal crystal structure of $\text{Ca}_2\text{CuO}_2\text{Cl}_2$. The square coordination of copper with its four nearest-neighbor oxygen ions in the CuO_2 planes is shown. The chlorine ions are located in the apical site above and below the copper. Black arrows indicate one of the possible magnetic structures. (bottom right) Temperature dependence of the fitted intensity of the averaged Bragg reflections $(\frac{1}{2}, \frac{1}{2}, \frac{5}{2})$ and $(\frac{1}{2}, \frac{1}{2}, \frac{7}{2})$ and a power law fit (red). From Ref. [4].



Dispersion of $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ measured using Cu L_3 RIXS. The red, continuous line is a calculation for a classical spin-1/2 2D Heisenberg model with nearest-neighbor exchange and the blue, dashed line is a calculation including further exchange terms which is described in the text. (inset) 2D Brillouin zone showing high-symmetry points. The first Brillouin zone boundary is represented by a thick black square, while the magnetic Brillouin zone boundary is represented by a dashed line. The region where we measured is shown as two thick red lines along Γ -X and Γ -M. From Ref. [4].