ESRF	Experiment title: Local structure study of the La dopant in the superconductor $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ by La-*K* EXAFS	**Experiment number:** **HE 2644**
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Names and affiliations of applicants (* indicates experimentalists):

Jürgen Röhler	Universität zu Köln, 50937 Köln, Germany
Christoph Trabant	Universität zu Köln, 50937 Köln, Germany
Johanna Frielingsdorf	Universität zu Köln, 50937 Köln, Germany
Rabia Djemour	Universität zu Köln, 50937 Köln, Germany
Victor Martovitsky	Lebedev Physical Institute, 11991 Moscow, Russia
Alicia Krapf	Humboldt-Universität zu Berlin, D 12489 Berlin, Germany
Recardo Manzke	Humboldt-Universität zu Berlin, D 12489 Berlin, Germany

Report: We have measured the La *K* - EXAFS of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ single crystals (size ≈ 2 x 2 x 0.1mm^3) in transmission geometry **(E || a, b)**. Spectra up to k = 17 Å^{-1} were recorded from nine crystals with La concentrations between x = 0.22 and 0.83, and at low temperatures, T = 30 - 300 K. In all crystals

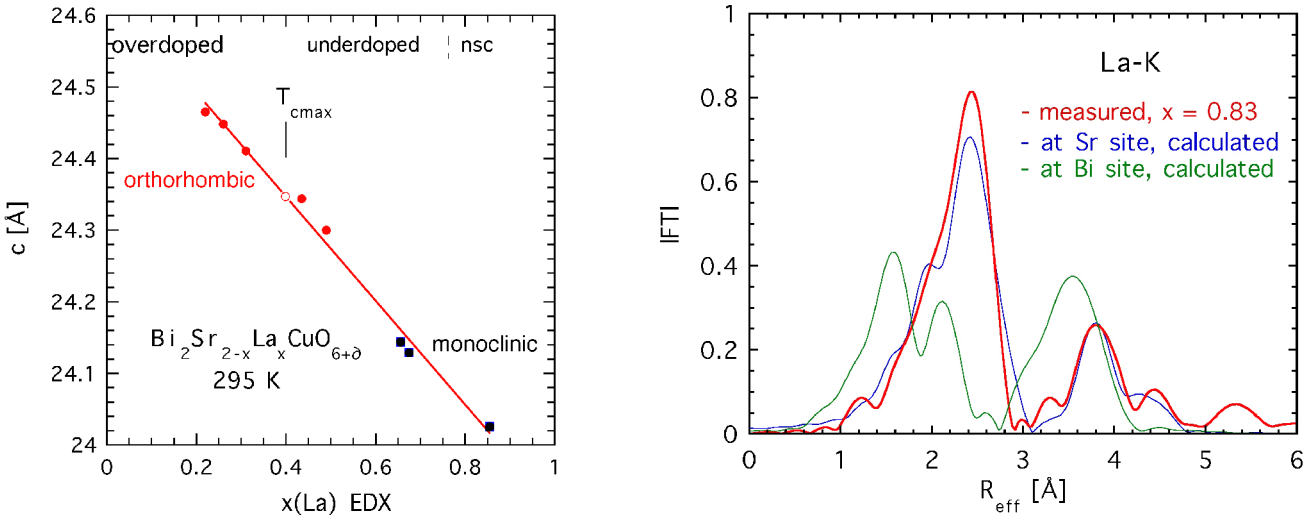

Fig. 1 *Left*: *c*-axis Parameter *vs.* La concentration (determined with EDX) of the crystals under investigation. T_{cmax} = 25 K. Red dots: predominantly orthorhombic supercells (≥ 60%). Black squares: predominantly monoclinic supercells (≥ 60%). Underdoped crystals are stacks of orthorhombic and monoclinic layers alternating along *c*, each ≈ 80 Å thick. Overdoped crystals are phase segregated into optimum doped and other blocks. *Right*: La-*K* Fourier transform spectra: as measured (red), La at the Sr site (blue, FEFF 8.1 calculation), and La at the Bi site (green, FEFF 8.1 calculation).

lanthanum is found substituting Sr, not Bi, see Fig. 2 *left*.. Within the accuray set by our data analysis in real space, see Fig. 1 *right*, we exclude even a partial substitution of Bi by La. This finding indicates that the phase transformation from the monoclinic to the orthorhombic supercell is driven by another mechanism than a site change of the La dopant. Most likely La forms a strongly distorted complex $(La\text{-}O)^+$ including the interstitial oxygens next to the apical oxygen ("site A"), thereby being displaced from the nominal Sr site. The RDF with $(La\text{-}O)^+$ is depicted in Fig. 3 *left*. The static disorder in the *nn* environment of La is strong and overides the thermal disorder even at 300 K. σ^2 (disorder) >> σ^2 (thermal), see Fig. 2 *right*.

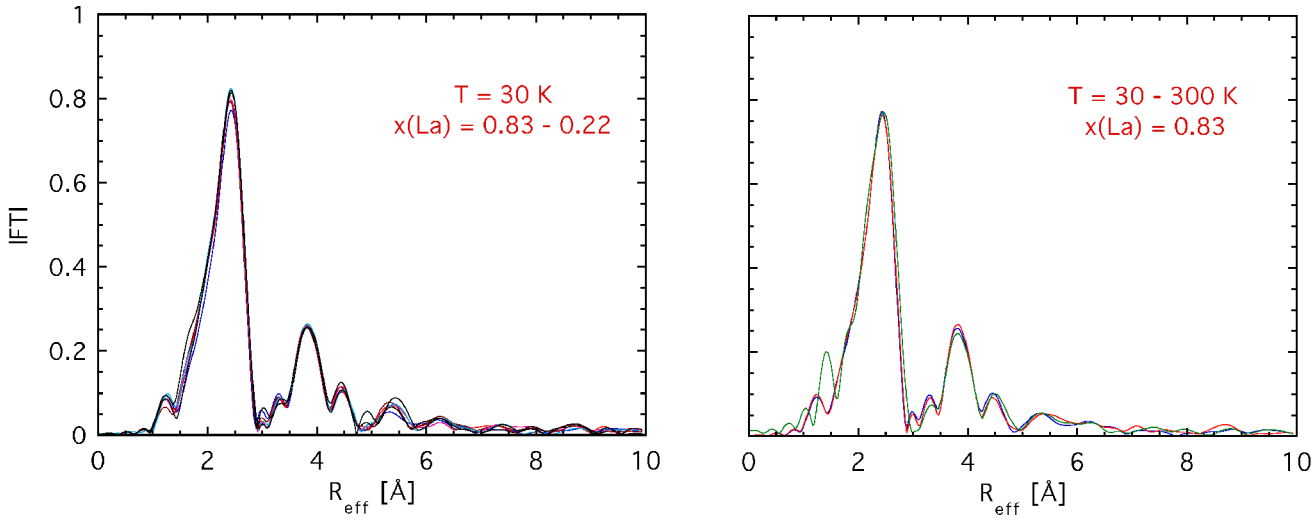

Fig. 2 *Left:* La *K* Fourier transform spectra $|FT(\chi k^2)|$ from $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ at $T = 30$ K with nine different concentrations between x=0.83 and 0.22. *Right:* from the x = 0.83 crystal at different T.

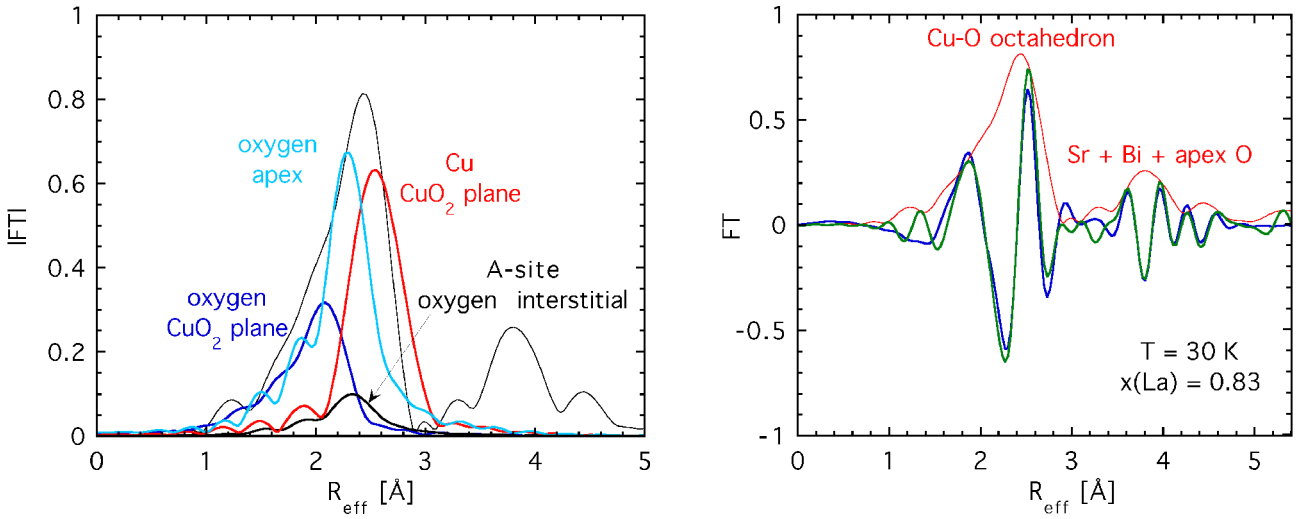

Fig. 3 *Right:* Fit to the Fourier transform spectrum (imaginary part) between R_{eff} = 1.1 and 4.5 Å using the FEFF8.1 code and FEFFIT. Green: measured, blue: fit. *Left:* Deconvolution of the first peak into the shells from the *nn* planar oxygens (blue), the *nn* apical oxygens, the *nn* Cu, including the A-site oxygen interstitial. La is found being displaced by 0.5 Å from its nominal crystallographic position. Notably this local structure at the La site does not change with x(La). The $(La\text{-}O)^+$ complex acts as the effective dopant, not simply La^{3+}.

Literature:

[1] J. Röhler, C. Trabant, J. Frielingsdorf, R. Djemour, V. Martovitsky, L. Dudy, H. Dwelk, A. Krapf, Verhandl. DPG(VI)**43** 1/752 (2008).