

Supplementary information for

## Study of the temperature dependent local atomic displacements in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ superconductor

M.Y. Hacisalihoglu<sup>a,b,c</sup>, E. Paris<sup>a,d</sup>, B. Joseph<sup>a,e</sup>, L. Simonelli<sup>f</sup>, T. J. Sato, T. Mizokawa<sup>g</sup>, and N.L. Saini<sup>h</sup>

<sup>a</sup>Dipartimento di Fisica, Università di Roma "La Sapienza" - P. le Aldo Moro 2, 00185 Roma, Italy.

<sup>b</sup>Department of Physics, Recep Tayyip Erdogan University, 53100 Rize, Turkey.

<sup>c</sup>Department of Physics, Karadeniz Technical University, 61080 Trabzon, Turkey.

<sup>d</sup>Center for Life NanoScience@Sapienza, Istituto Italiano di Tecnologia, V.le Regina Elena 291, 00185 Rome, Italy.

<sup>e</sup>Elettra, Sincrotrone Trieste, Strada Statale 14, Km 163.5, Basovizza, Trieste, Italy.

<sup>f</sup>ALBA Synchrotron Light Facility, Crta. BP 1413, Km. 3.3, 08290 Cerdanyola del Valles, Barcelona, Spain.

<sup>g</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Sendai 980-8577, Japan.

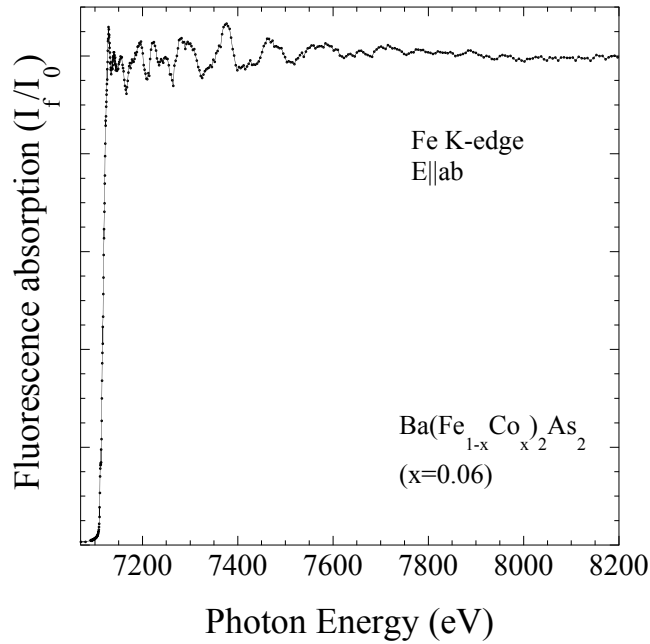
<sup>h</sup>Department of Applied Physics, Waseda University, Tokyo 169-8555, Japan.

1. Fluorescence x-ray absorption  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  ( $x=0.06$ ).

2. Fluorescence EXAFS on single crystal samples: self-absorption correction

## 1. Fluorescence x-ray absorption Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> (x=0.06):

The Fe K-edge fluorescence absorption spectra were obtained by collecting Fe K $\alpha$  fluorescence photons (emission energy 6405 eV) using solid-state fluorescence detector with the resolution of  $\sim 300$  eV at this photon energy. Therefore no contribution from Co K-edge (emission energy and 6930 eV) is seen in the absorption spectrum (Figure S1). Nevertheless, the k-range used in the present analysis is limited to  $14 \text{ \AA}^{-1}$ , and any small contribution due to Co K-edge should not have any appreciable effect on the derived structural parameters.



**Figure S1:** Polarized Fe K-edge x-ray absorption spectrum measured on Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> superconductor (x=0.06) using fluorescence mode. The absorption spectrum was measured by collecting Fe K $\alpha$  fluorescence photons using a multi-element Ge-detector.

## 2. Fluorescence EXAFS on single crystal samples: self-absorption correction

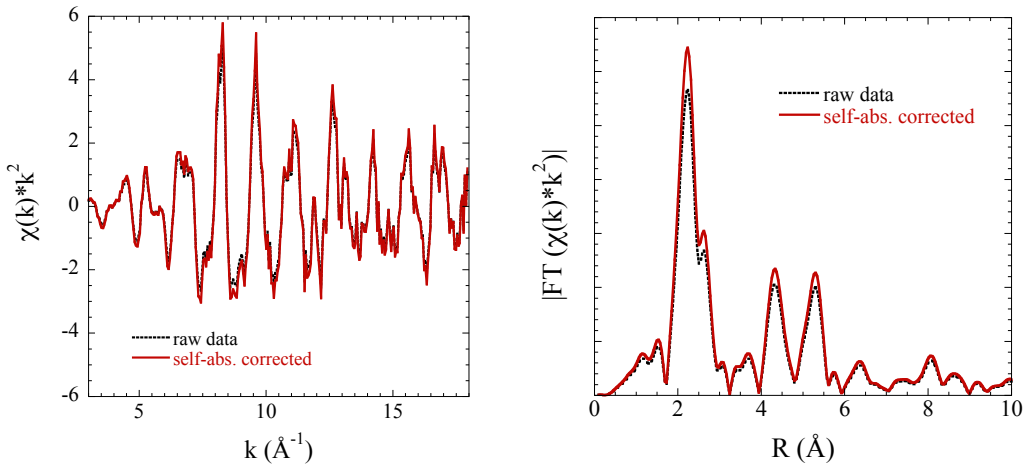
The EXAFS of concentrated samples, as the case of the title system, measured in the fluorescence mode strongly depend on the detection geometry through the self-absorption effect. On the other hand, fluorescence mode is also one of the most suitable modes to study x-ray absorption of single crystal samples, especially for which desired thickness for transmission absorption is highly non-trivial, as the case of the Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub>

system. It is possible to calculate the absorption (and hence the correction due to the fluorescence mean free path) knowing the experimental geometry, a very common procedure in the field. Tröger et al [Tröger et al, Phys. Rev. B 46, 3283 (1992)] have described a simple procedure to deal with the self-absorption effect. Here, the self-absorption term  $S(E)$  is defined as:

$$S(E) = \frac{\mu_{Fe}(E)}{\mu_{tot}(E) + \mu_{tot}(E_F)g} ; \text{ here } \mu_{Fe}(E) \text{ is energy dependent absorption due to}$$

absorber (Fe),  $\mu_{tot}(E)$  is total absorption,  $\mu_{tot}(E_F)$  is total absorption at fluorescence

emission energy and  $g$  is the geometrical factor defined as  $g = \frac{\sin \phi}{\sin \theta}$  with  $\phi$  and  $\theta$  being angles of incidence and detection with respect to the sample surface (about  $80 \pm 5$  and  $10 \pm 5$  degree respectively in the present experiments). Incidentally the self-absorption correction in the used geometry is not that big as can be judged from the EXAFS spectra shown as a ready reference (Figure S2). It is worth mentioning that, since the self-absorption for a specific sample measured in a specific geometry depends solely on the geometry, it may affect the absolute value of the DW factor, however, should not have any impact on the main conclusion that is based on a variation across the superconducting transition.



**Figure S2:** (left) Fluorescence self-absorption corrected Fe K-edge EXAFS on  $Ba(Fe_{1-x}Co_x)_2As_2$  ( $x=0.06$ ) at 20 K is plotted with the raw data. The Fourier transforms of the corrected and uncorrected EXAFS are shown revealing the effect of fluorescence self-absorption.