Supporting Information:

Chemical bonding effects in Sc compounds studied by the X-ray absorption and X-ray photoelectron spectroscopies.

Anna Zimina*

Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany and Institute for Chemical Technology and Polymer Chemistry,

Karlsruhe Institute of Technology, Engesserstrasse 18-20, 76128 Karlsruhe, Germany

Aline Léon

European Institute for Energy Research, Emmy Noether Strasse 11, 76131 Karlsruhe, Germany

Ralph Steininger

Institute for Photon Science, Karlsruhe Institute of Technology,

Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

(Dated: July 7, 2023)

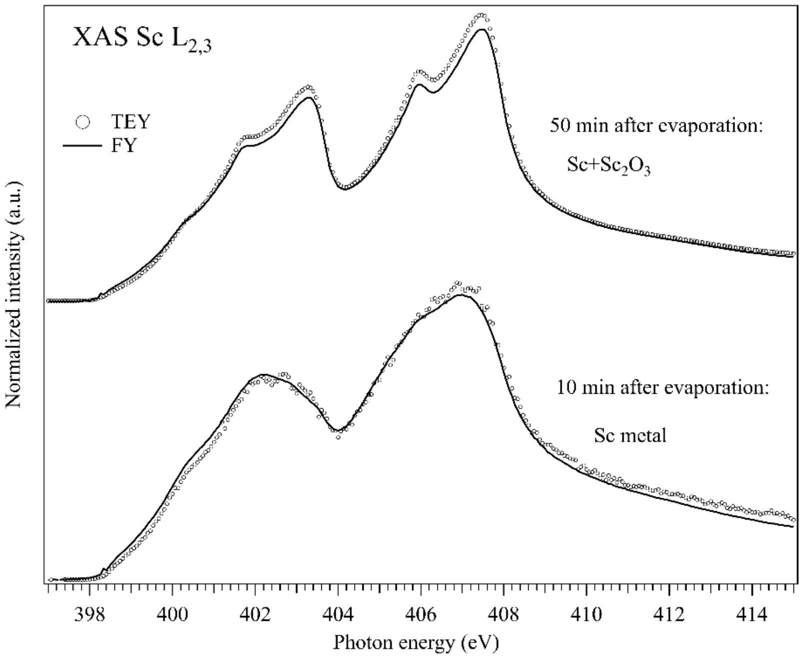

Fig. S1. TEY-XAS (circles) and FY-XAS (solid line) Sc $L_{2,3}$ spectra of the fresh prepared layer of Sc metal on Cu substrate (after 10 min, the transfer from the preparation chamber in vacuum) and after 50 min under the photon radiation in 10^{-8} mbar. For the metallic scandium the electron correlation effects are less traceable by Sc K XAS, compared to the ionic compounds with empty d states discussed later and the changes in spectrum of metallic scandium due to light oxidation is less drastic compare to effects observed for Sc K XAS on $ScBr_3$, for instance.

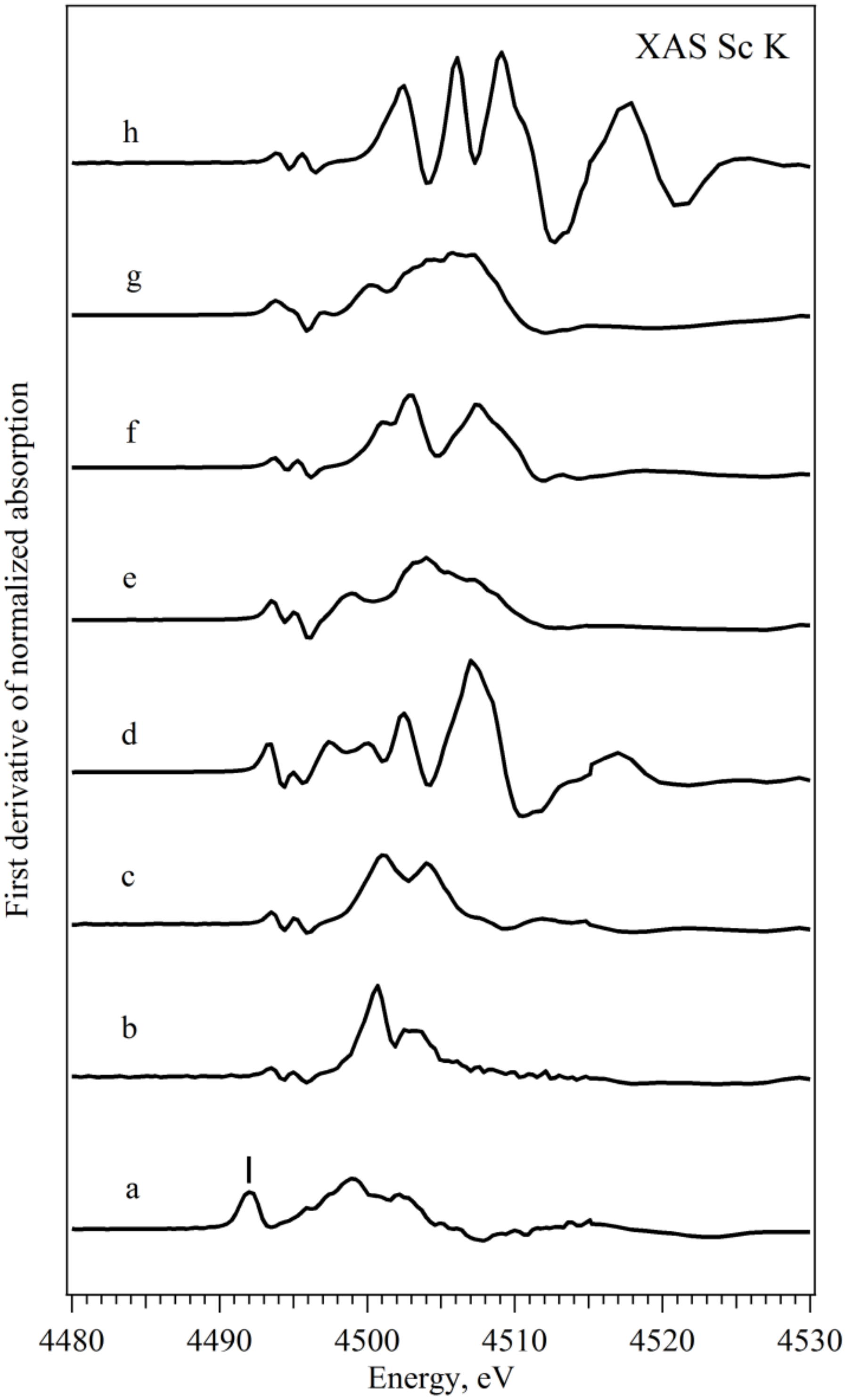

Fig. S2. First derivative of normalized XAS Sc K spectra of different Sc compounds: (a) Sc metal, (b) $ScBr_3$, (c) $ScCl_3$, (d) Sc_2O_3, (e) $Sc_2(CO_3)_3$, (f) $Sc_2(SO4)_3$, (g) $Sc(NO_3)_3$, (h) ScF_3. The vertical line marks the position of the absorption edge of the Sc metal.

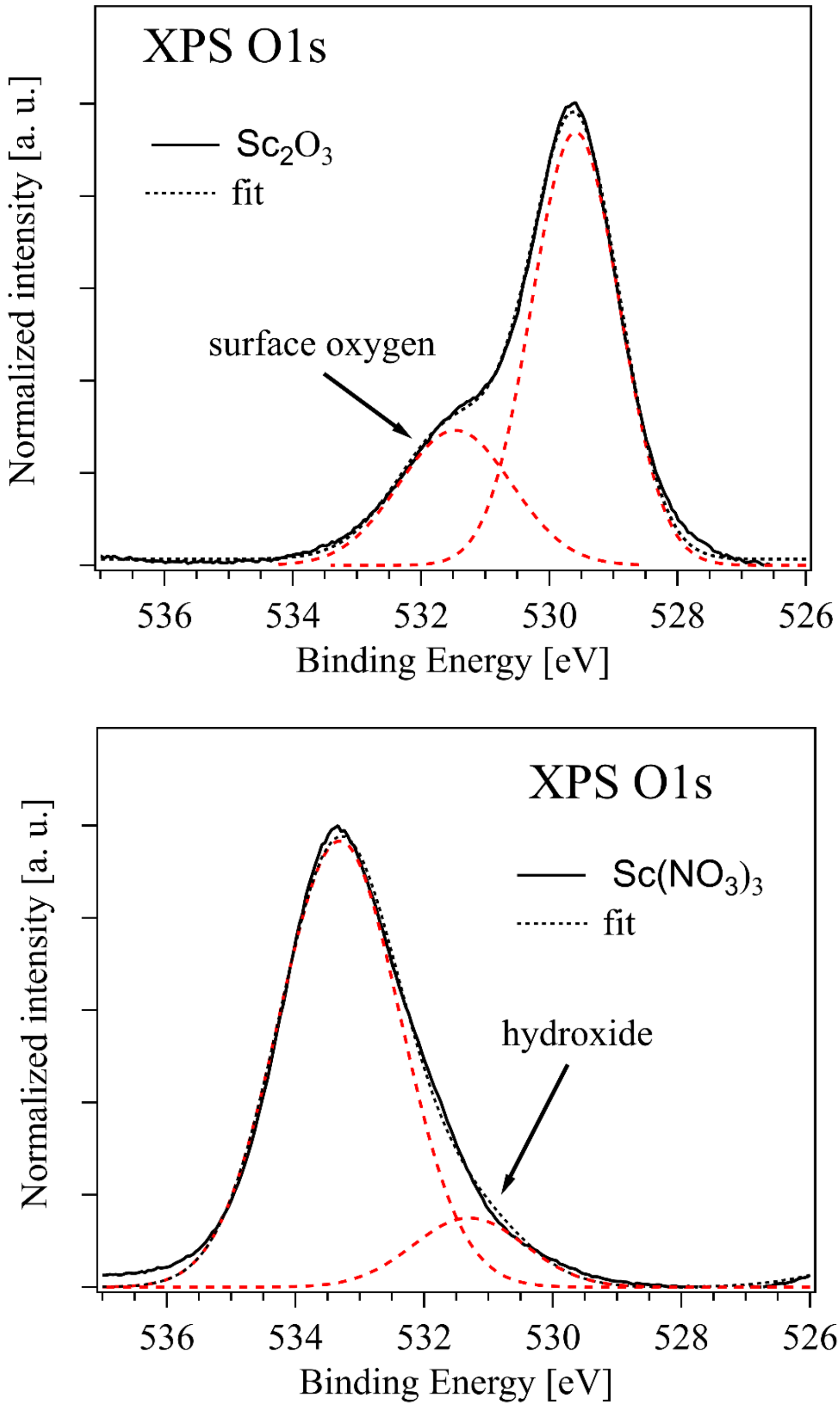

Fig. S3. Results of the peak decomposition analysis of the O 1s XPS data on Sc_2O_3 and $Sc(NO_3)_3$.

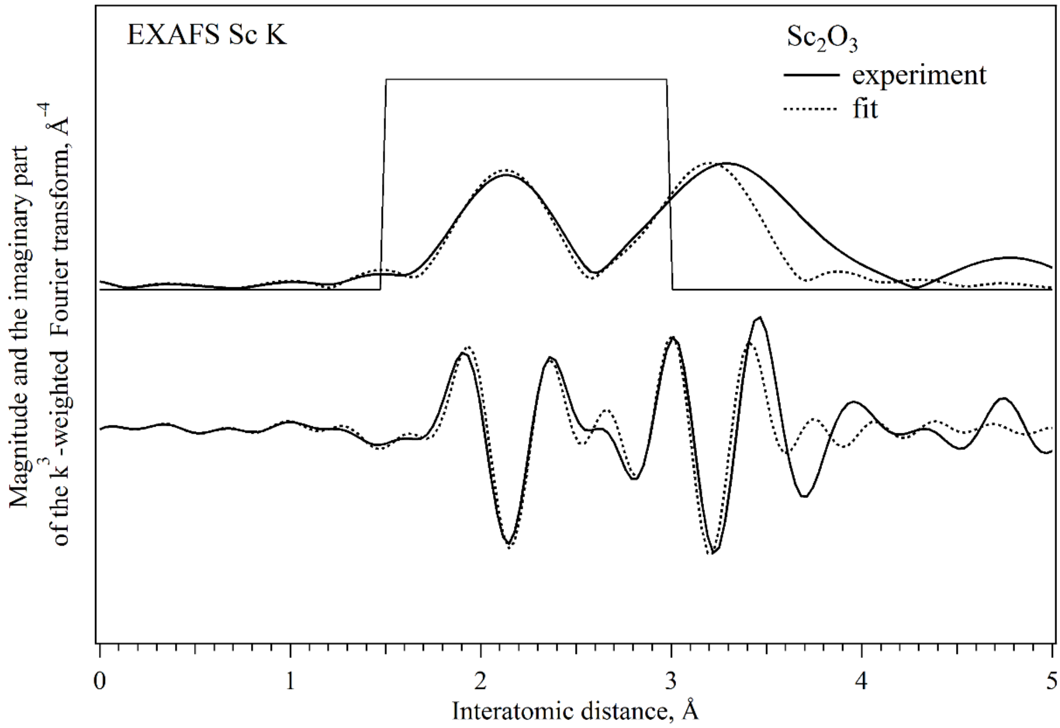

Fig. S4: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of Sc_2O_3, the fitting range is marked by thin solid line.

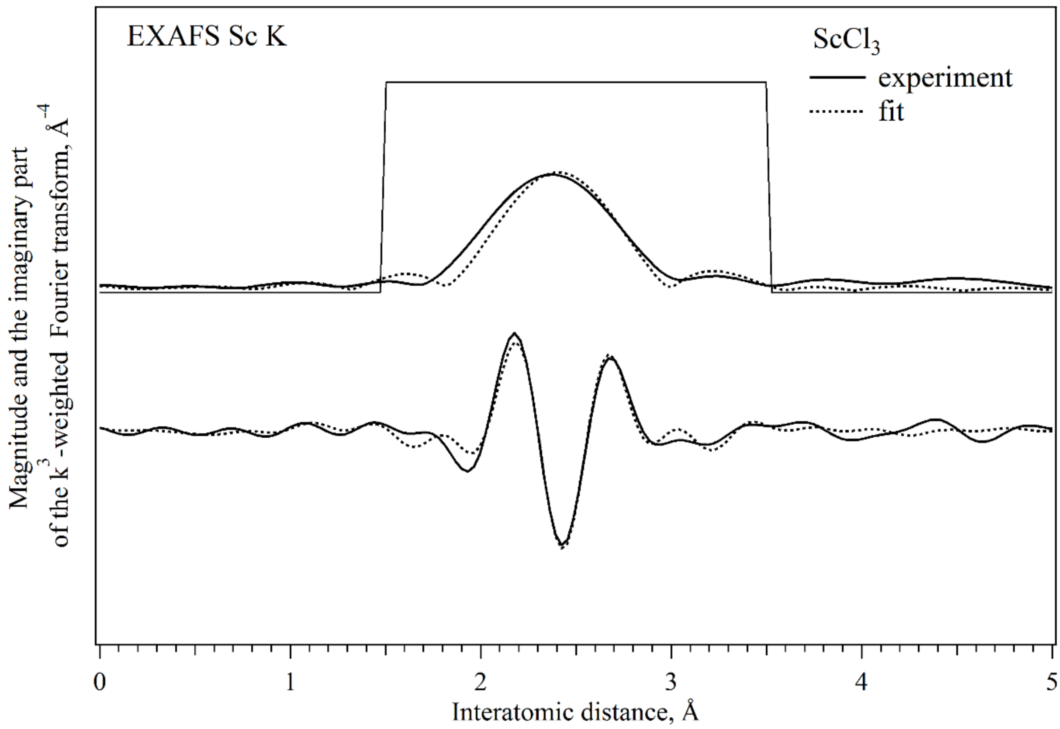

Fig. S5: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of $ScCl_3$, the fitting range is marked by thin solid line.

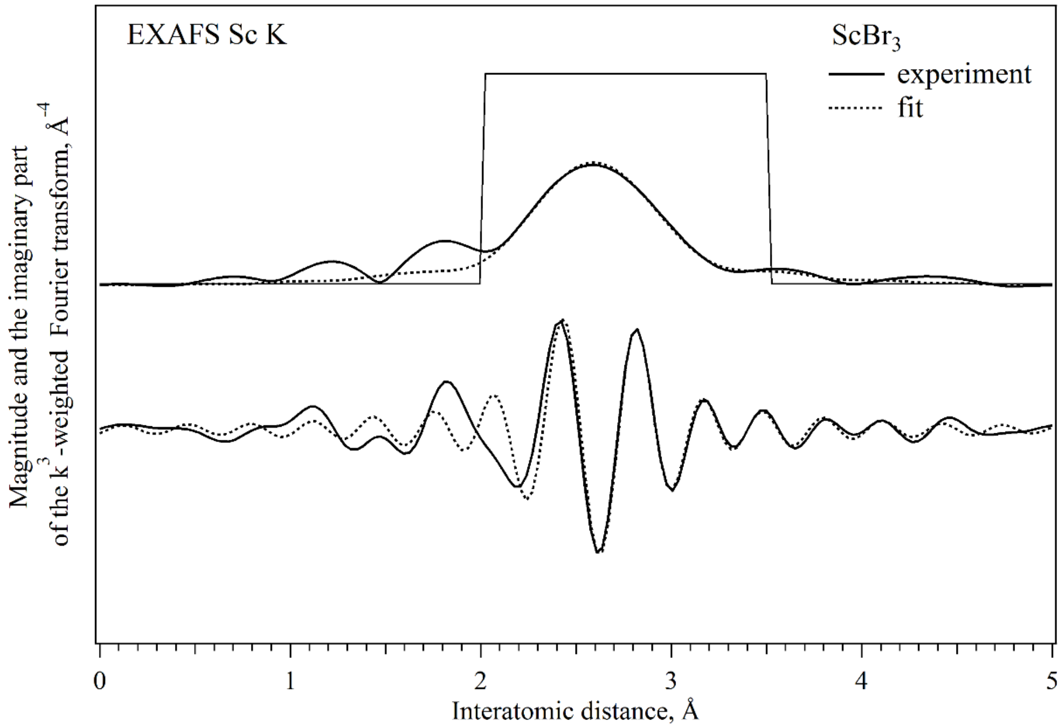

Fig. S6: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of $ScBr_3$, the fitting range is marked by thin solid line.

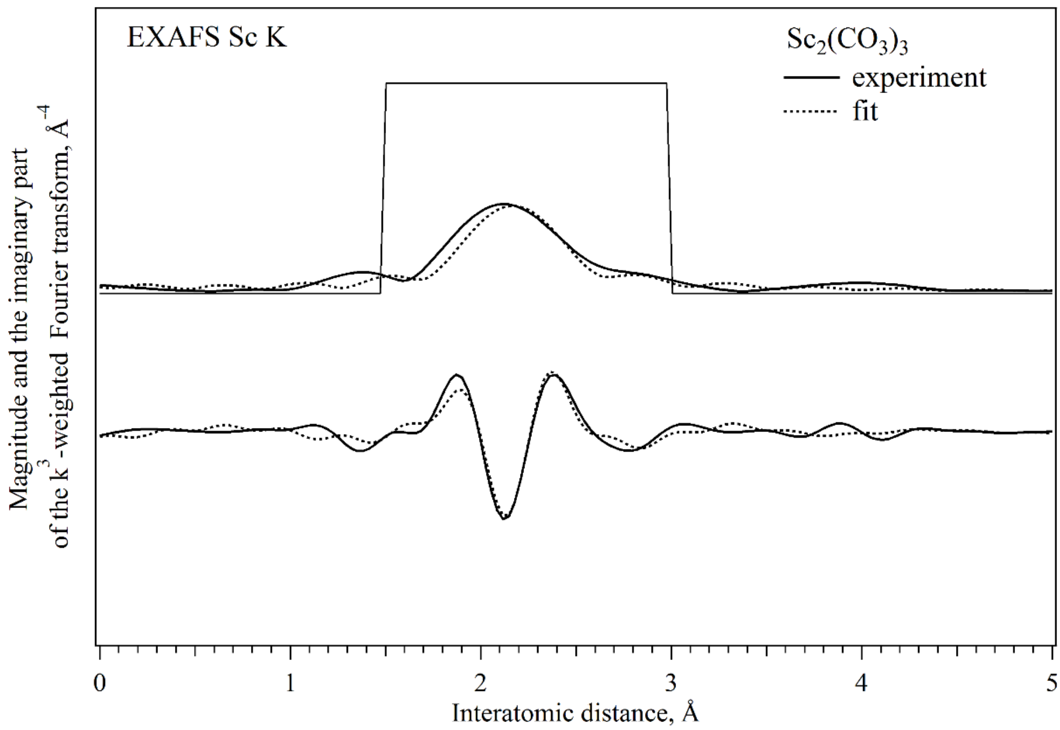

Fig. S7: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of $Sc_2(CO_3)_3$, the fitting range is marked by thin solid line.

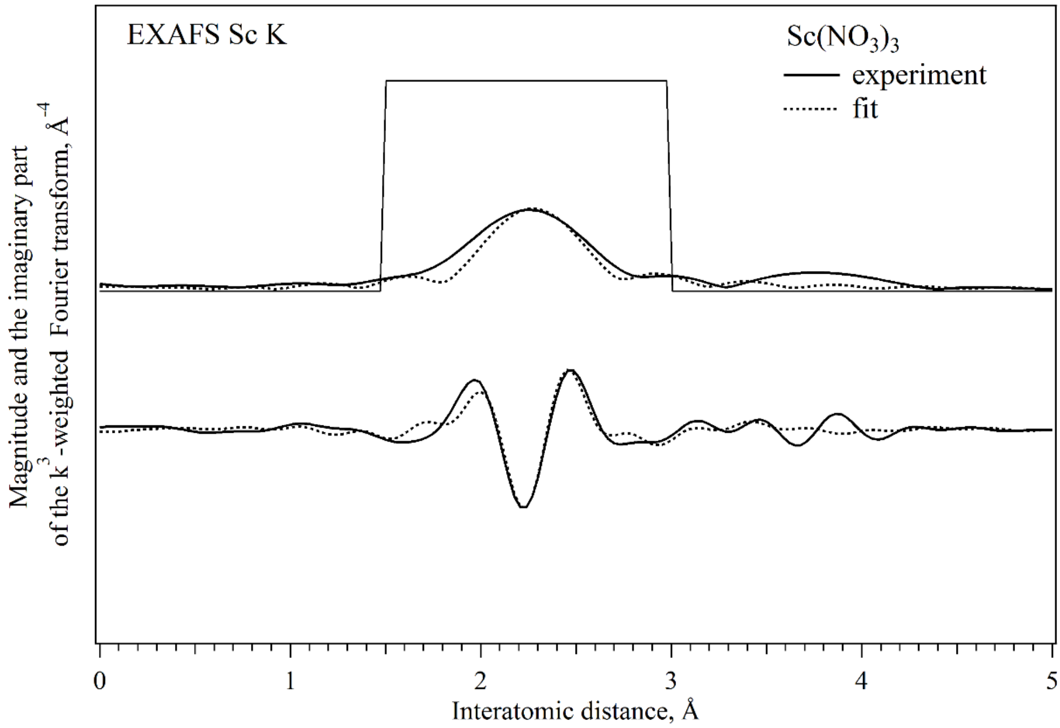

Fig. S8: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of $Sc(NO_3)_3$, the fitting range is marked by thin solid line.

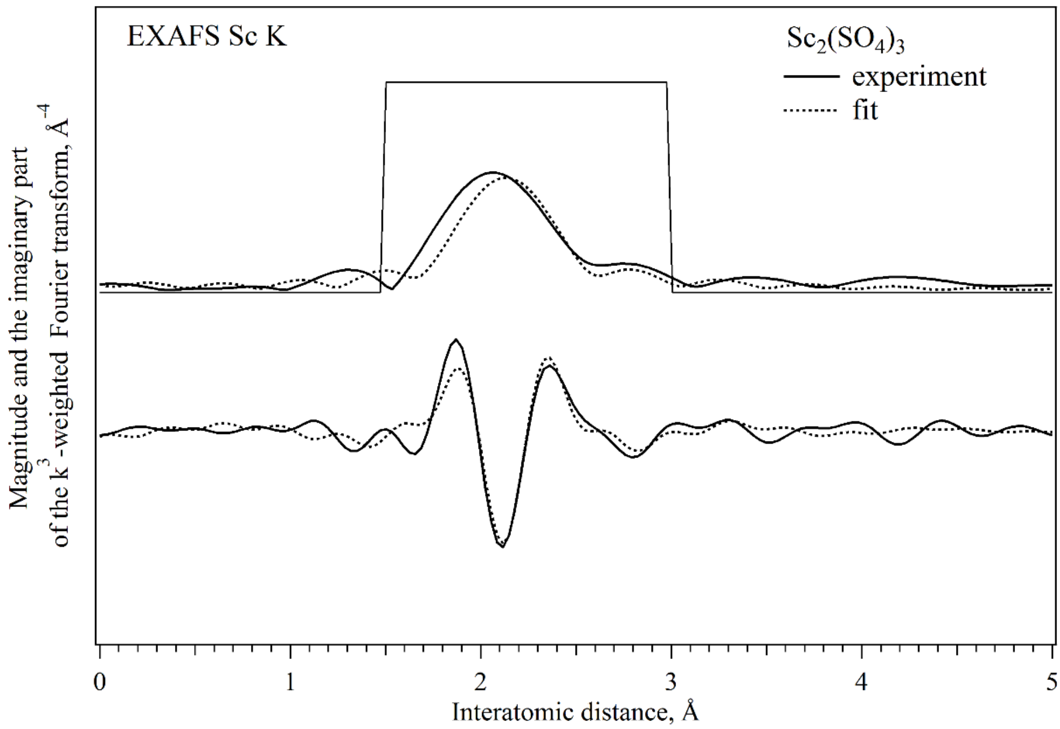

Fig. S9: Experimental (solid line) and fitted (dotted line) magnitude and the imaginary part of the FT of $Sc_2(SO_4)_3$, the fitting range is marked by thin solid line.