



**The Abdus Salam
International Centre for Theoretical Physics**



2332-19

**School on Synchrotron and FEL Based Methods and their Multi-Disciplinary
Applications**

19 - 30 March 2012

XAS data analysis

G. Aquilanti
Sincrotrone Trieste

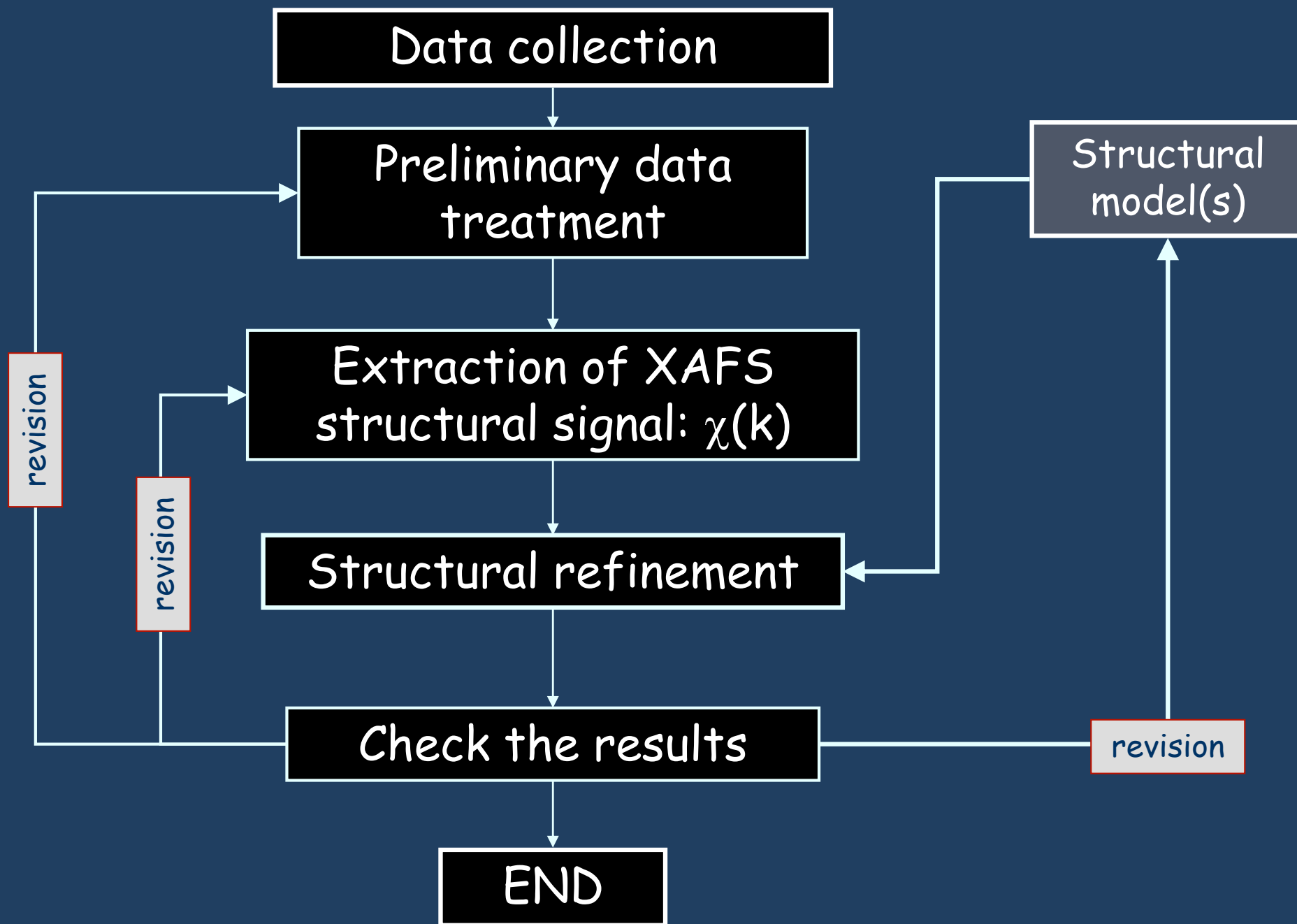
Introduction to the EXAFS data analysis

Giuliana Aquilanti
Elettra Laboratory

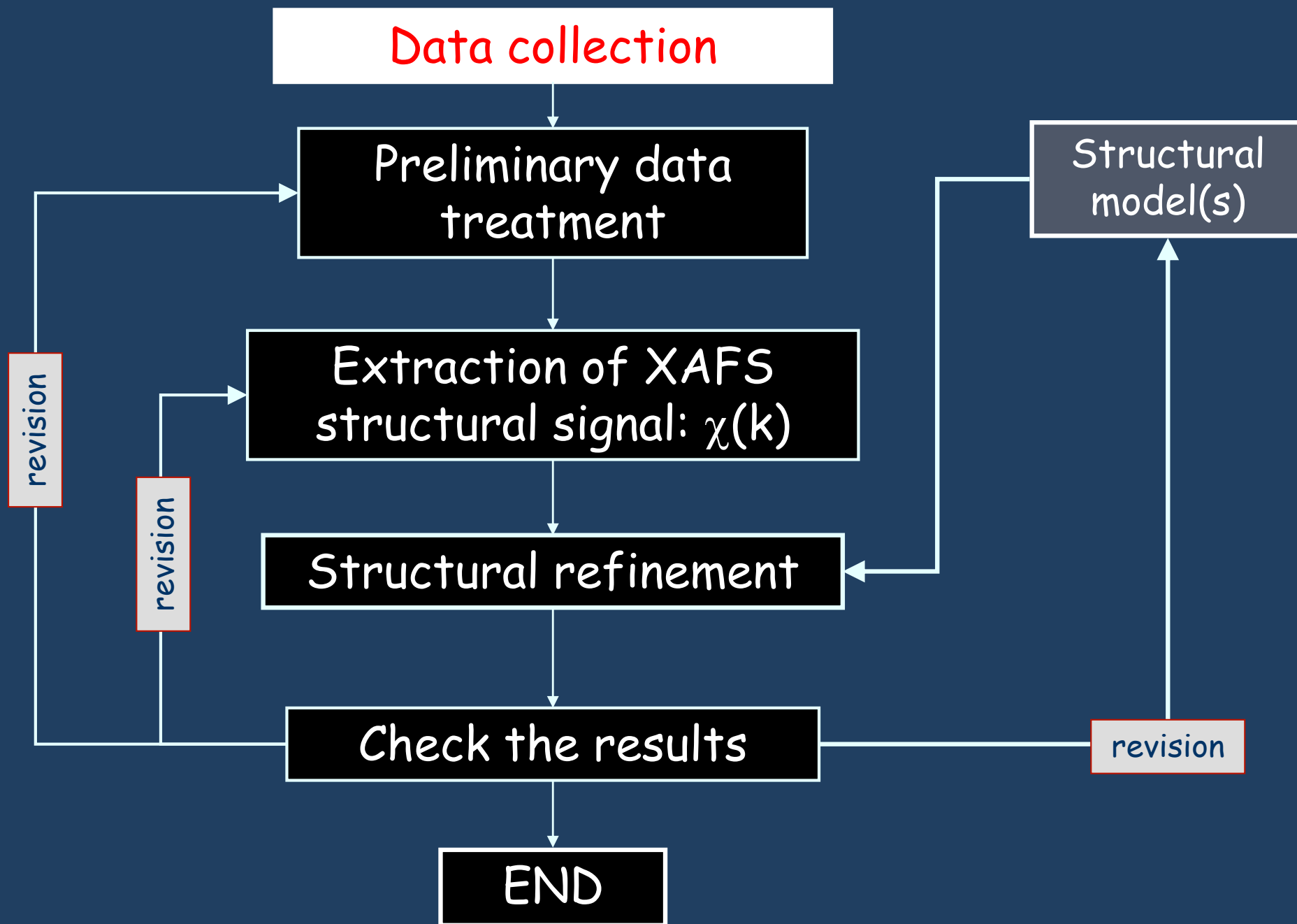


Material almost integrally taken from Carlo Meneghini: EXAFS tutorial at Synchrotron Radiation school of Duino 2011

XAFS study: from experiment to results



XAFS study: from experiment to results

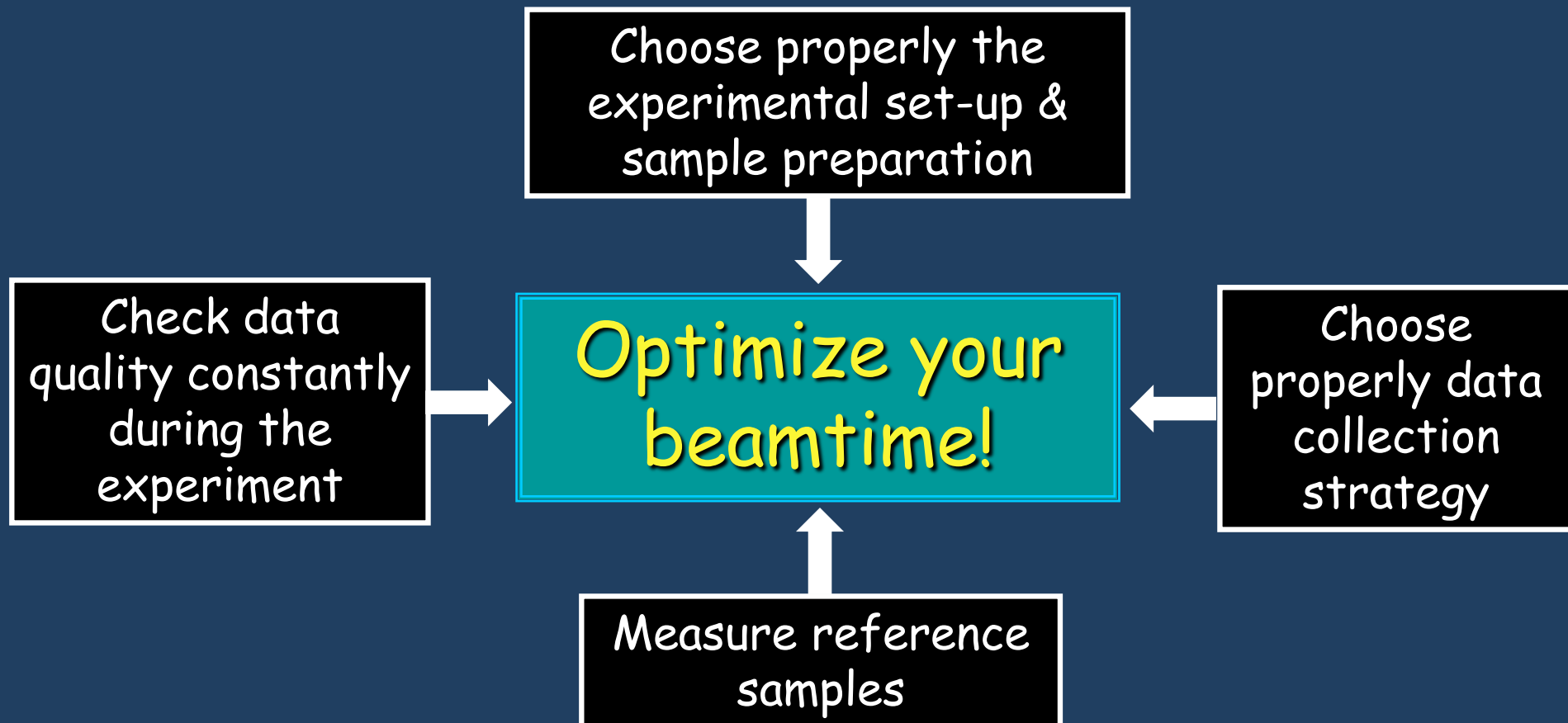


Data collection

Considerations:

- 1) Proposal submission + proposal evaluation + beamtime scheduling = 6 to 12 months
- 2) Difficult to have new beamtime in case of proposal failure

- Check the proposal submission deadlines
- discuss your experiment with local contacts



Data collection

Choose properly the experimental set-up & sample preparation

- For massive concentrated samples: **TRANSMISSION**

Jump $0.5 \leq \Delta\mu t \leq 1.5$

Total absorption $\mu t \leq 2.$



inhomogeneities, holes, not parallel surfaces, etc...

- For thin concentrated or thin diluted samples: **FLUORESCENCE**

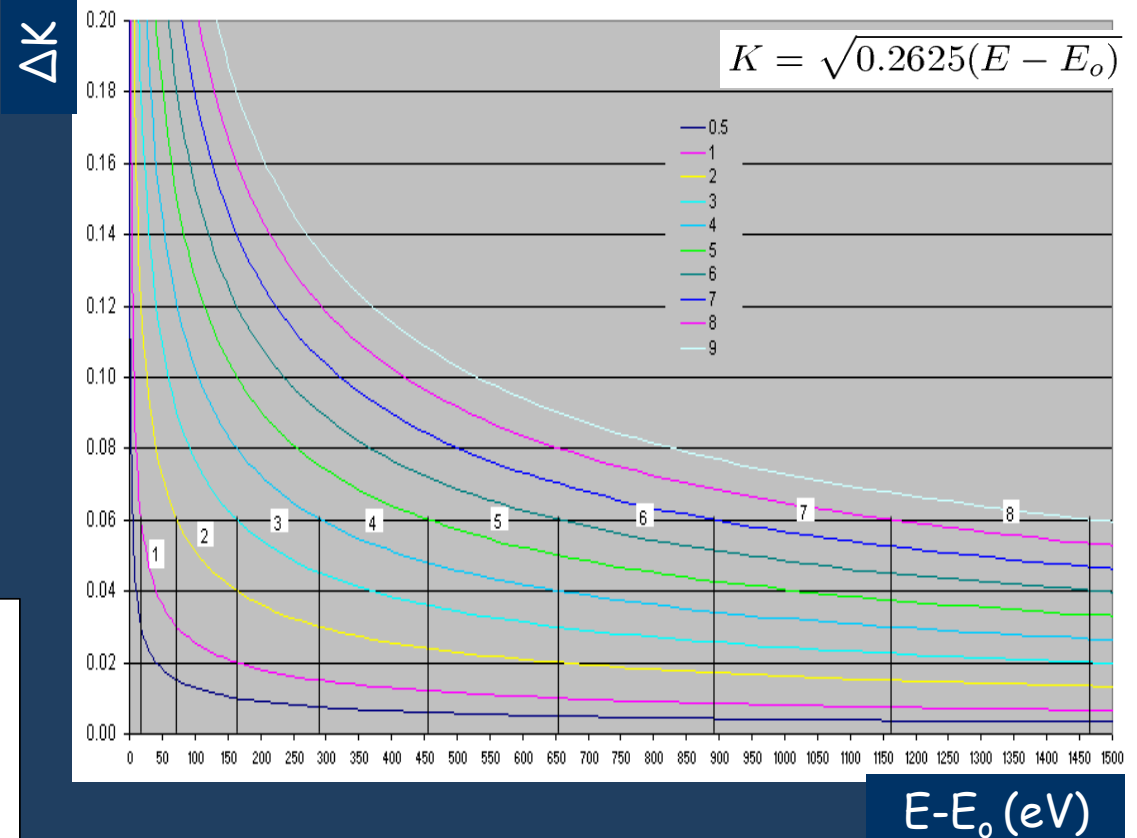
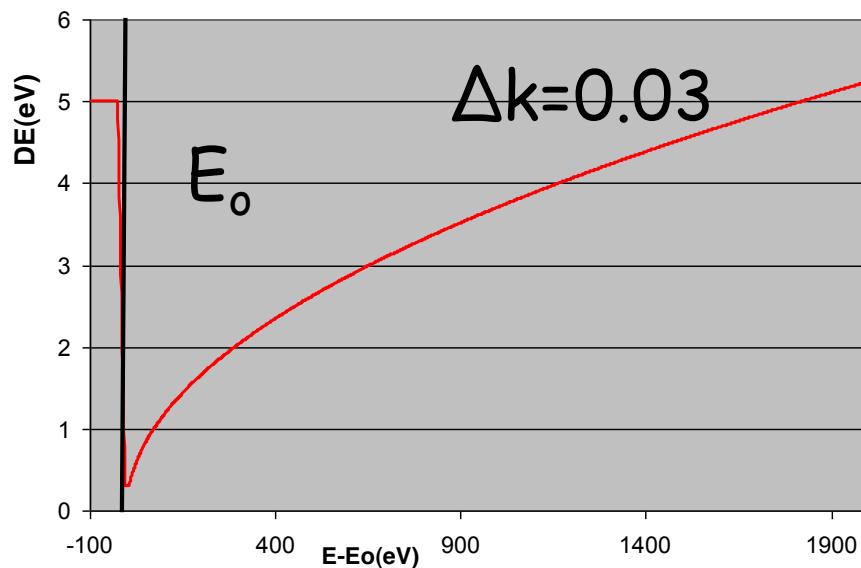


Self absorption, detector linearity, Bragg reflections

Data collection

Choose properly the data collection strategy

- Acquisition time per point
- Single scan or repeated scans
- ΔE or Δk step

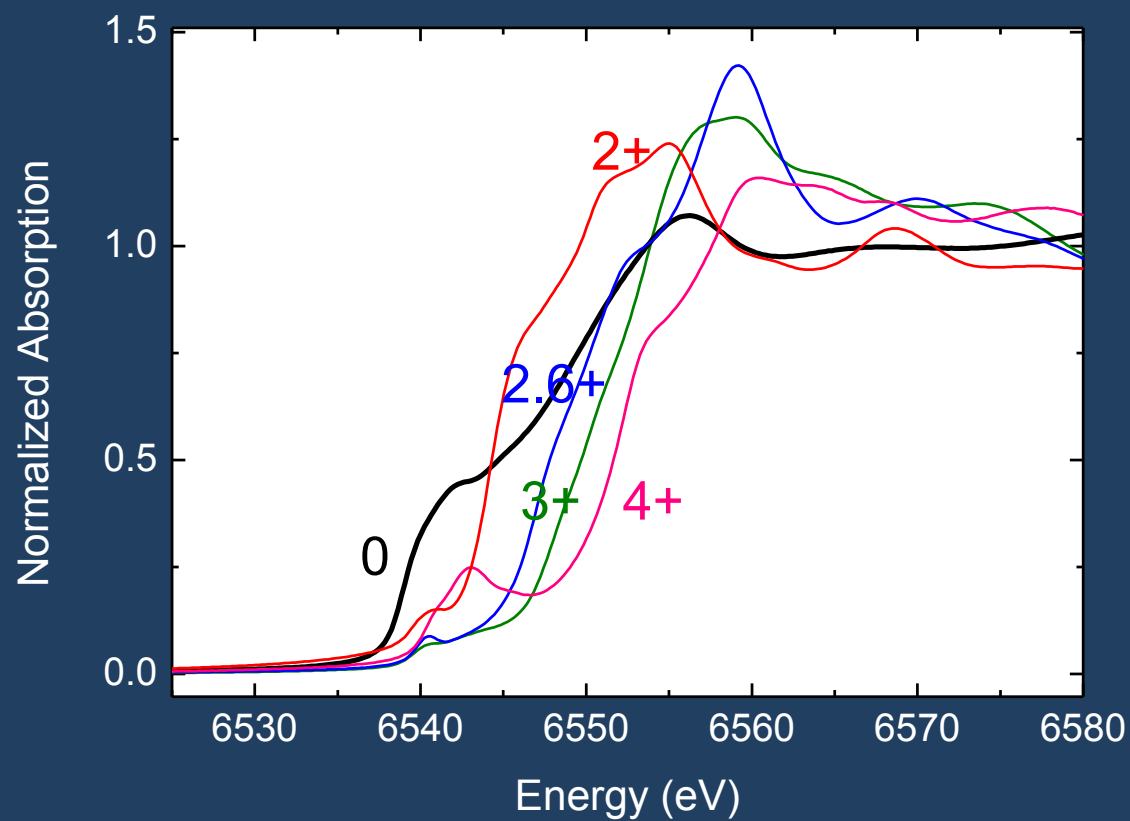
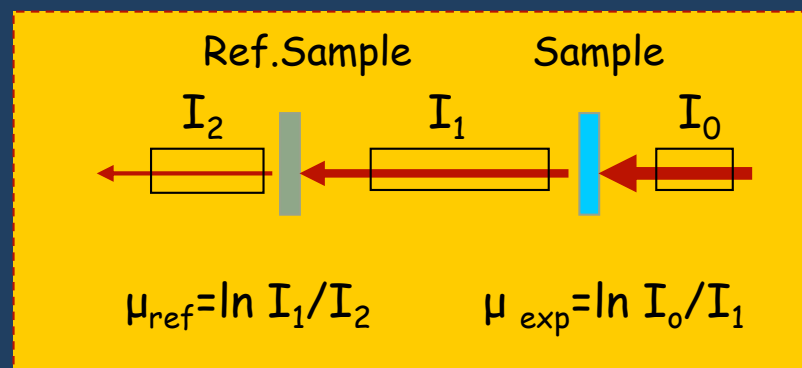


Constant Δk acquisition

- Optimizes the number of collected points
- More efficient
- Faster

Data collection

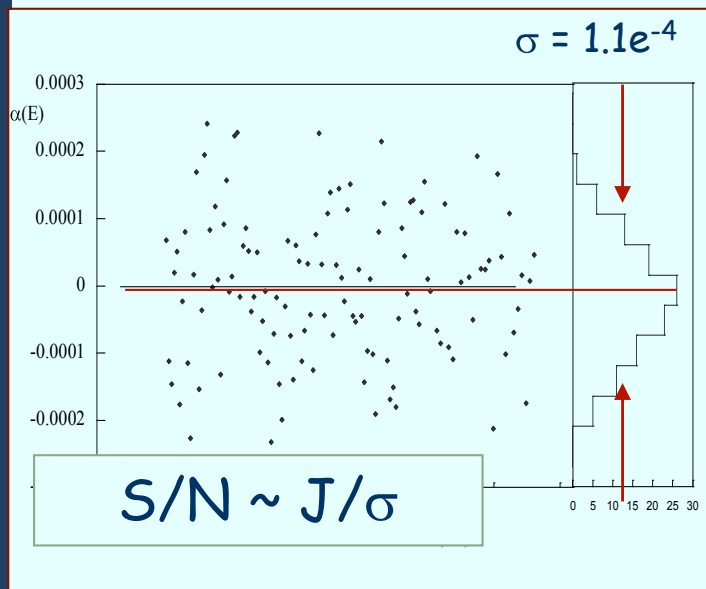
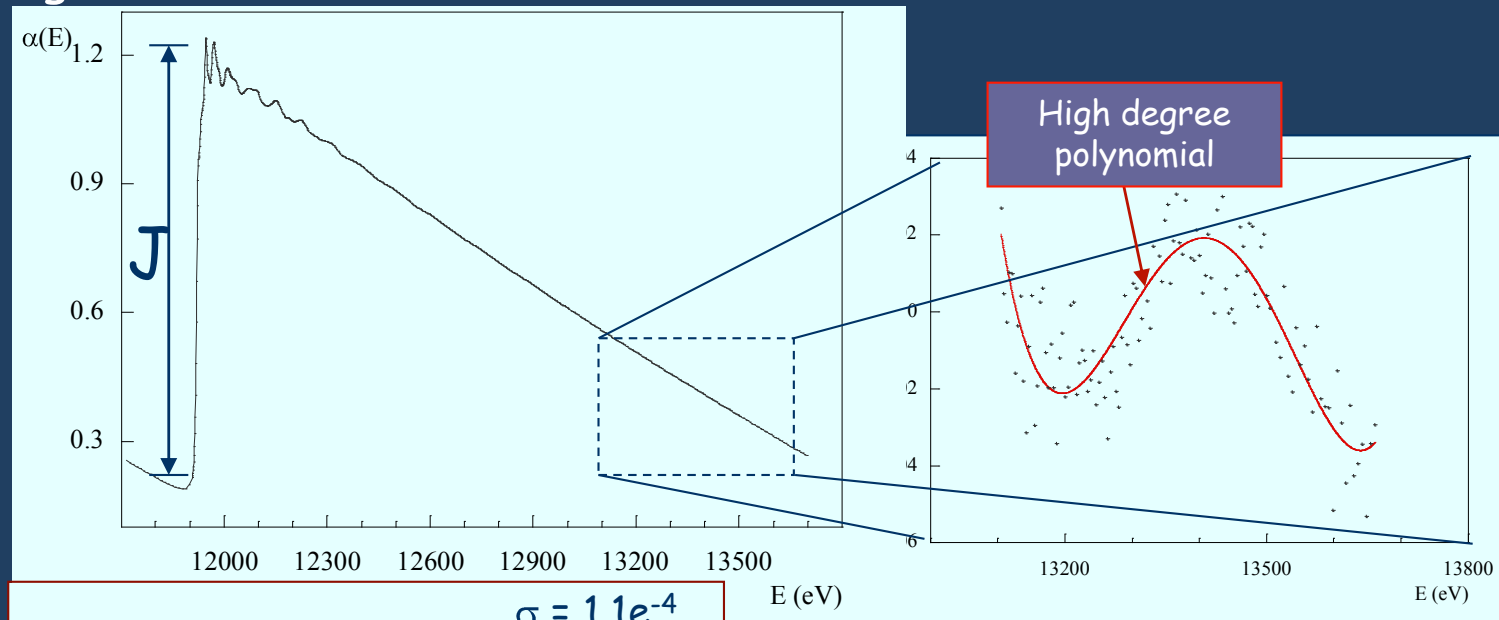
Measure reference samples



Data collection

Check data quality constantly during the experiment

- Evaluate signal/noise ratio



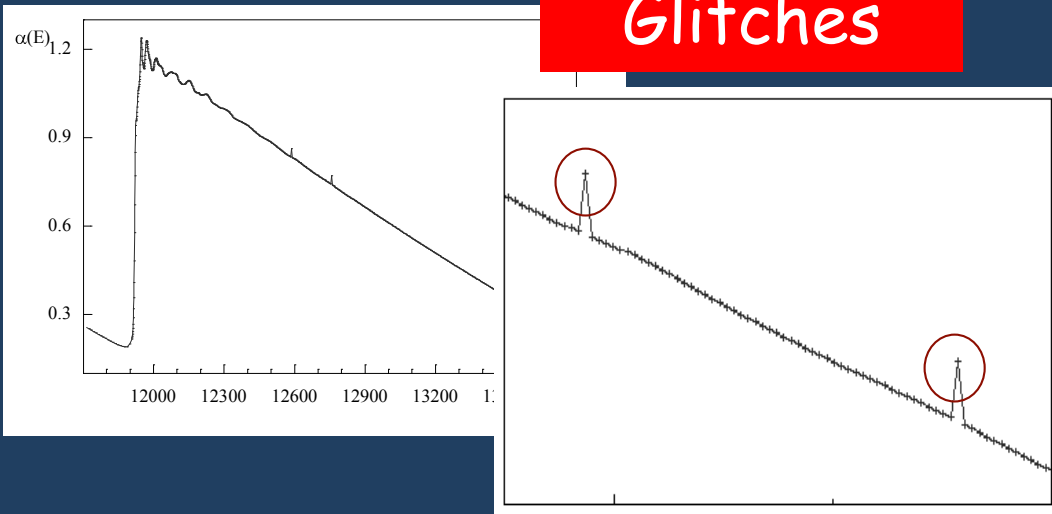
S/N ratio should be less than 10^{-3}

Data collection

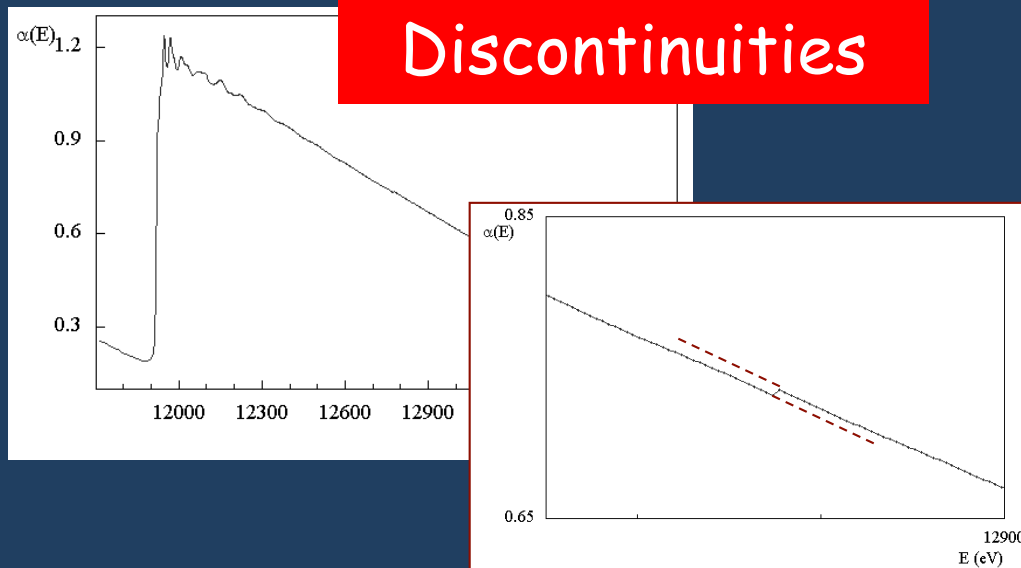
Check data quality constantly during the experiment

- Check for:

Glitches



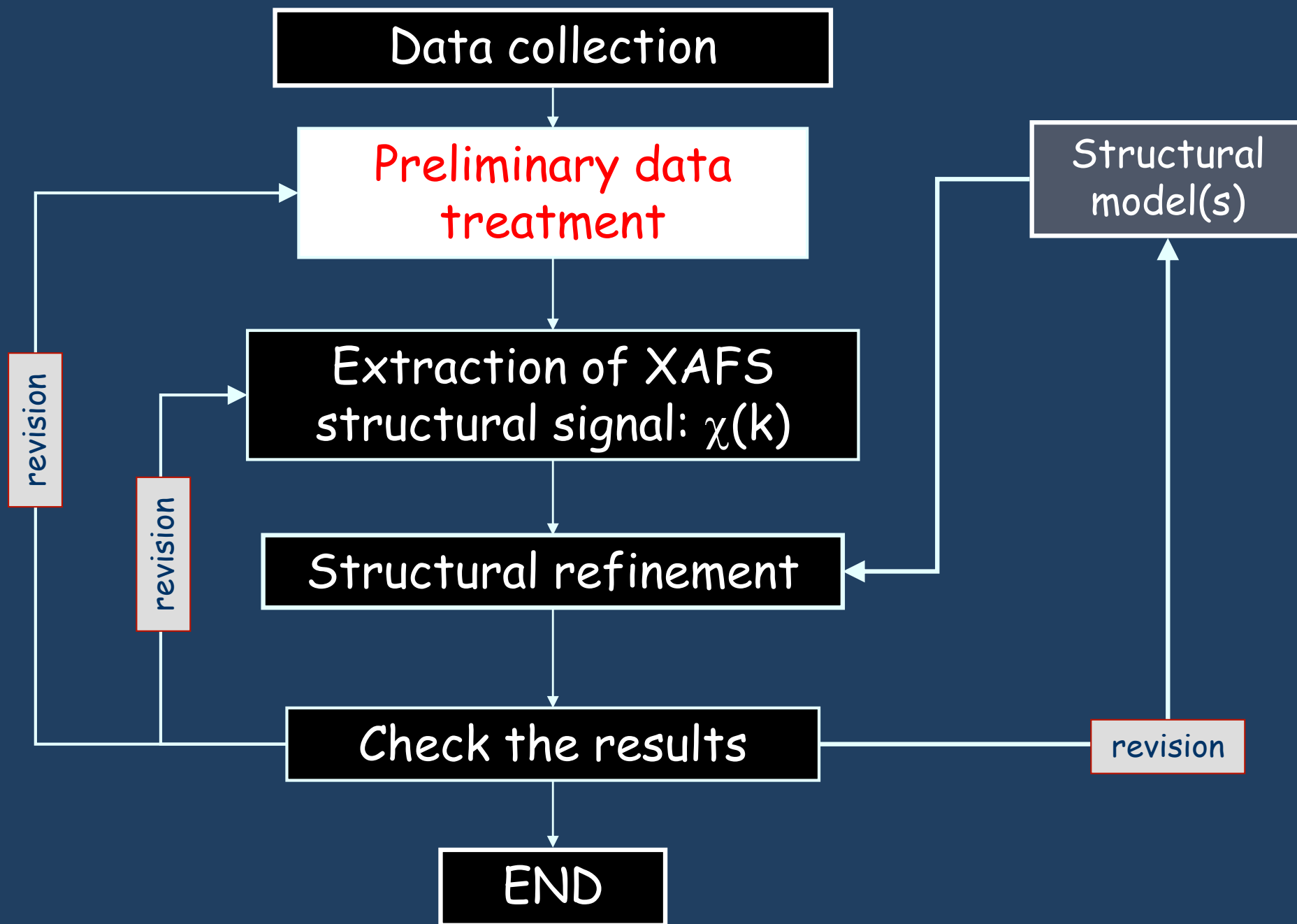
Discontinuities



edge shift

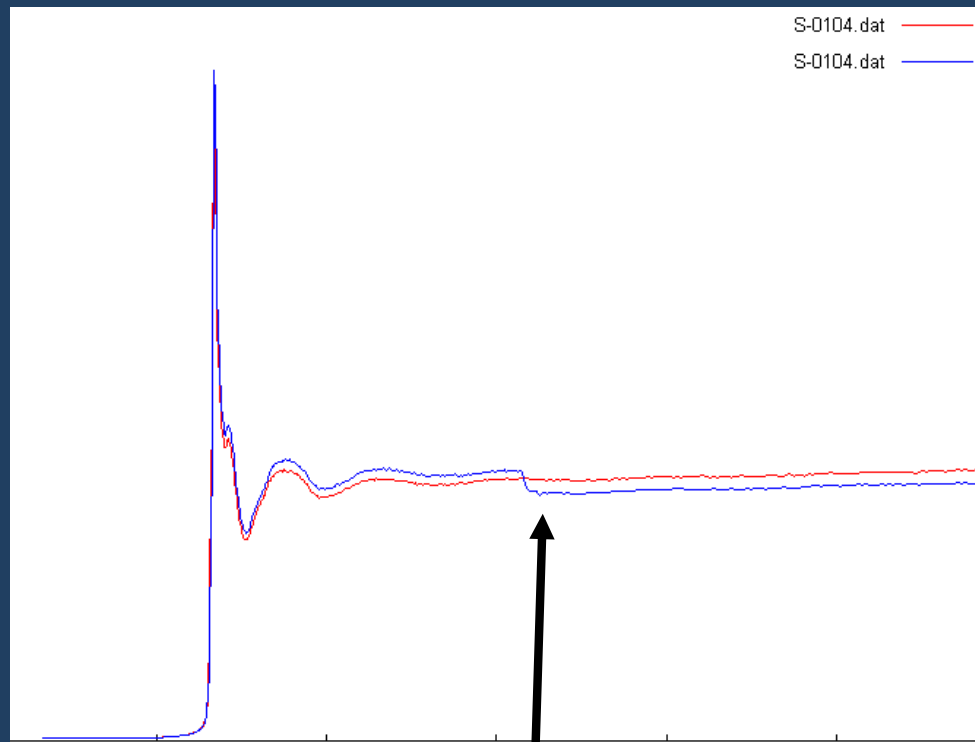


XAFS analysis: from experiment to results

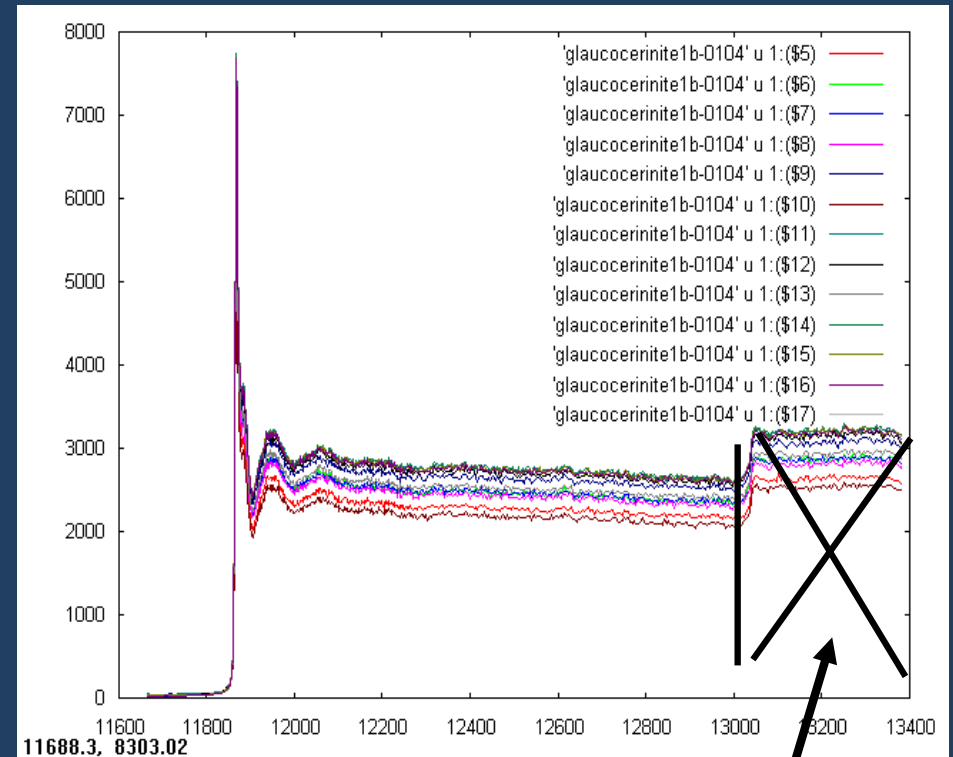


Preliminary data treatment

Choose the best spectra and useful data regions



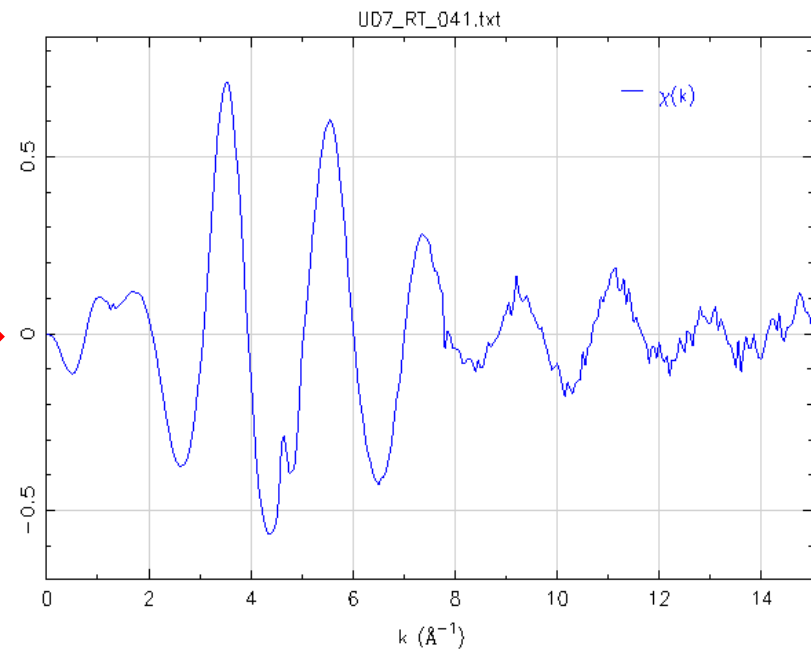
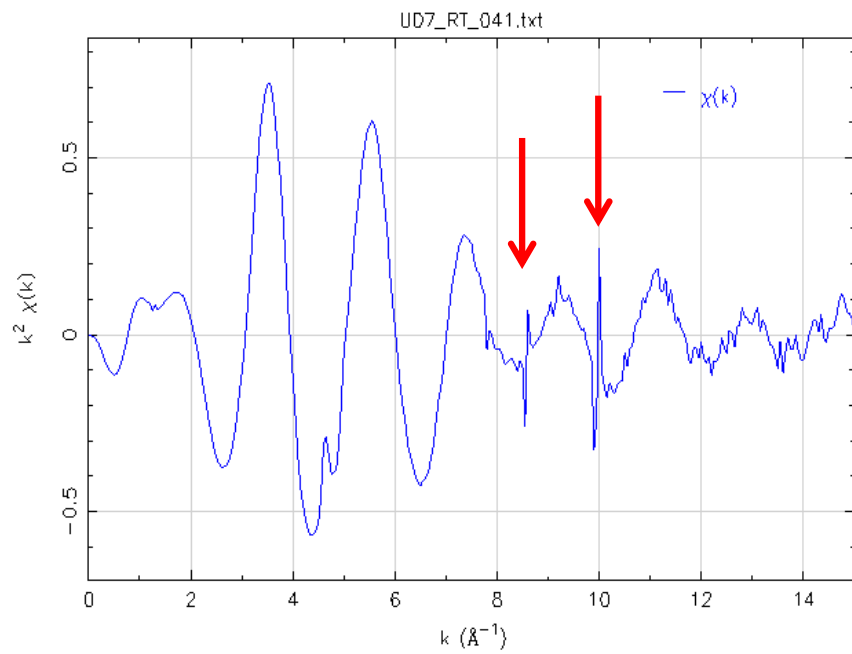
do not use the blue one!



do not use data beyond 13000 eV !

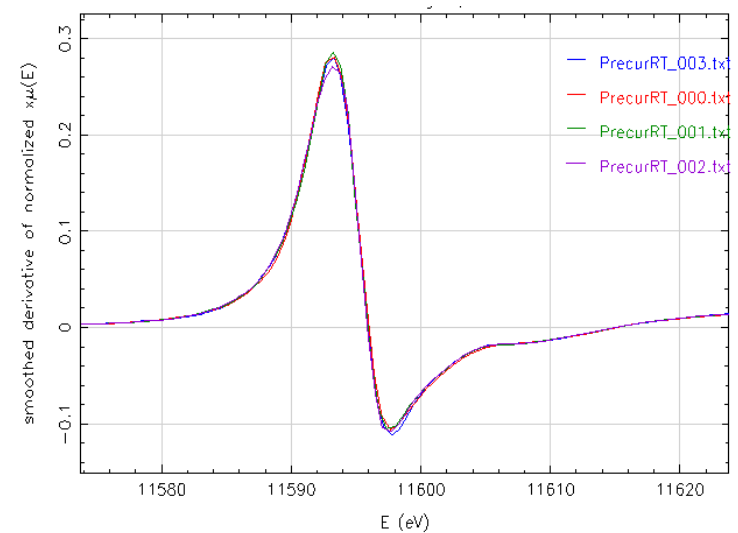
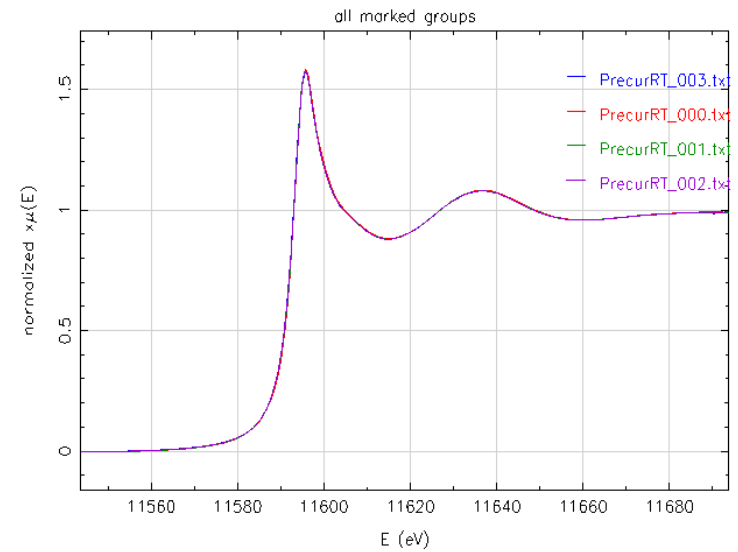
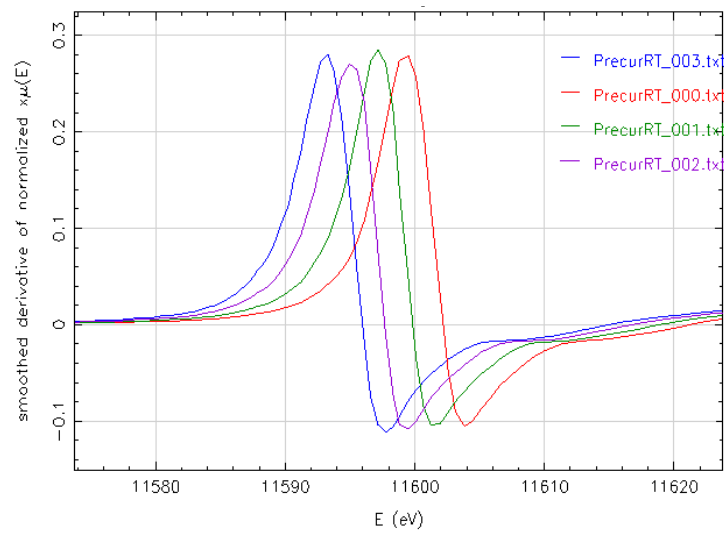
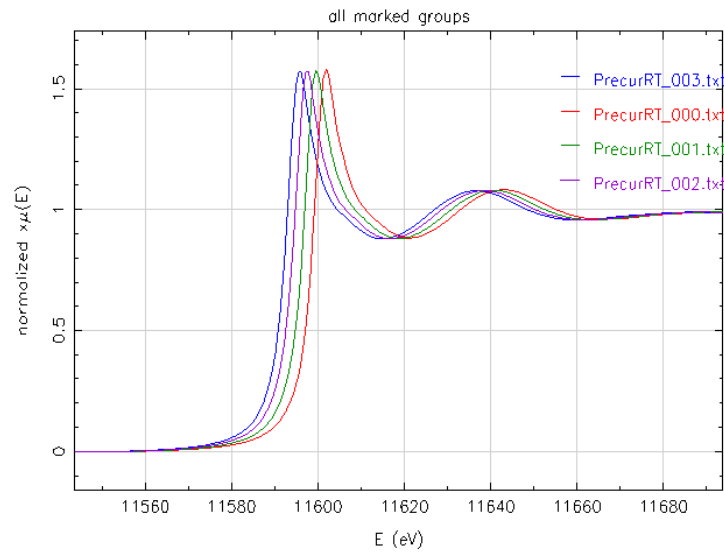
Preliminary data treatment

De-glitch



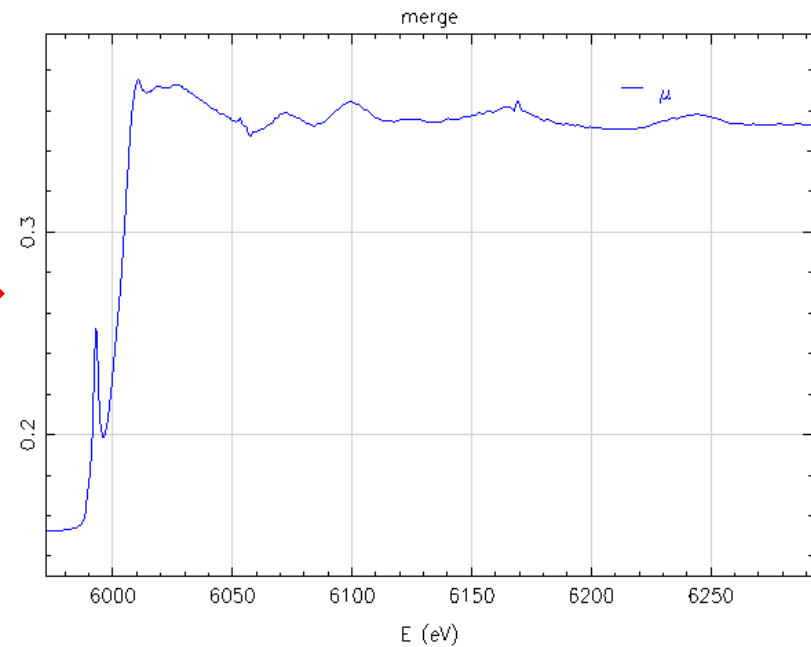
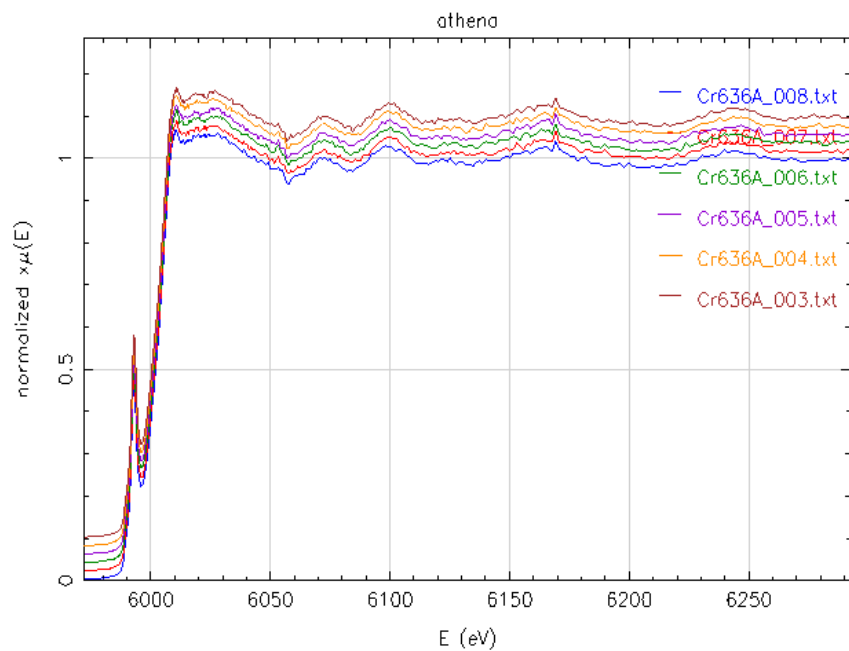
Preliminary data treatment

Align



Preliminary data treatment

Average



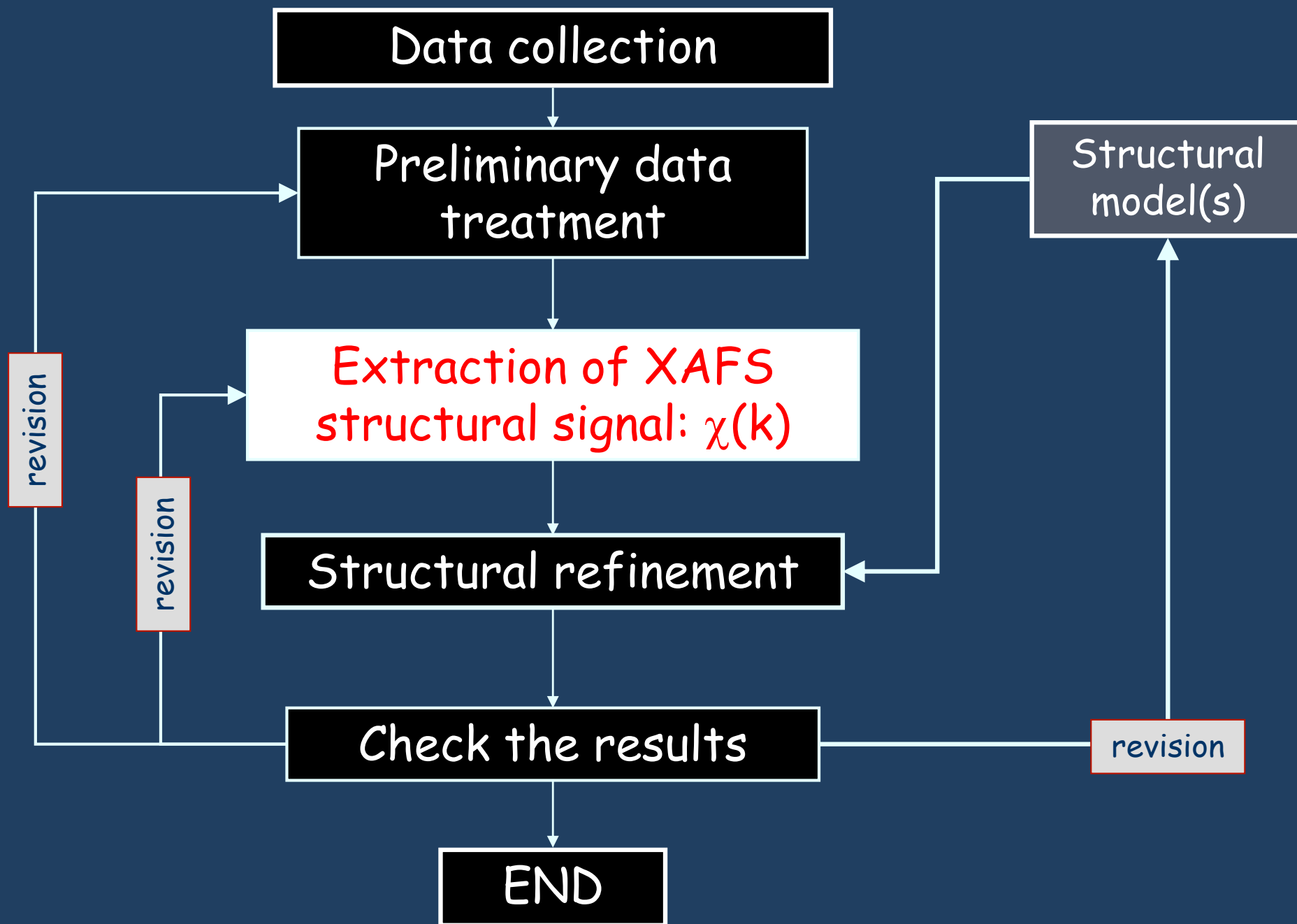
Preliminary data treatment

Preliminary data treatment is boring, it may be long...
While you are waiting for your data collection to finish...

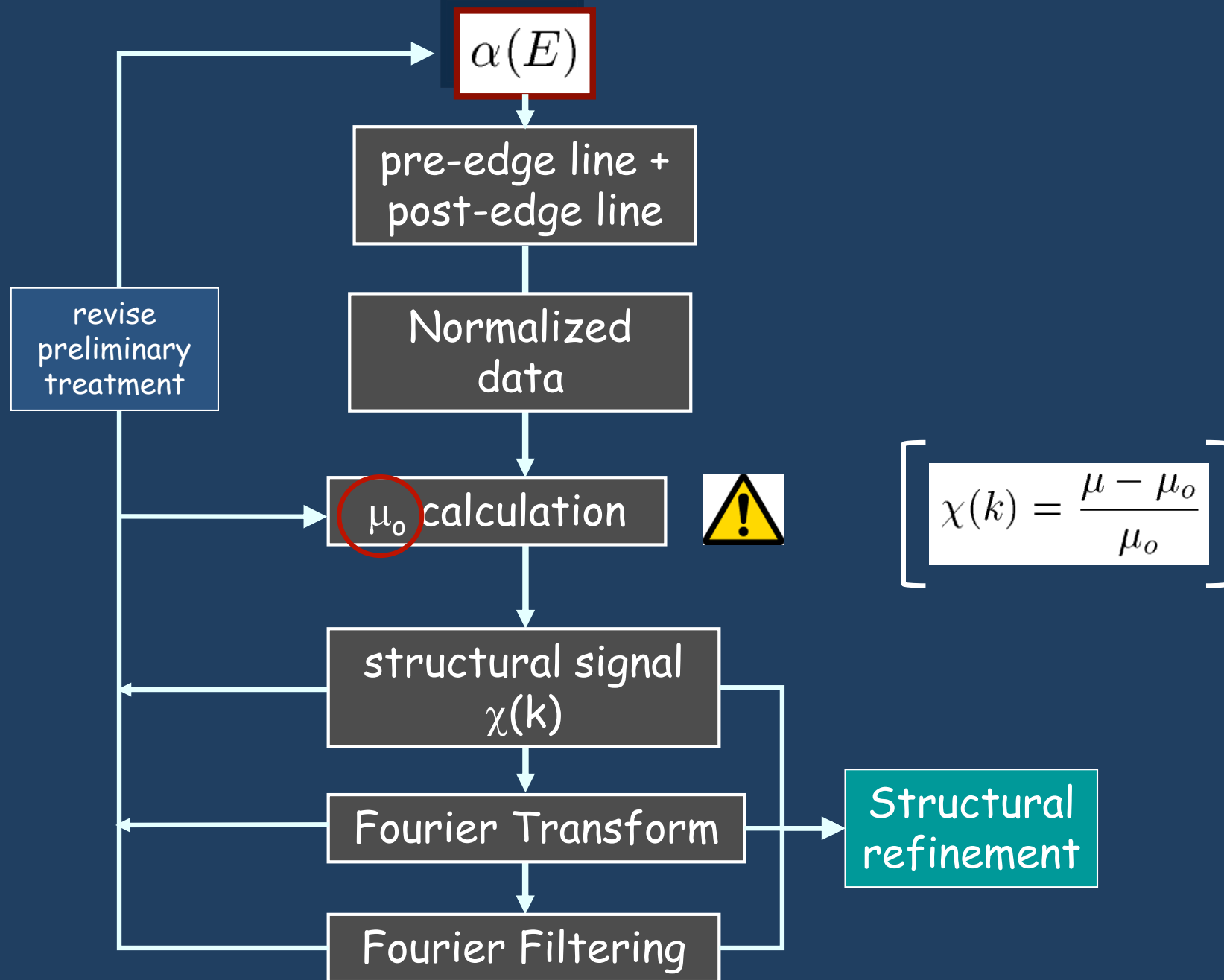
**Do it on already collected data!!
You will save your time at home!!**



XAFS analysis: from experiment to results



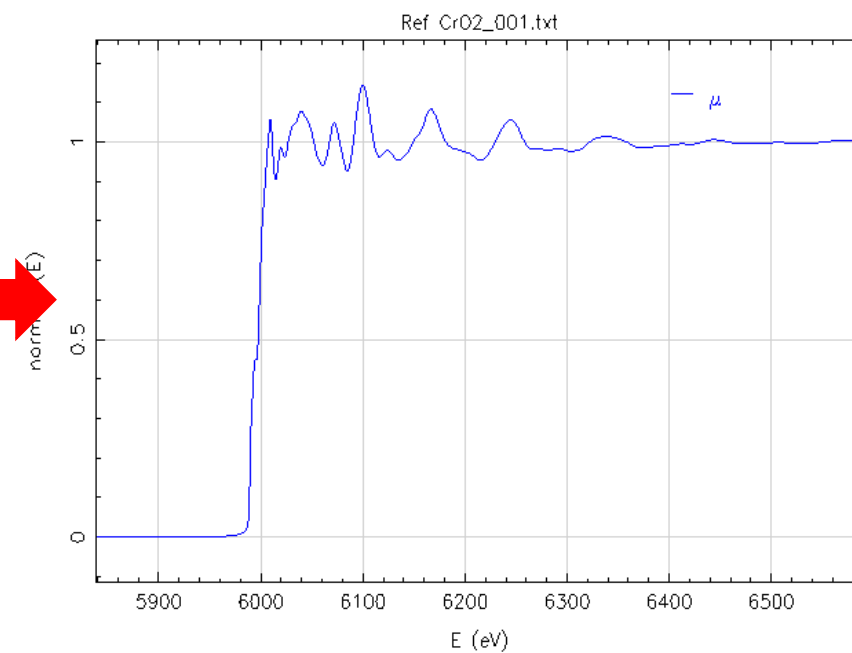
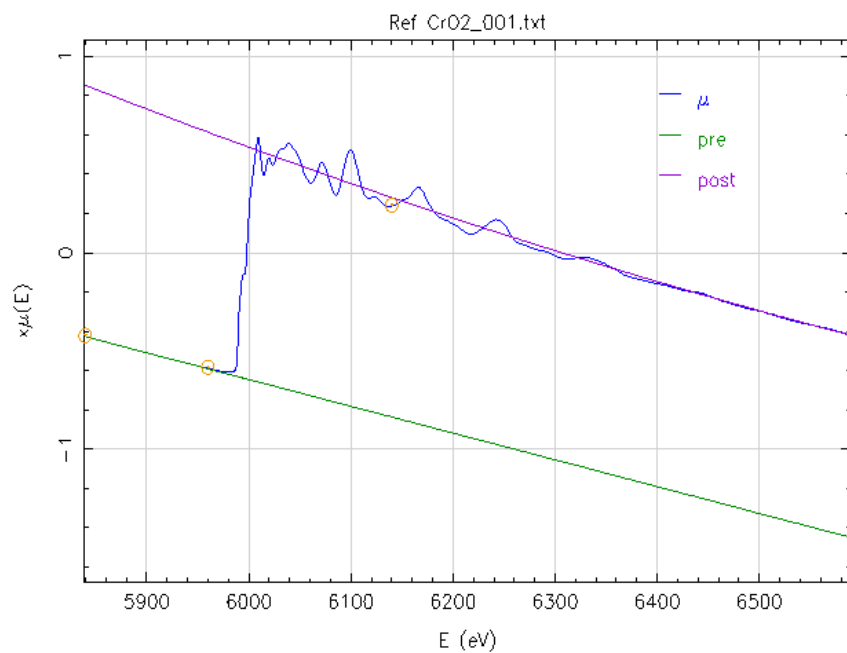
Extraction of the EXAFS signal



Extraction of the EXAFS signal

pre-edge line + post-edge line

Normalized data

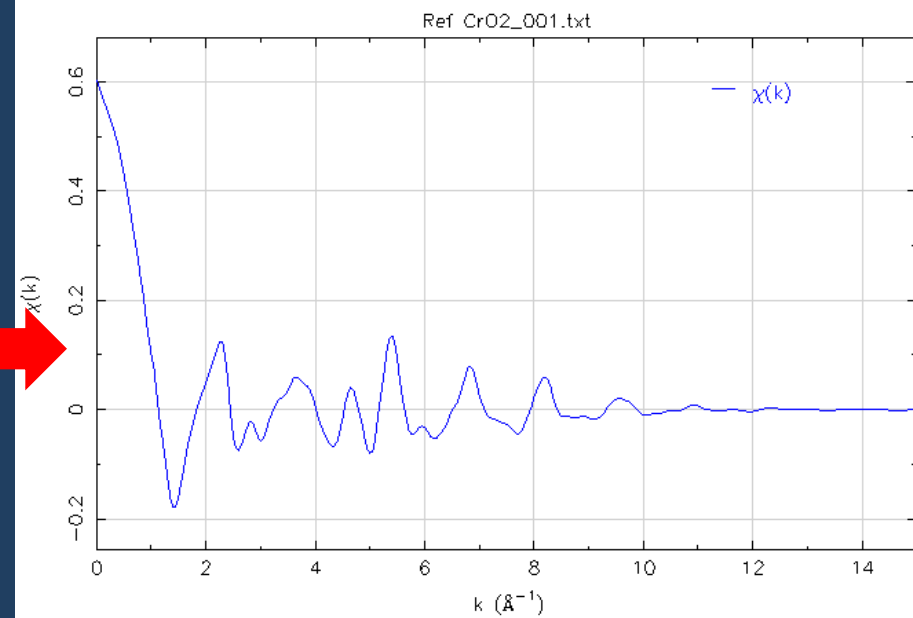
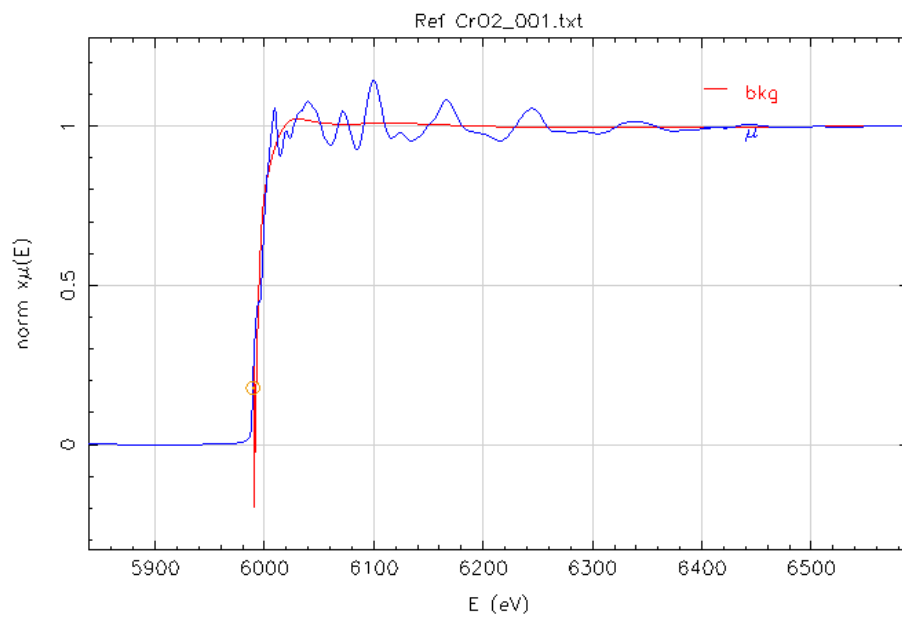


Extraction of the EXAFS signal

μ_0 calculation



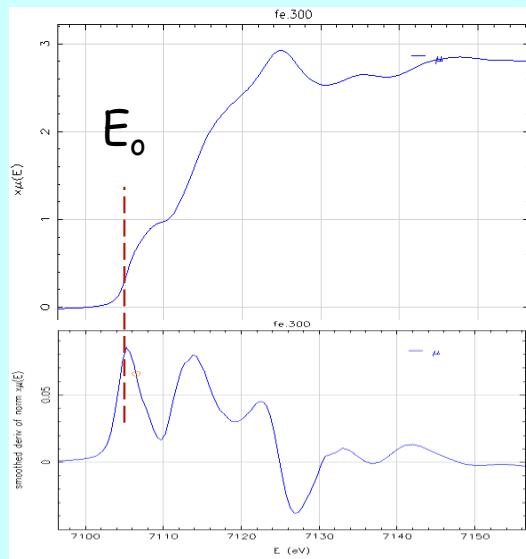
structural signal $\chi(k)$



Extraction of the EXAFS signal

μ_0 calculation

1) Define E_0



E_0 will allow to set the starting point of $\chi(k)$.

It is generally taken at the maximum of the 1st derivative of the absorption

2) Calculate μ_0

μ_0 is the bare atom atomic background.

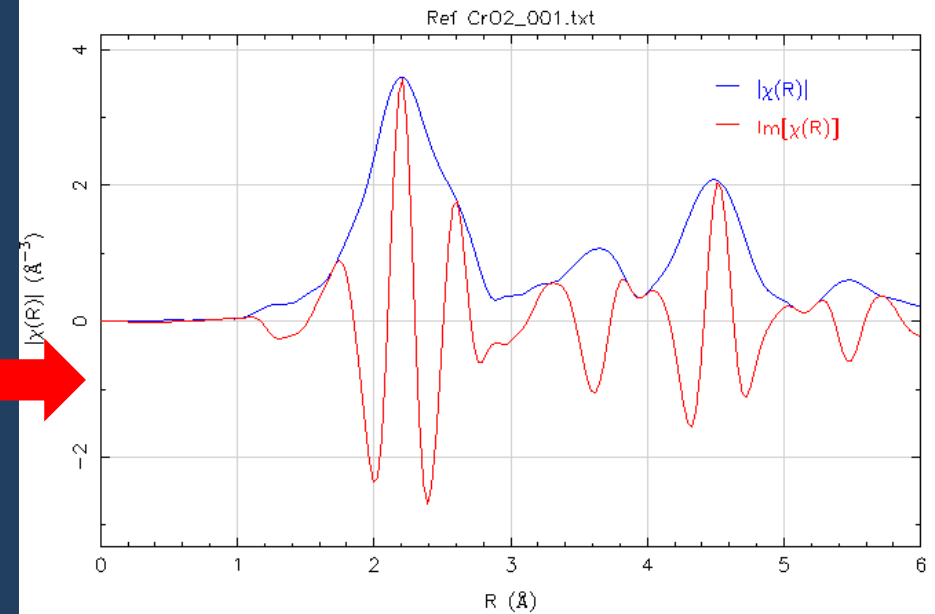
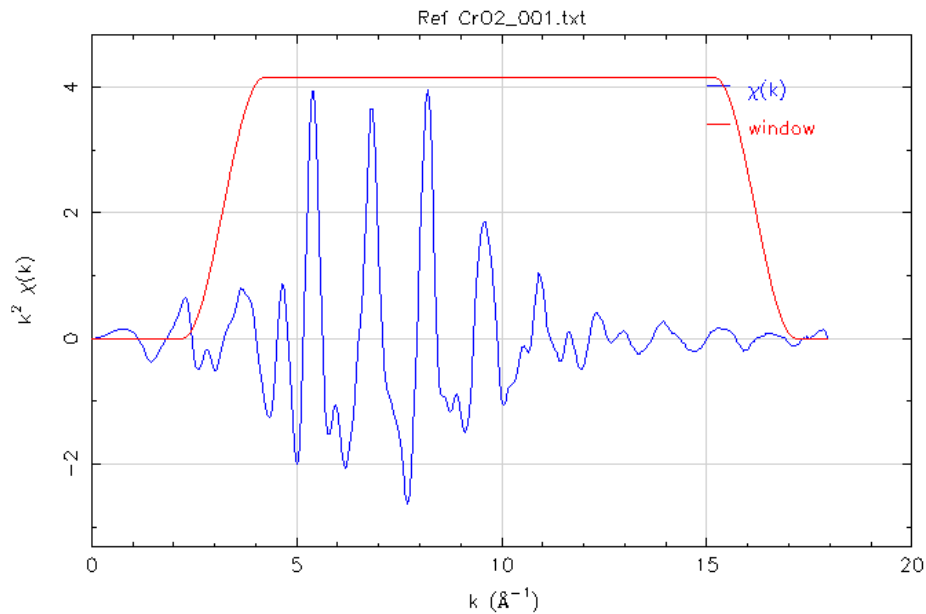
It is calculated empirically as a smooth curve across the data.

Different XAFS data analysis softwares apply different (equivalent) approaches

3) Subtract μ_0 from μ

Extraction of the EXAFS signal

Fourier Transform

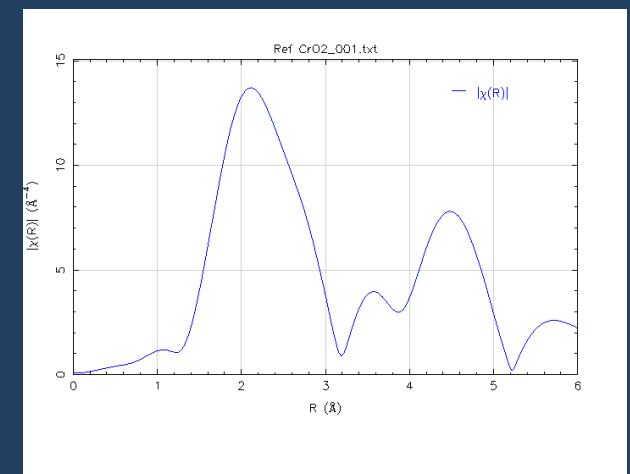
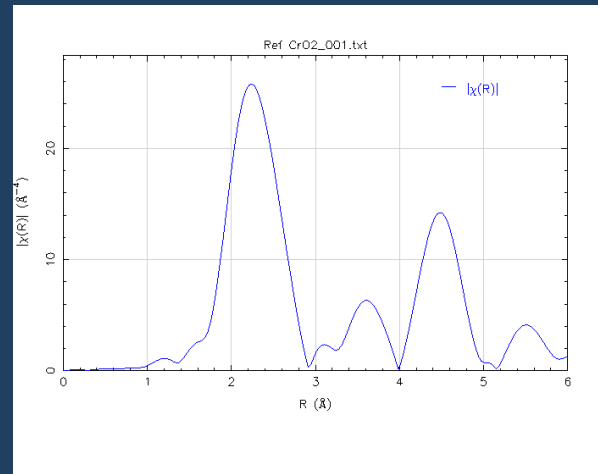
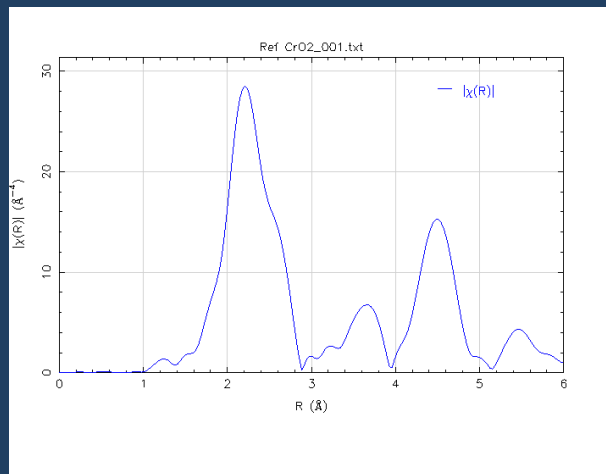
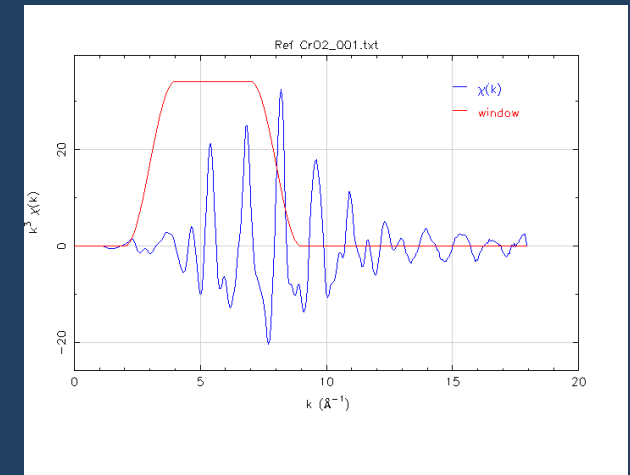
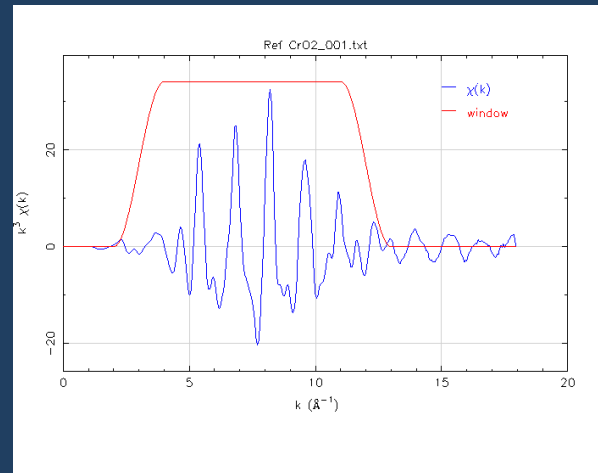
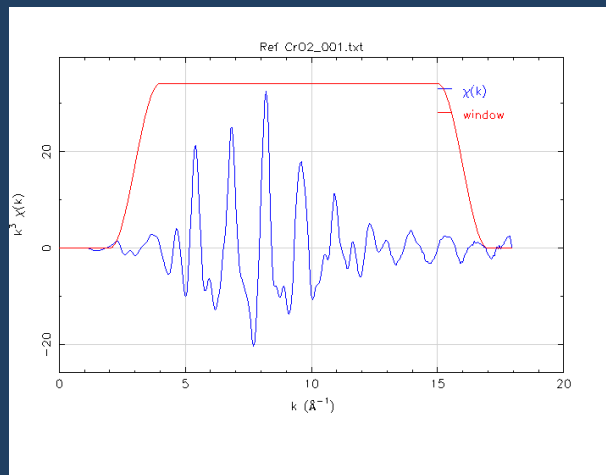


FT shows more intuitively the main structural features in the real space: the FT modulus represent a pseudo-radial distribution function (RDF)

$|\text{FT}|$ peaks represent interatomic correlation

Peak position are not the true correlation distances due to the phase shift effect

Fourier Transform - window size effect



Minor effects are given by type of windows (Hanning, Kaiser-Bessel, Sine) and apodization

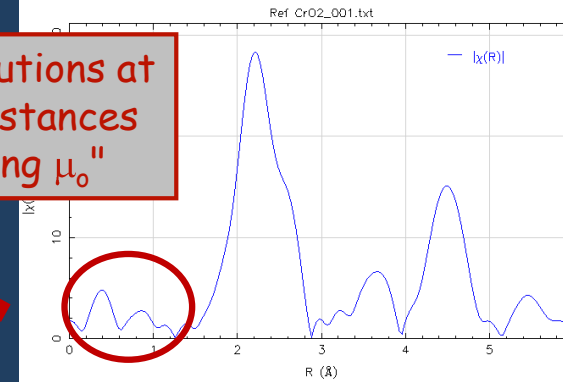
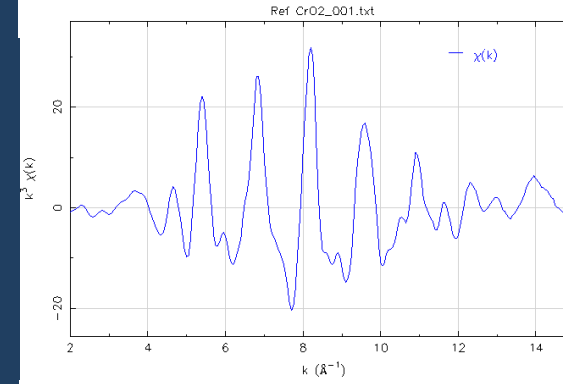
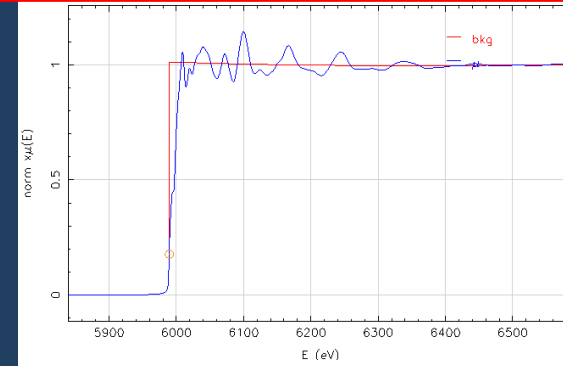
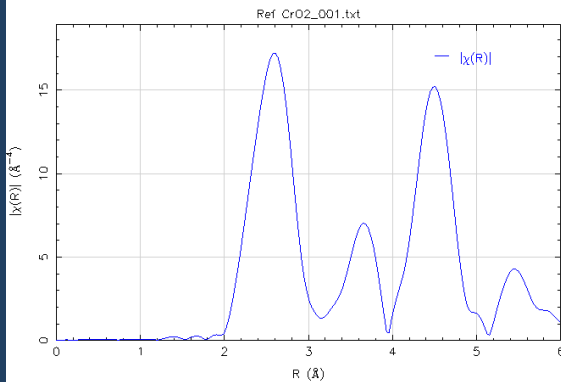
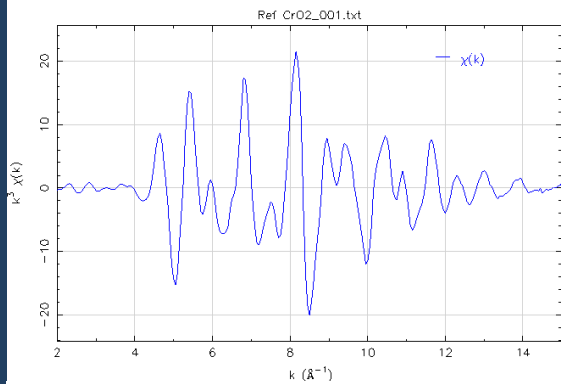
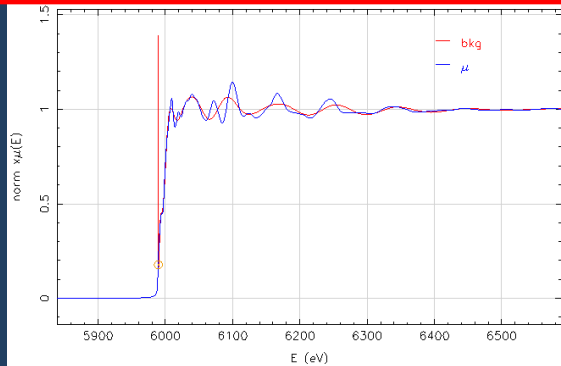
Extraction of the EXAFS signal



DO NOT REMOVE TRUE
STRUCTURAL FEATURES



DO NOT DO THE
OPPOSITE ERROR

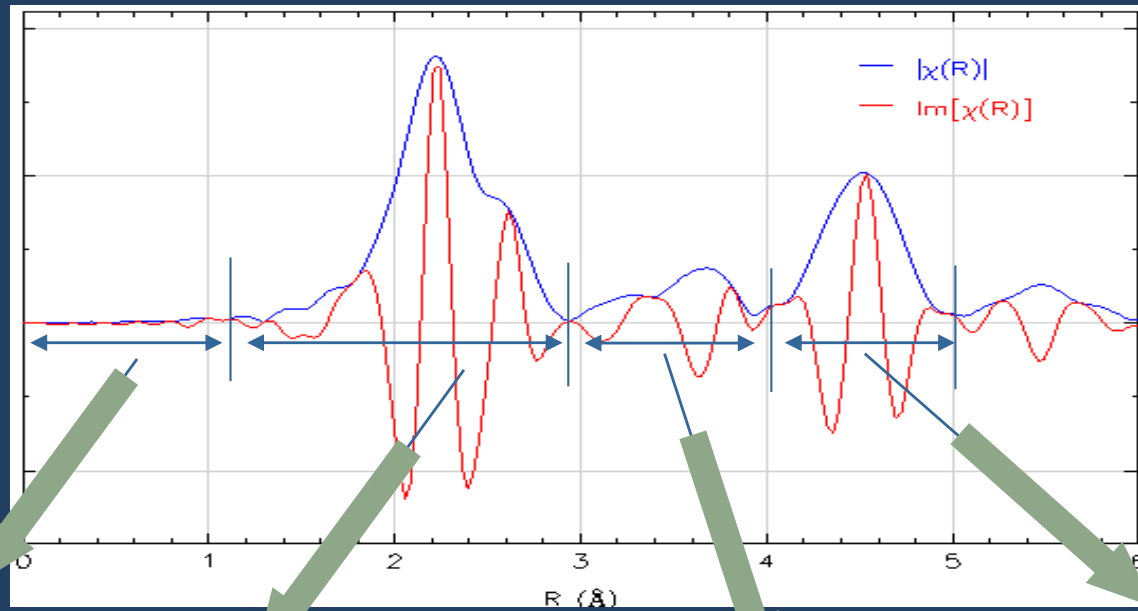


Large |FT| contributions at
low (unphysical) distances
may signify "wrong μ_0 "

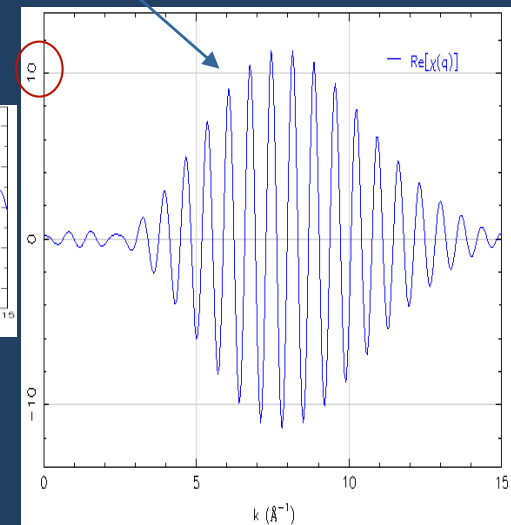
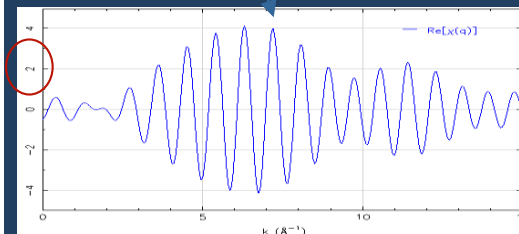
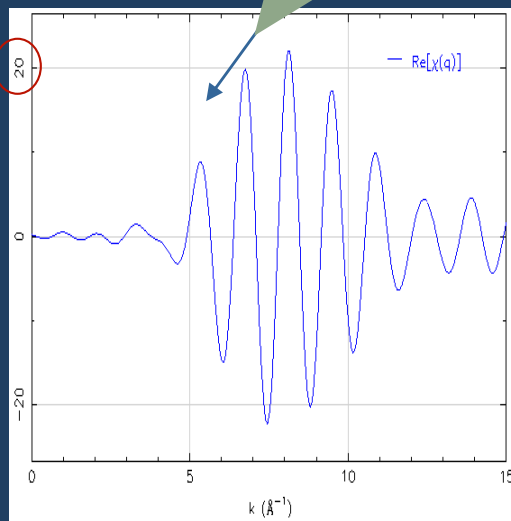
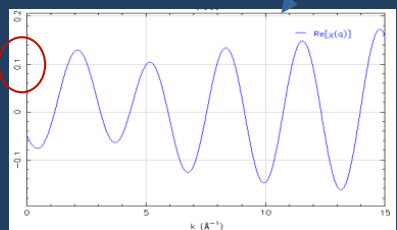
Extraction of the EXAFS signal

Fourier Filtering

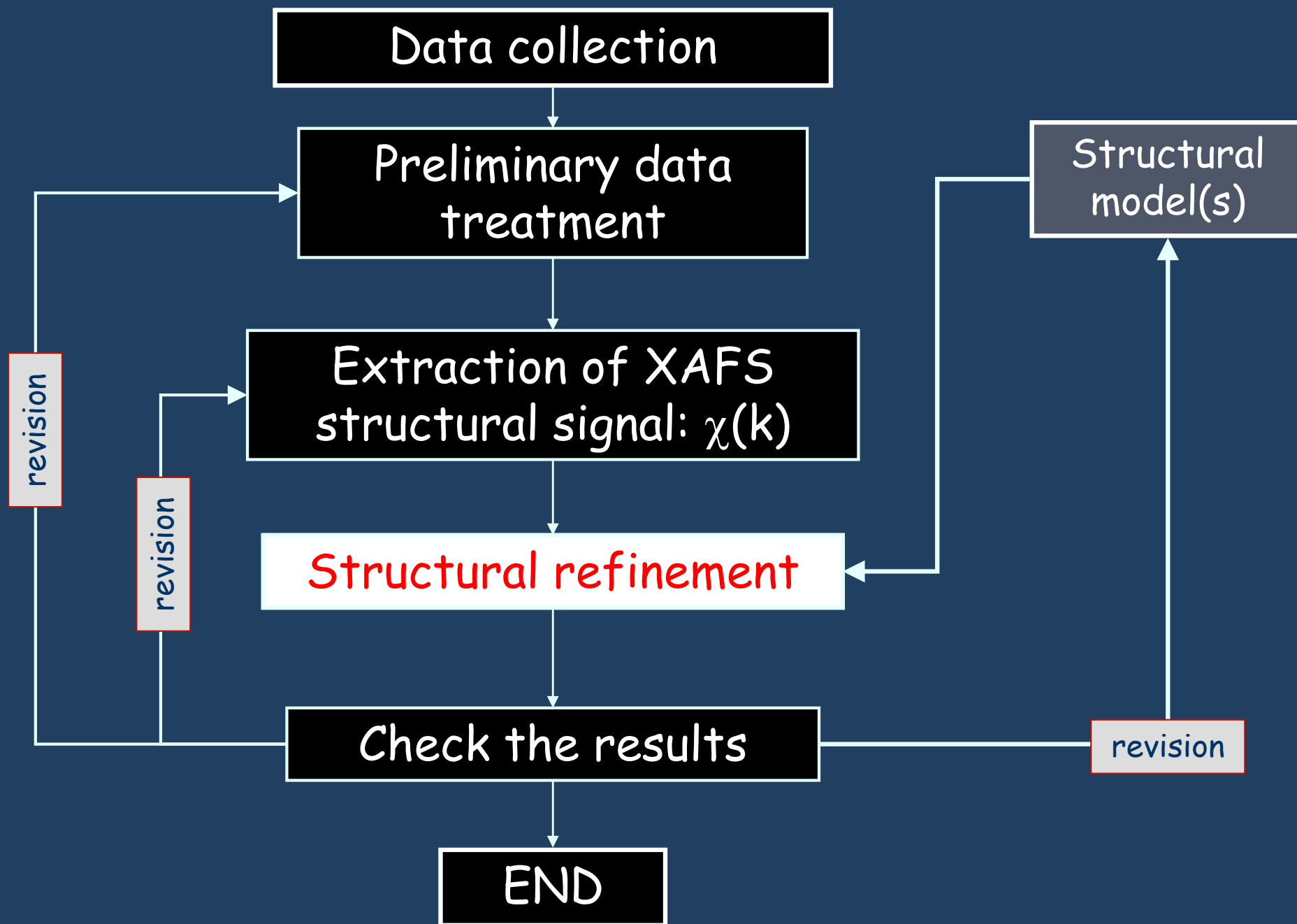
Fourier filtering allows isolating contributions of selected regions of the FT



Background contribution



XAFS analysis: from experiment to results

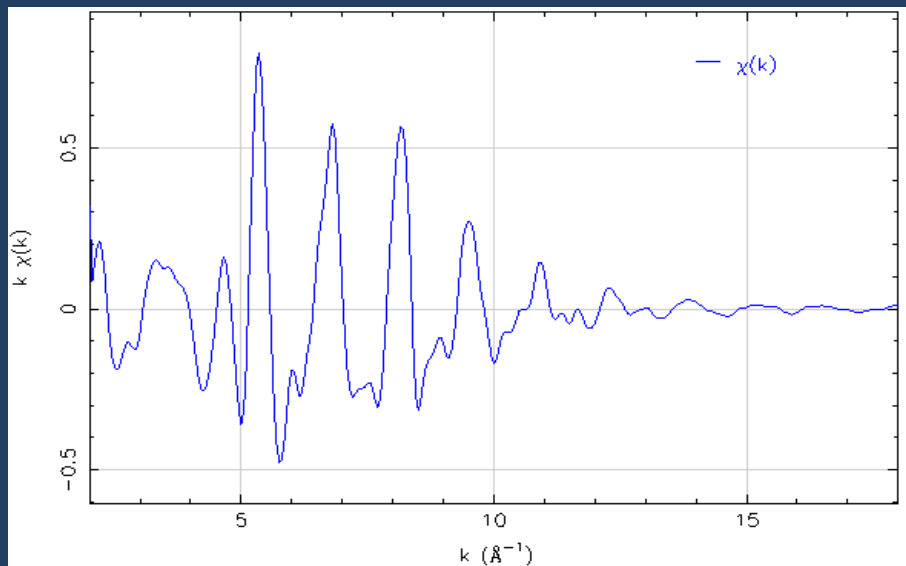


Structural refinement

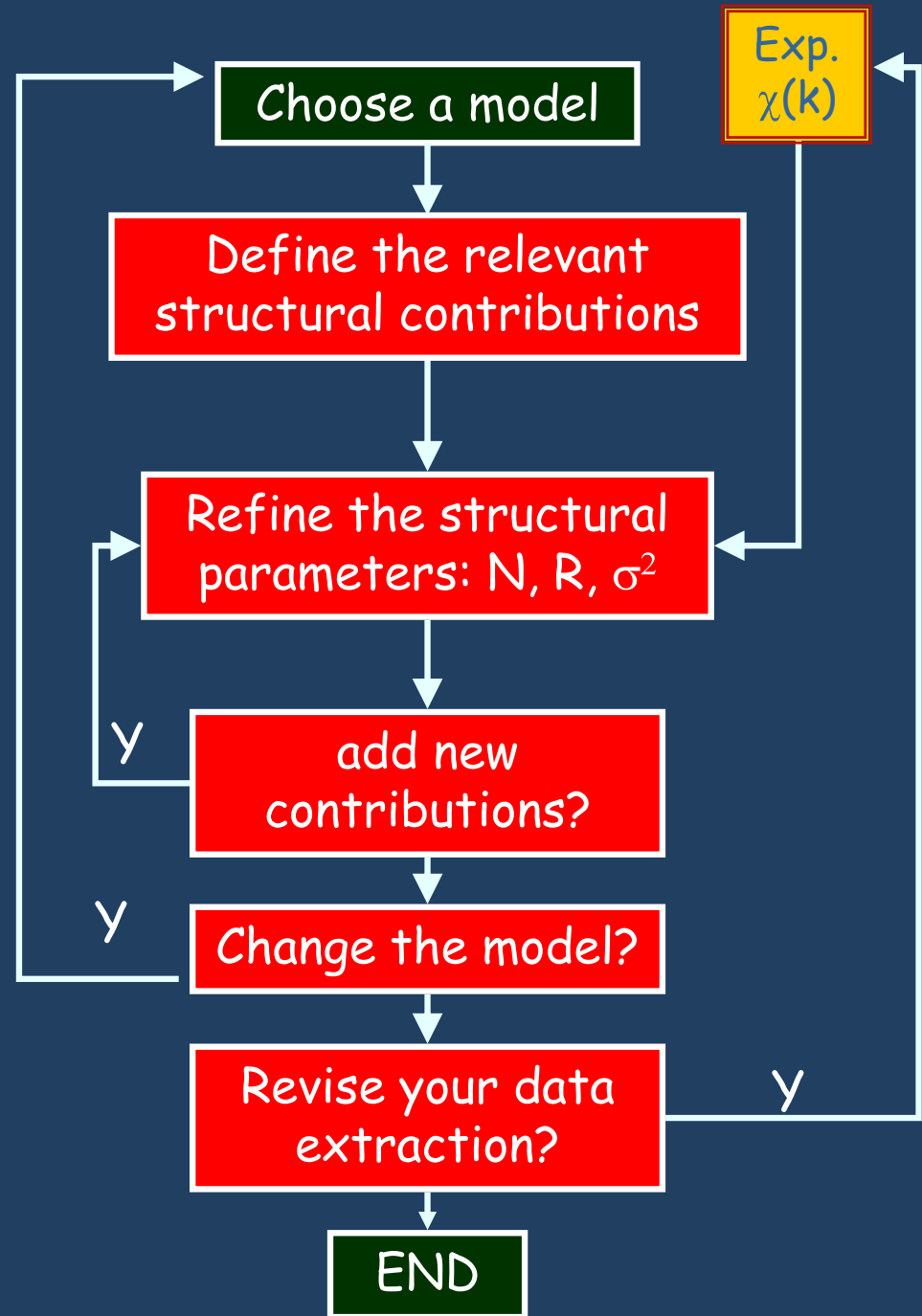
Theoretical $\chi(k)$

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

Experimental $\chi(k)$



Require data analysis programs



Structural refinement

Choose a model

How to find a model structure

How to visualize the structure

How to calculate distances and geometries



Barns.ill.fr

English Russian

<http://database.iem.ac.ru/mincryst/>

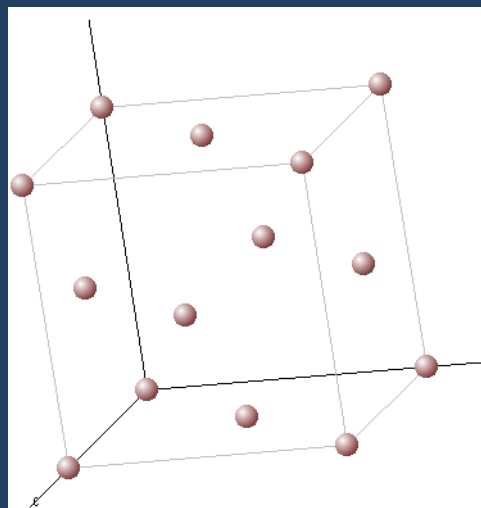
ICSD database

PowderCell for Windows
Version 2.4
8.03.2000

W.Kraus & G. Nolze
Federal Institute for Materials Research and Testing
Rudower Chaussee 5, 12489 Berlin, Germany

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G.Nolze: Tel. +49 -30 - 8104 3109, E.mail: gert.nolze@bam.de

scientific support:
Günter Reck (BAM) guenter.reck@bam.de IPAP
Berd Müller (Uni Jena) bernd.mueller@uni-jena.de Size and Strain
U. Müller (Uni Kassel) subgroup data



ATOMS on the Web

<http://millenia.cars.aps.anl.gov/cgi-bin/atoms/atoms.cgi>

Run ATOMS Clear Reset

Gold

Titles

Operational Parameters

Space Group: Fm-3m Rmax: 6 Edge:

Output Type: feff6.inp Shift:

Lattice Constants and Angles

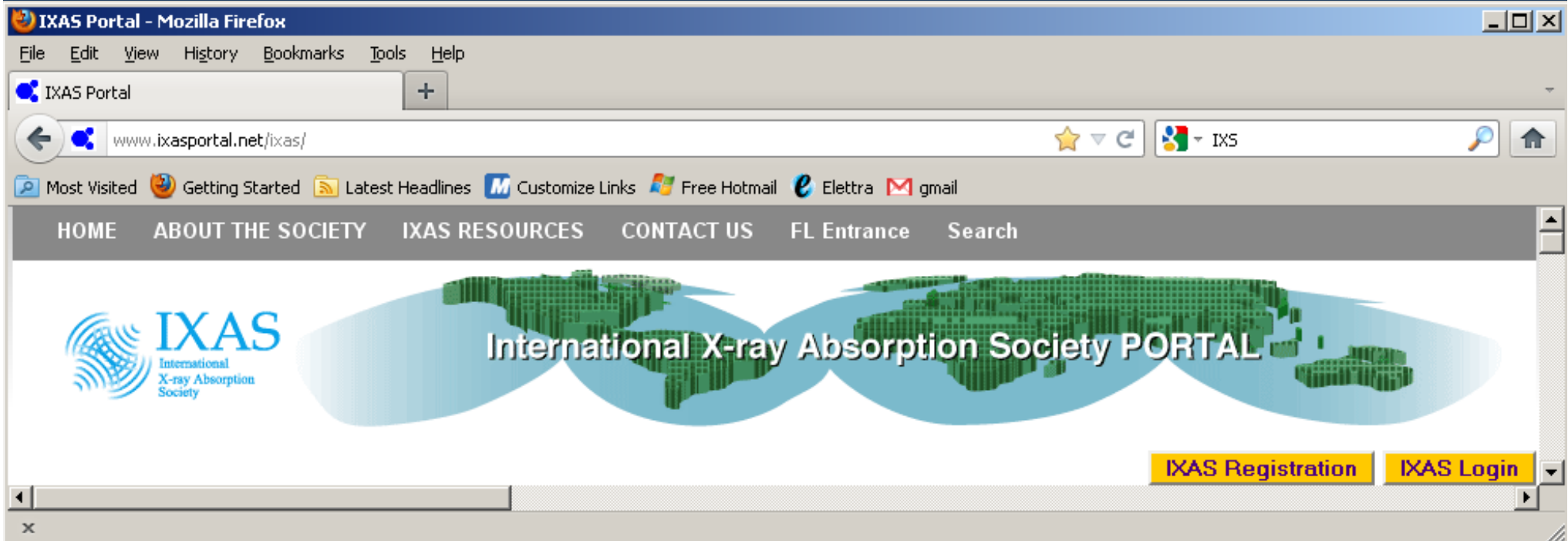
A: 4.08 B: 4.08 C: 4.08
Alpha: 90 Beta: 90 Gamma: 90

Run ATOMS Clear Reset

Table of Crystallographic Sites

Cent.	Element	X	Y	Z	Tag
1	Au	0	0	0	Au

XAFS data analysis softwares



<http://www.xafs.org/>



<http://cars9.uchicago.edu/ifeffit/>

Click DOWNLOADS

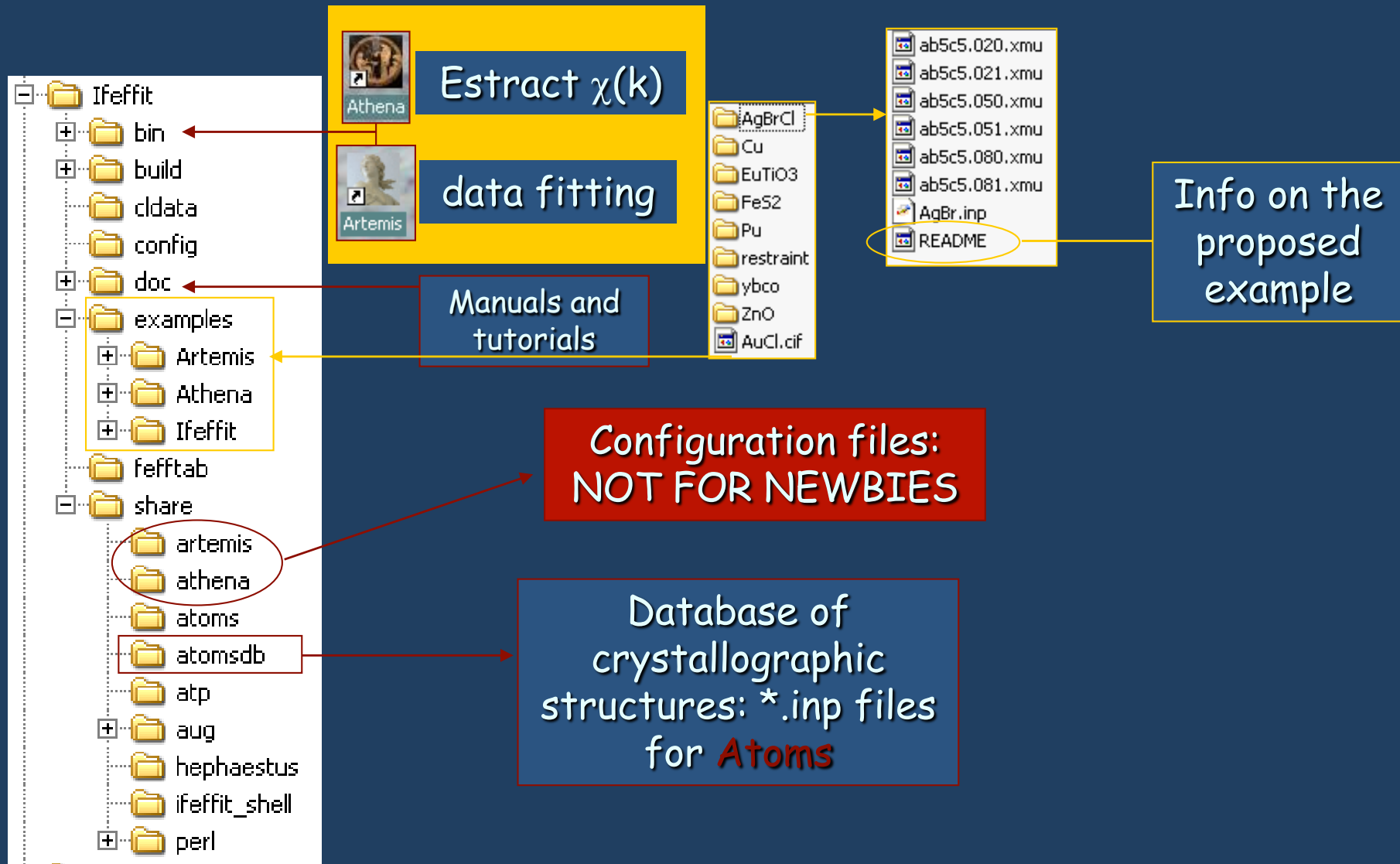
Click [ifeffit-1.2.11.exe](#)

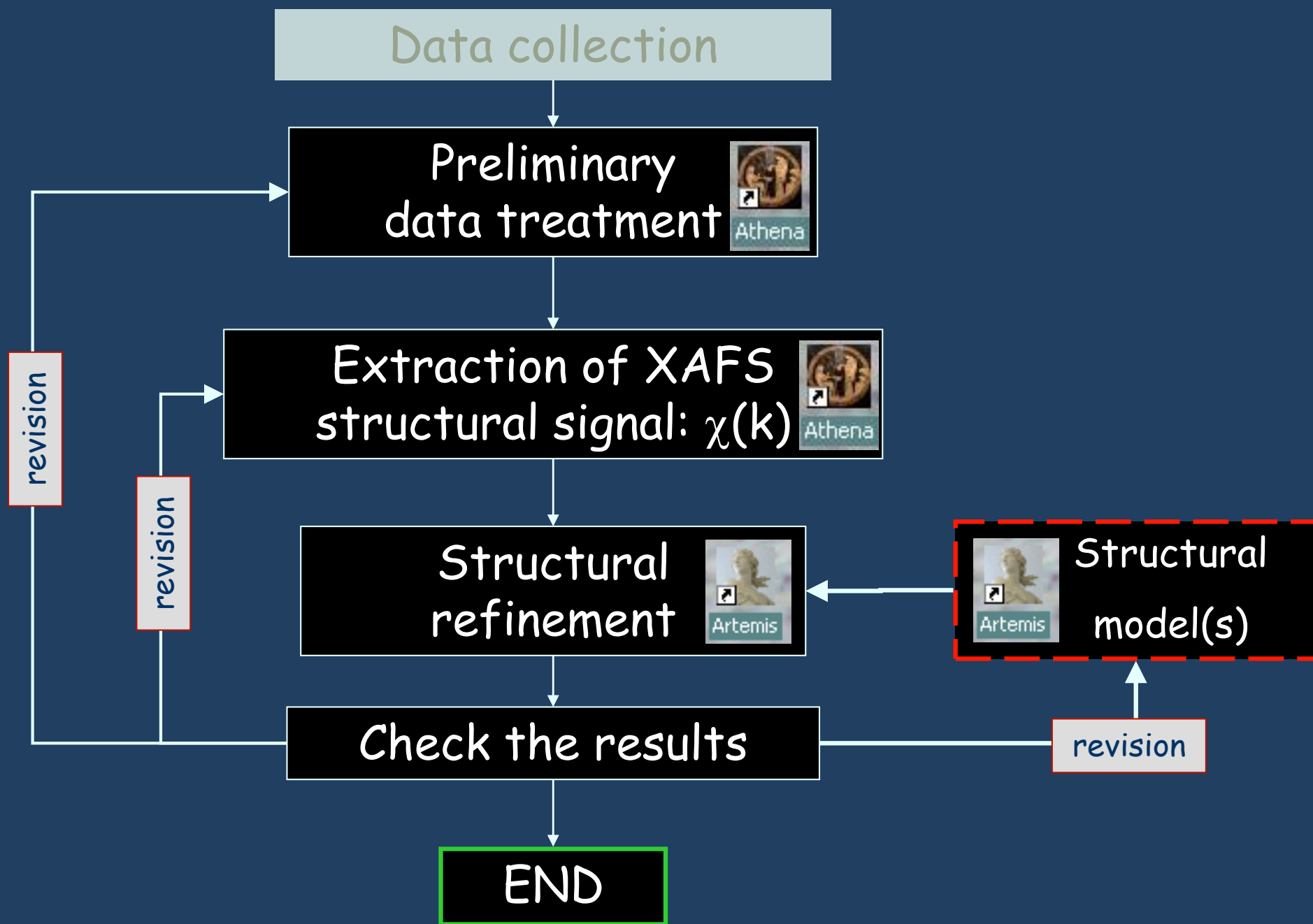
Install Ifeffit.exe



1. **athena** GUI for Data Processing with Ifeffit 
2. **artemis** GUI for XAFS Fitting with Ifeffit 
3. **hephaestus** GUI for general x-ray properties of the elements
4. **sixpack** GUI for XAFS Processing and Fitting with Ifeffit
5. **feff6** Stand-alone program for ab initio EXAFS calculations
6. **atoms** Stand-alone, command line crystallography->feff.inp
7. **autobk** Stand-alone background removal program
8. **feffit** Stand-alone FEFF fitting program
9. **ifeffit** command-line version of Ifeffit

Inside the Ifeffit directory







Preliminary data treatment & Extraction of XAFS structural signal: $\chi(k)$

The screenshot shows the Athena software interface with the following sections:

- Project:** Current group: **cu_foil_10k.dat** (circled in red). File: E:/Duino_ago09/Examples/Cu_10K/cu_foil_10k.dat. Z: Cu, Edge: K, E shift: 0, Importance: 1.
- Background removal:** E0: 8977.58, Rbkg: 1.0, k-weight: 2, Edge step: 2.32667, Pre-edge range: -150 to -30, Normalization range: 150 to 2284.89, Spline range: k: 0.0 to 25.019, E: 0.000 to 2384.861.
- Forward Fourier transform:** k-range: 2 to 23.019, dk: 1, window type: hanning, Phase correction: no, arbitrary k-weight: 0.5.
- Backward Fourier transform:** R-range: 1 to 3, dr: 0.0, window type: hanning.
- Plotting options:** mu(E) [checked], background [checked], pre-edge line [unchecked], post-edge line [unchecked], Normalized [unchecked], Derivative [unchecked], Emin: -200, Emax: 800.

At the bottom, a status bar reads: "plotting in energy from group 'cu_foil_10k.dat' ... done!"

List of files (group) opened into Athena

Plot highlighted files

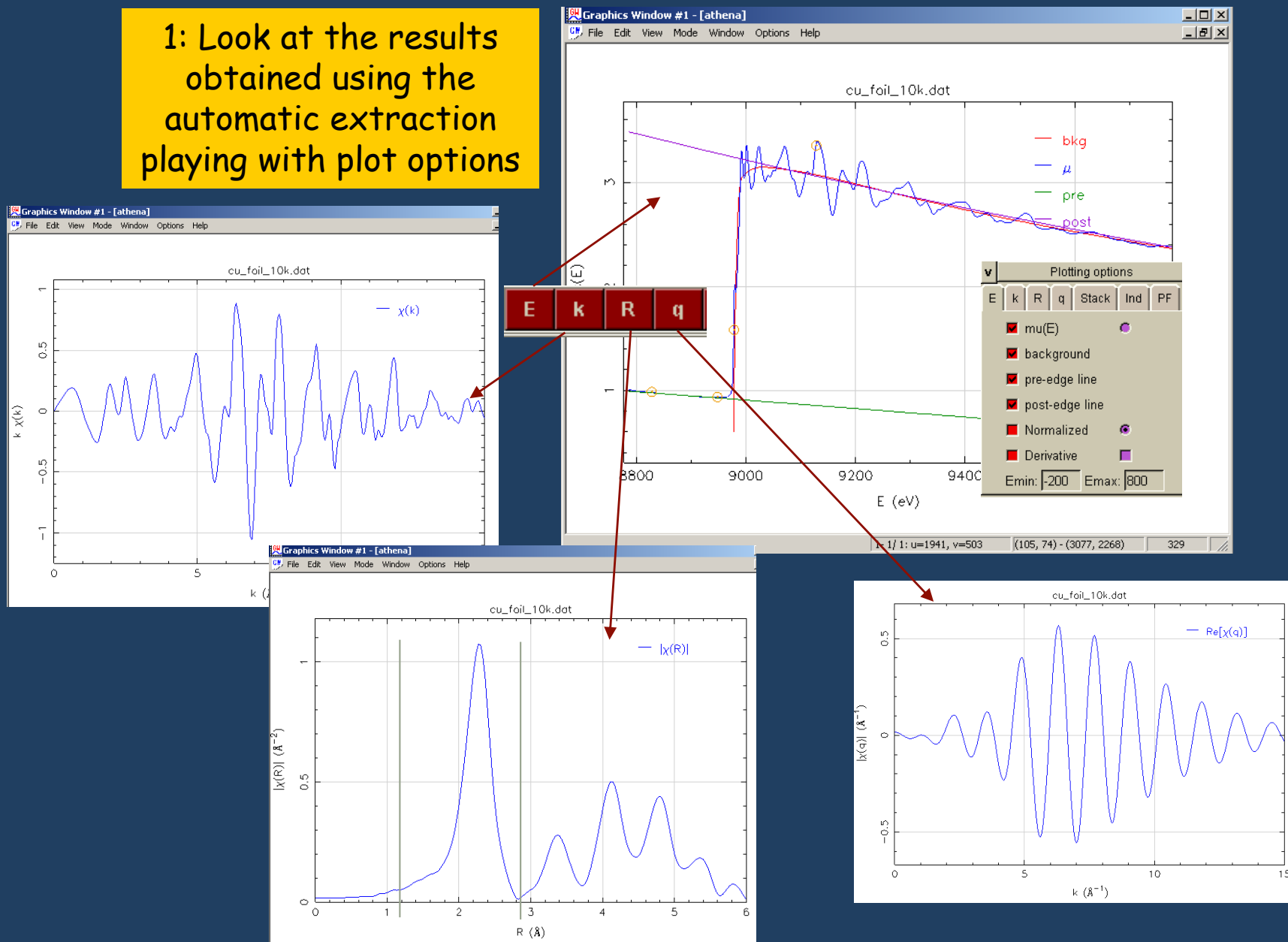
Plot (several) marked files

Options for plot

Example 1: Cu 10 K

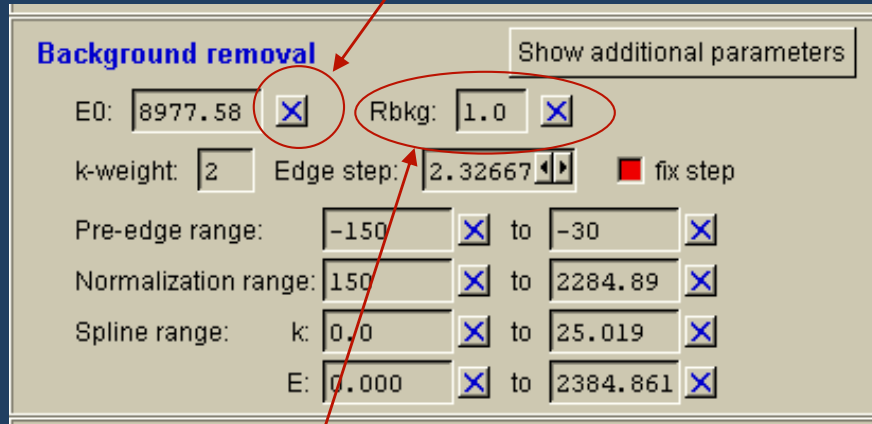
Open **cu010k.dat** into ATHENA

1: Look at the results obtained using the automatic extraction playing with plot options



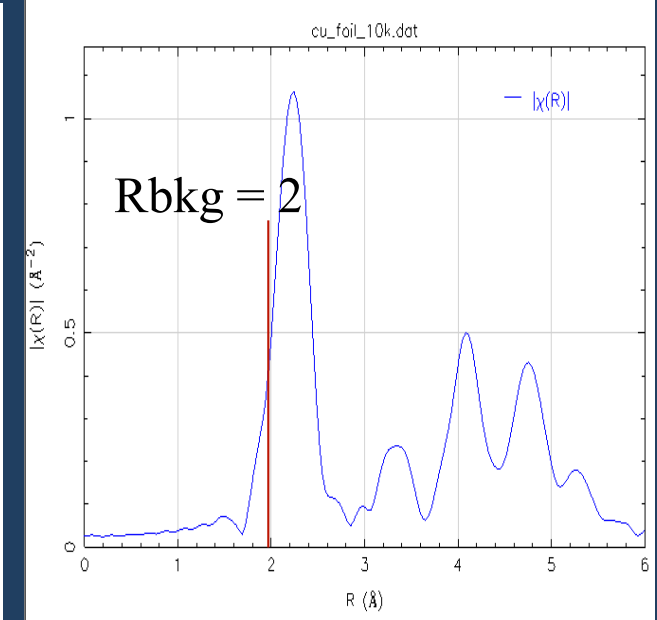
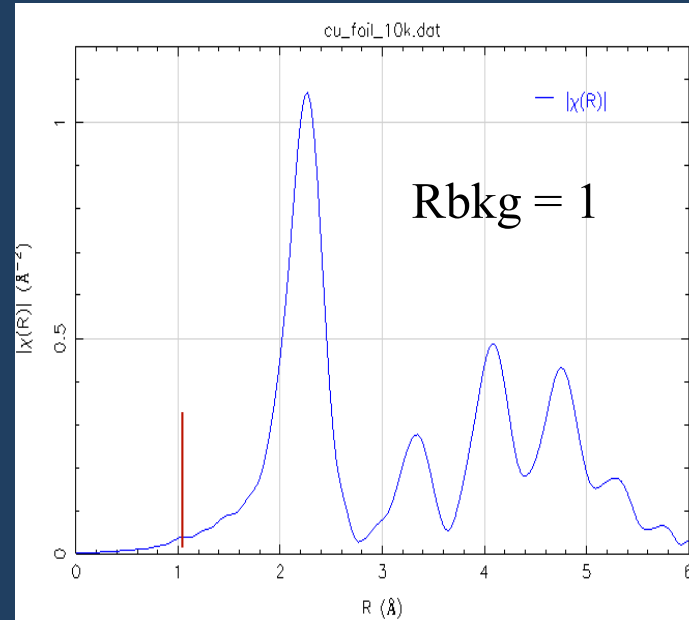
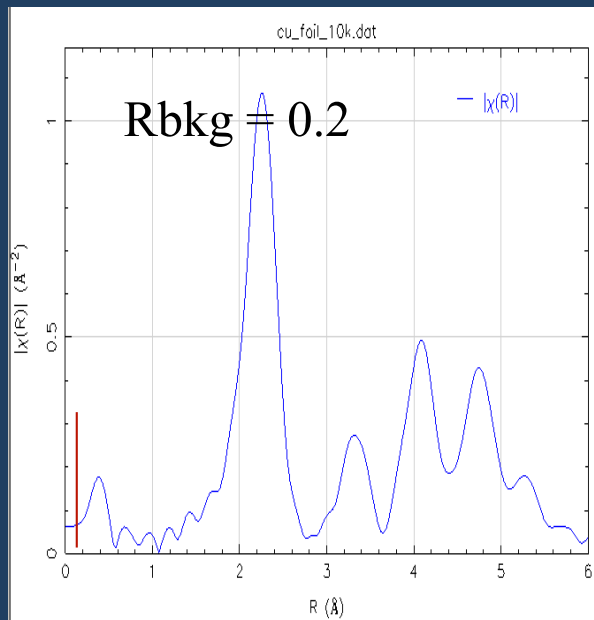
Takes the value from the cursor on the graph window

1: Look at the effects of changing background subtraction parameters



R cut off for automatic background calculation

- Change E_0
- Change R_{bkg}
-



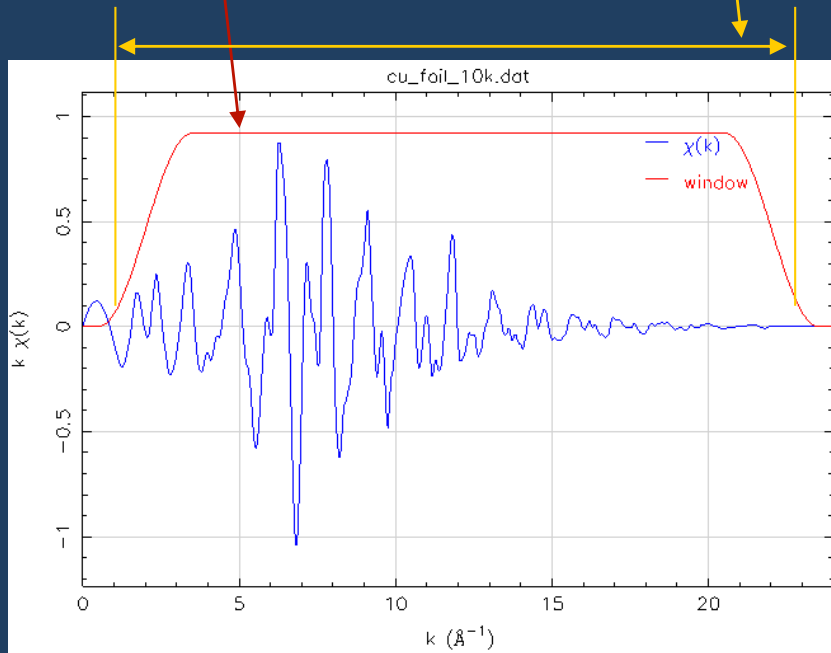
3: Look, in R space, at the effects of changing extraction and FT parameters

Forward Fourier transform

k-range: to

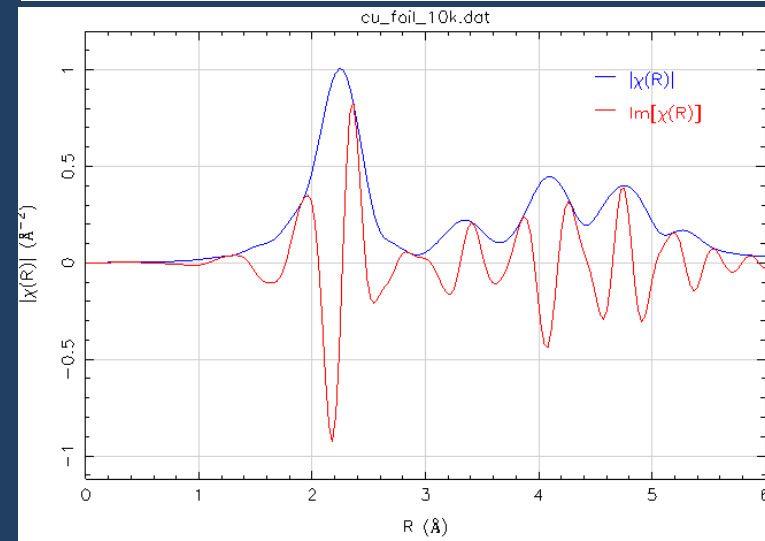
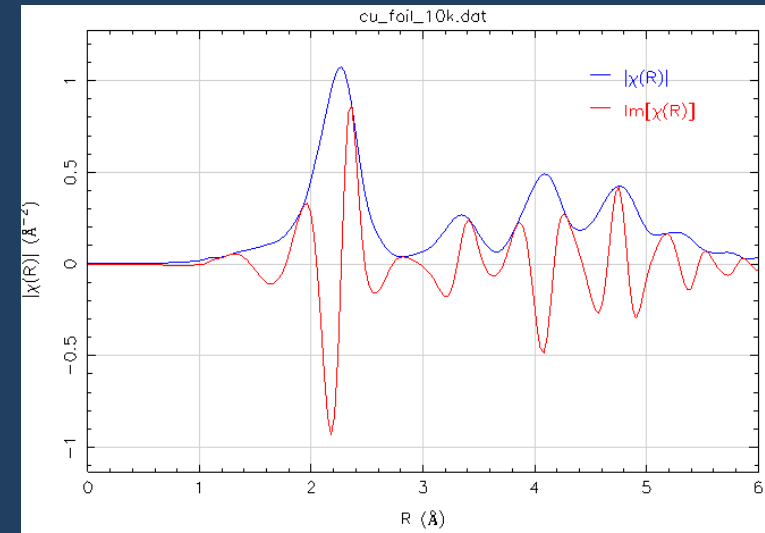
dk: window type:

Phase correction: no arbitrary k-weight:



0 1 2 3 kw

FT of: $k^{kw}(\chi(k))$

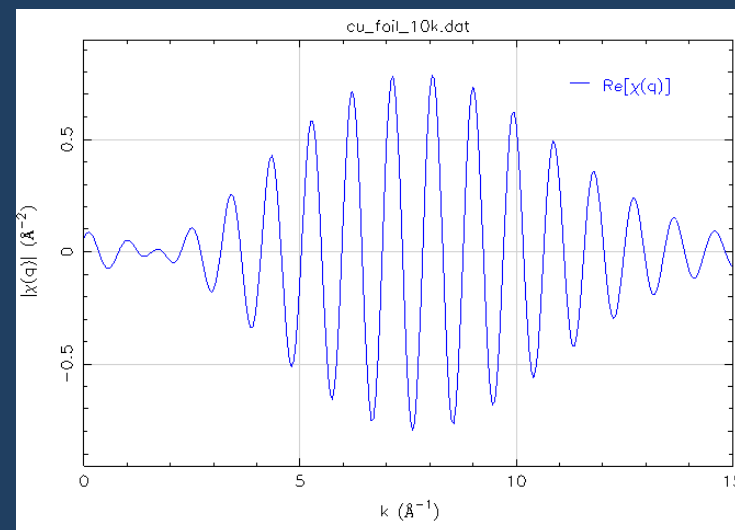
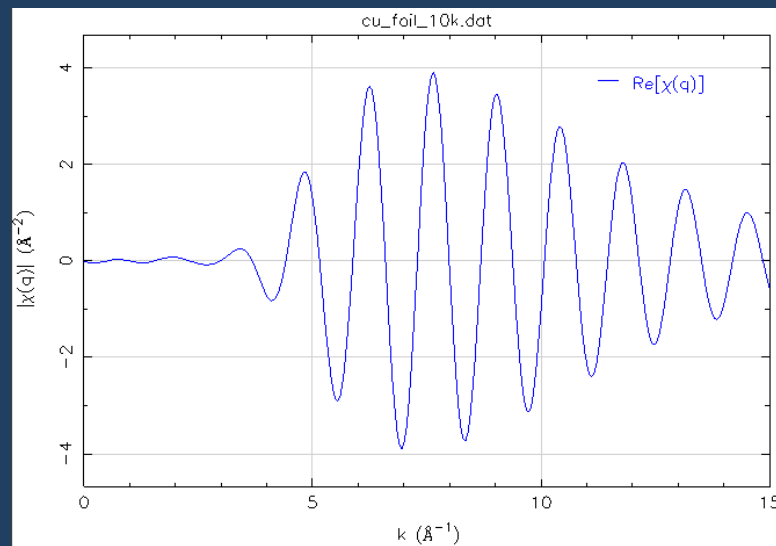
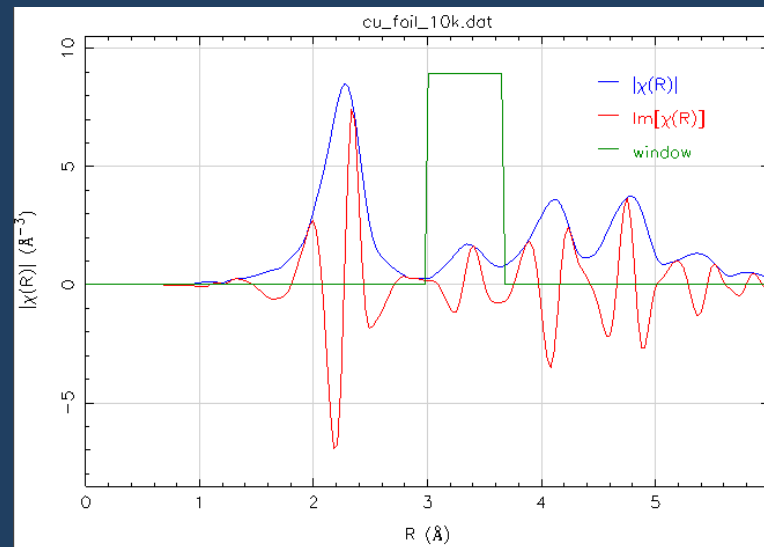
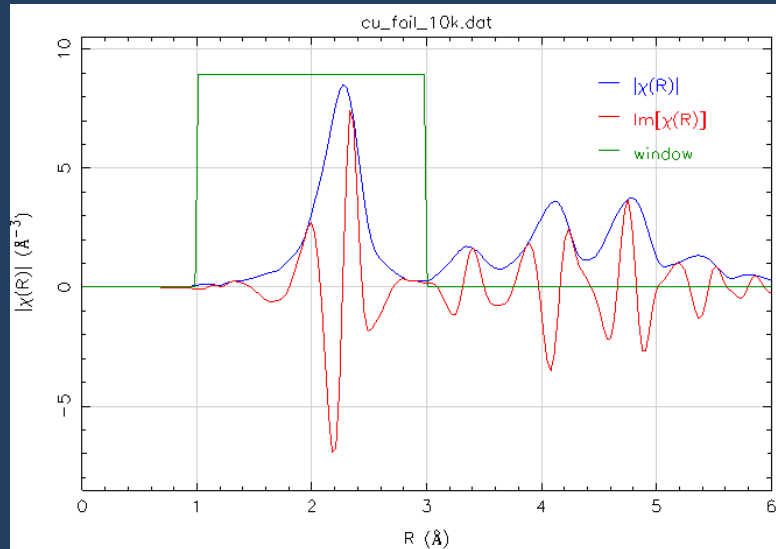


Backward Fourier transform

R-range: to

dr: window type:

4: Look, in q (Back Fourier) space, at the effects of changing BF parameters



5: Data pre-treatment

Data Merge Analysis - Settings

Calibrate energies

Align scans

Calibrate dispersive XAS

Deglitch

Truncate

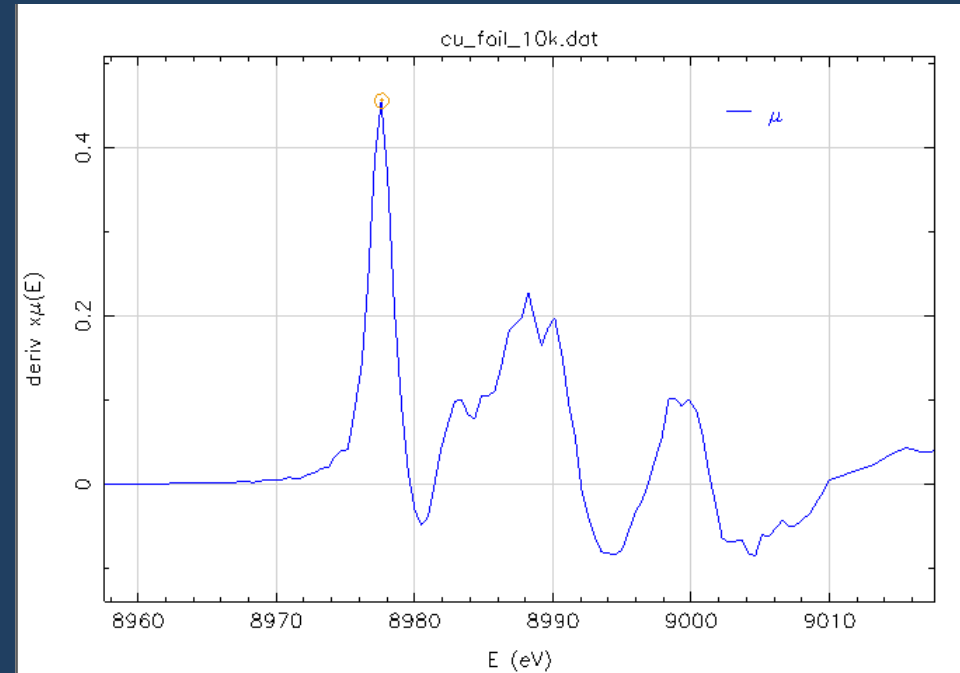
Rebin $\mu(E)$

Smooth $\mu(E)$

Convolute $\mu(E)$

Self Absorption

MEE correction



Data calibration

Group: cu_foil_10k.dat

Display: deriv(E)

Smoothing: 0

Reference at: 8977.58

Calibrate to: 8979

Select a point

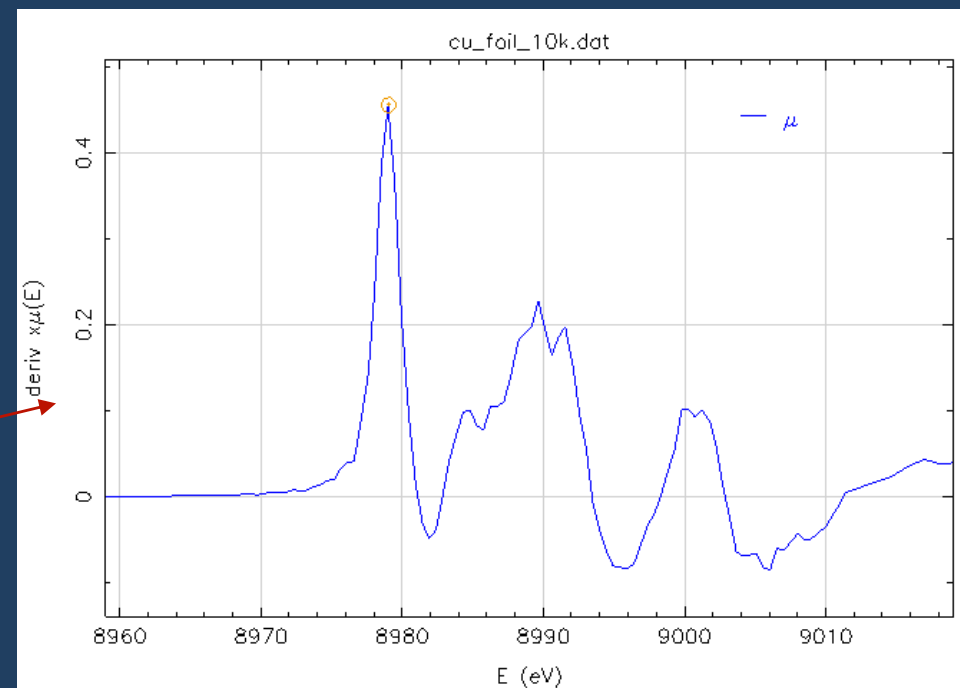
Find zero-crossing

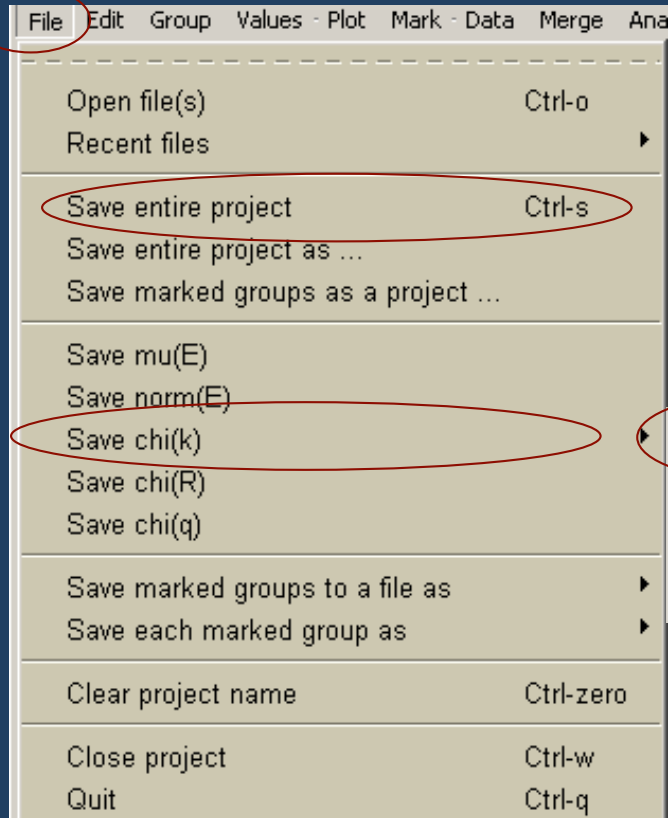
Replot

Calibrate

Document section: energy calibration

Return to the main window

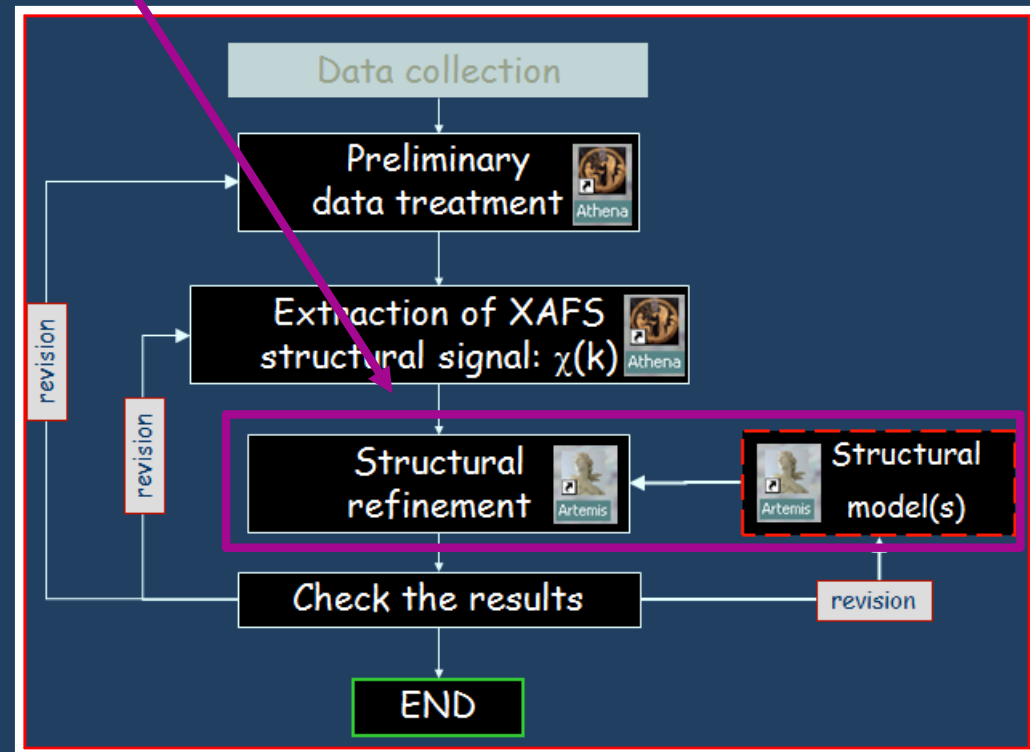




Save:

cu_foil_10k.dat.chi

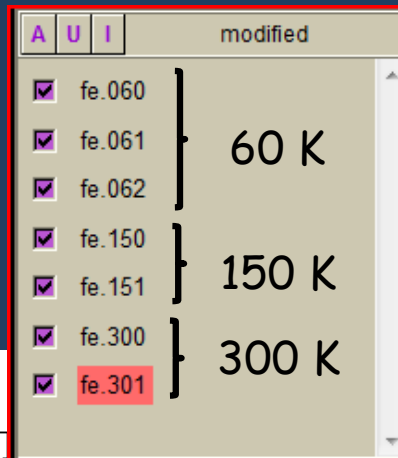
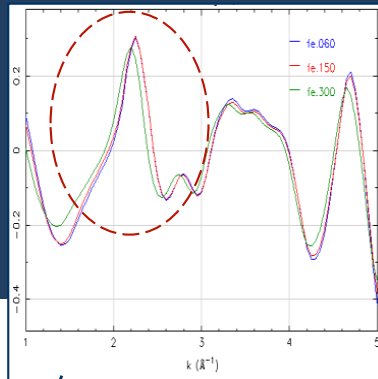
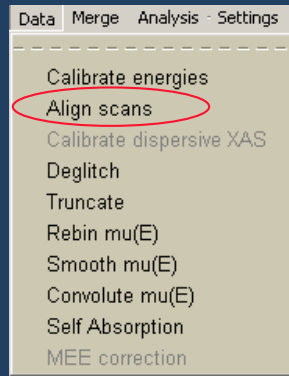
$\chi(k)$ is required for ARTEMIS



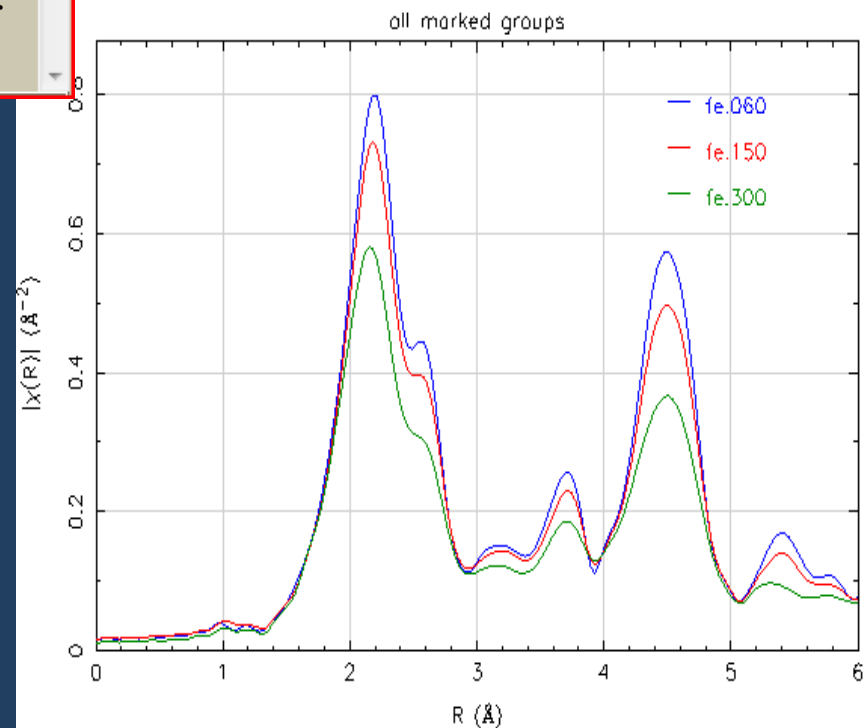
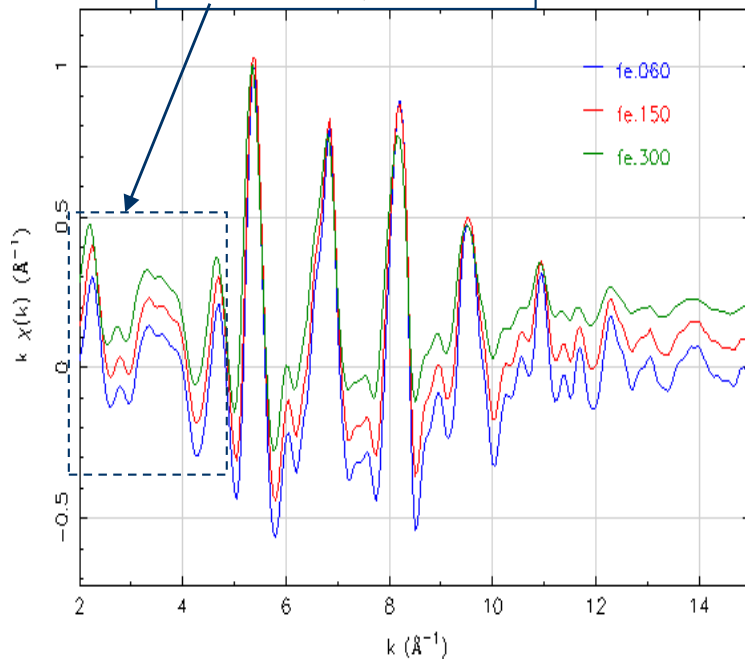
Working with several files

Go into the **Fe** directory

Open all the files (except README)
into Athena



Temperature
effect



5: Data treatment: Align E₀

- Data Merge Analysis Settings
- Calibrate energies
- Align scans
- Calibrate dispersive XAS
- Deglintch
- Truncate
- Rebin $\mu(E)$

Athena

Data alignment

Standard: fe.060

Other: fe.300

Plot as: derivative

Fit as: derivative

Shift by 0 eV

Auto align

Align all marked groups

Replot

-5 +5

-1 +1

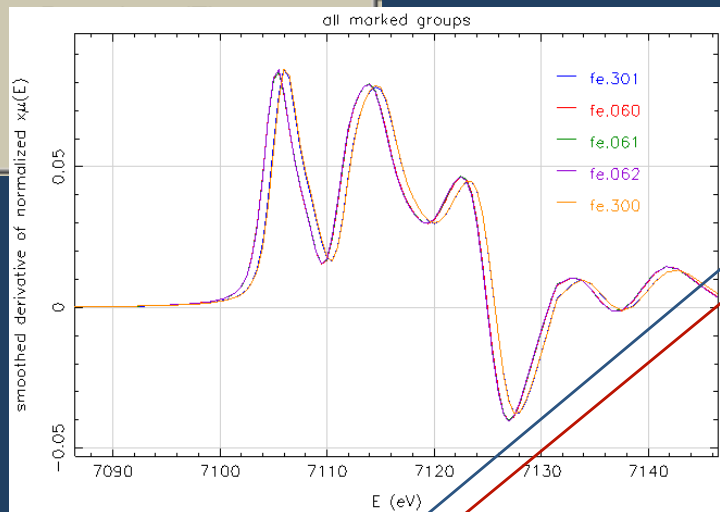
-0.5 +0.5

-0.1 +0.1

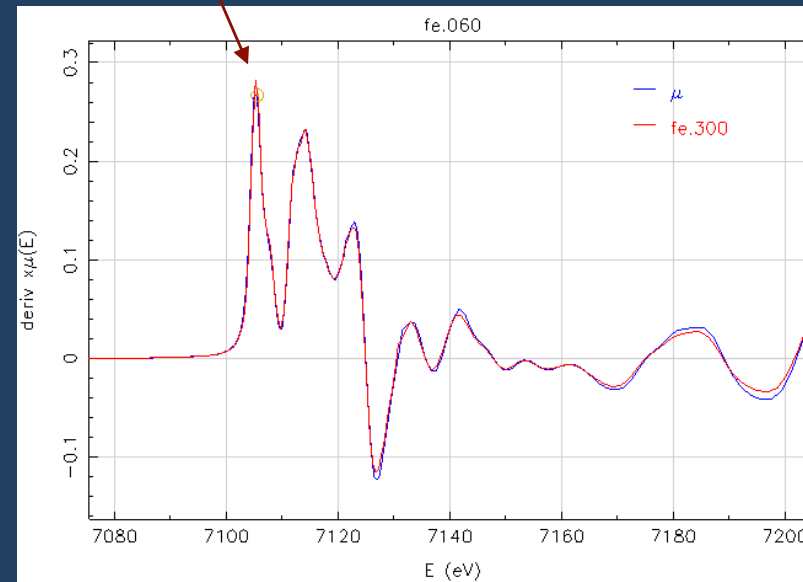
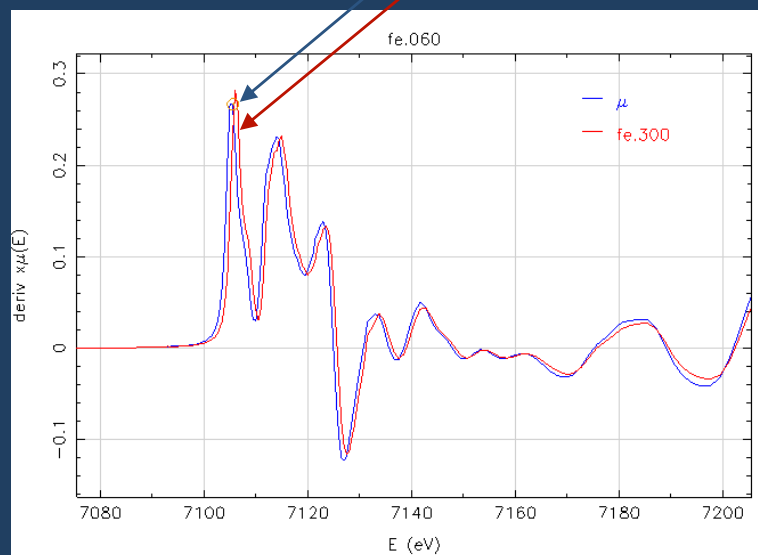
Restore value

Document section: aligning data

Return to the main window



E₀ appear shifted among the files



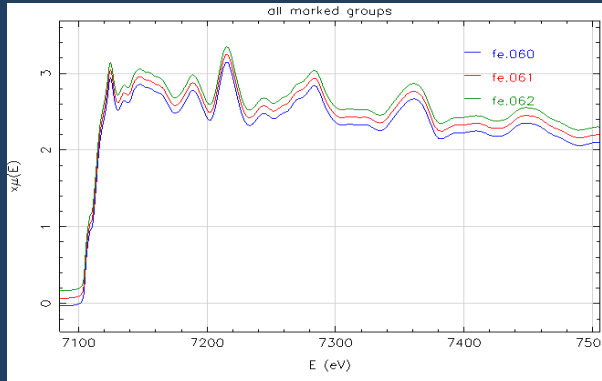
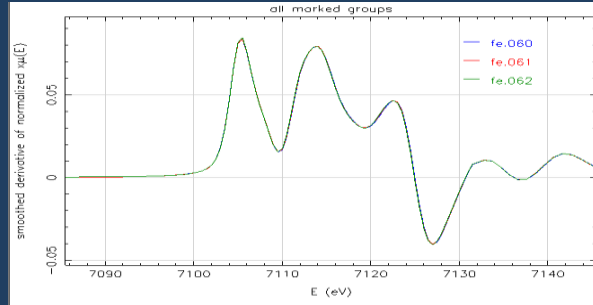
5: Data treatment: Merge several files

Merge Analysis - Settings Help

- Merge marked data in $\mu(E)$
- Merge marked data in $\text{norm}(E)$
- Merge marked data in $\chi(k)$

Weight by importance

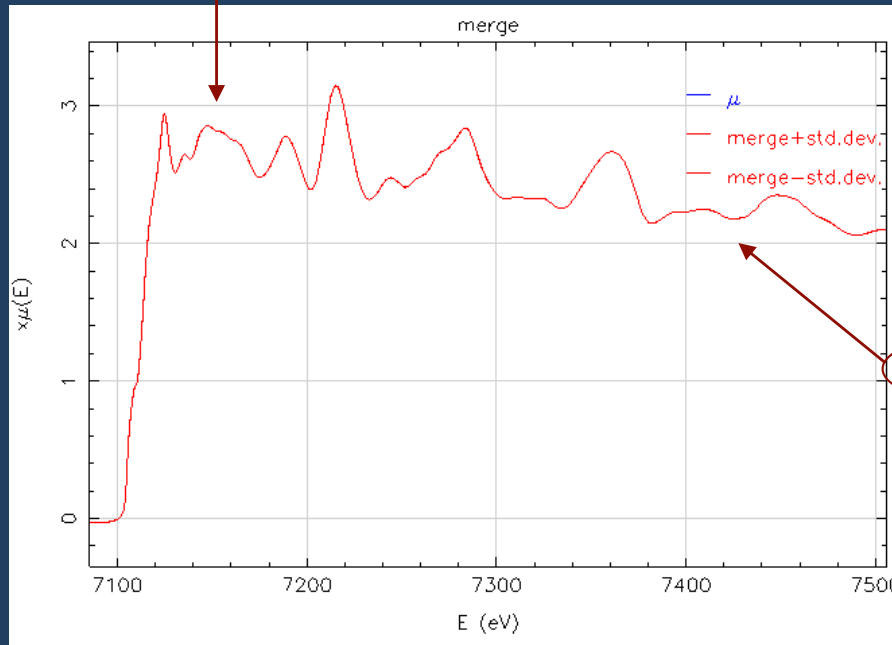
Weight by χ_{noise}



modified

- fe.301
- fe.060
- fe.061
- fe.062
- fe.150
- fe.151
- fe.300

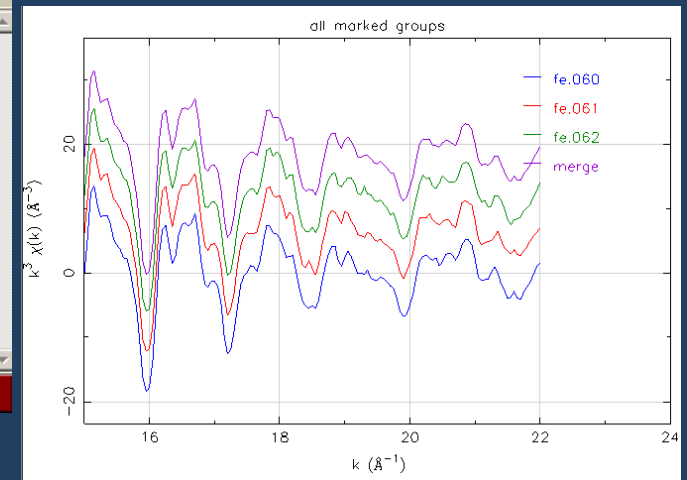
Fe 60 are aligned



modified

- fe.301
- fe.060
- fe.061
- fe.062
- fe.150
- fe.151
- fe.300
- merge

E k R q kq



Exercise:

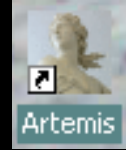
1. Read Fe Files
2. Align Fe files on order to have the same E_0
3. Merge files having the same T
4. Save $\chi(k)$ of merged files, these will be used for the structural analysis



Structural refinement

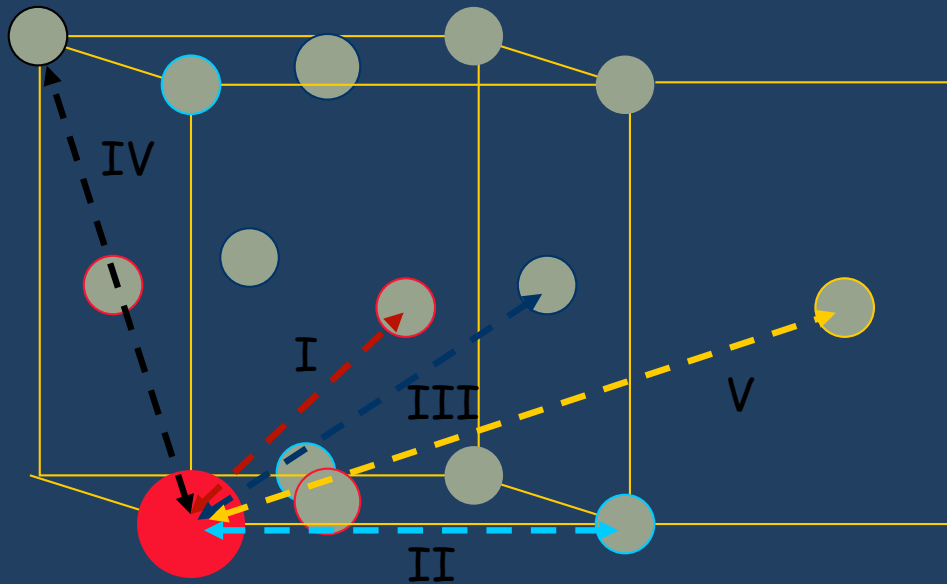


Structural model(s)



Cu-fcc

metal
SPG: fcc, f m 3 m (# 220)
a = 3.61 Å
Cu 0.0 0.0 0.0



Sh	R	N	$R_{Cu}(Å)$
I:	$a/\sqrt{2}$	12	2.553
II:	a	6	3.610
III:	$a \cdot \sqrt{1.5}$	24	4.421
IV:	$a \cdot \sqrt{2}$	12	5.105
V:	$a \cdot \sqrt{2.5}$	24	5.708
....			

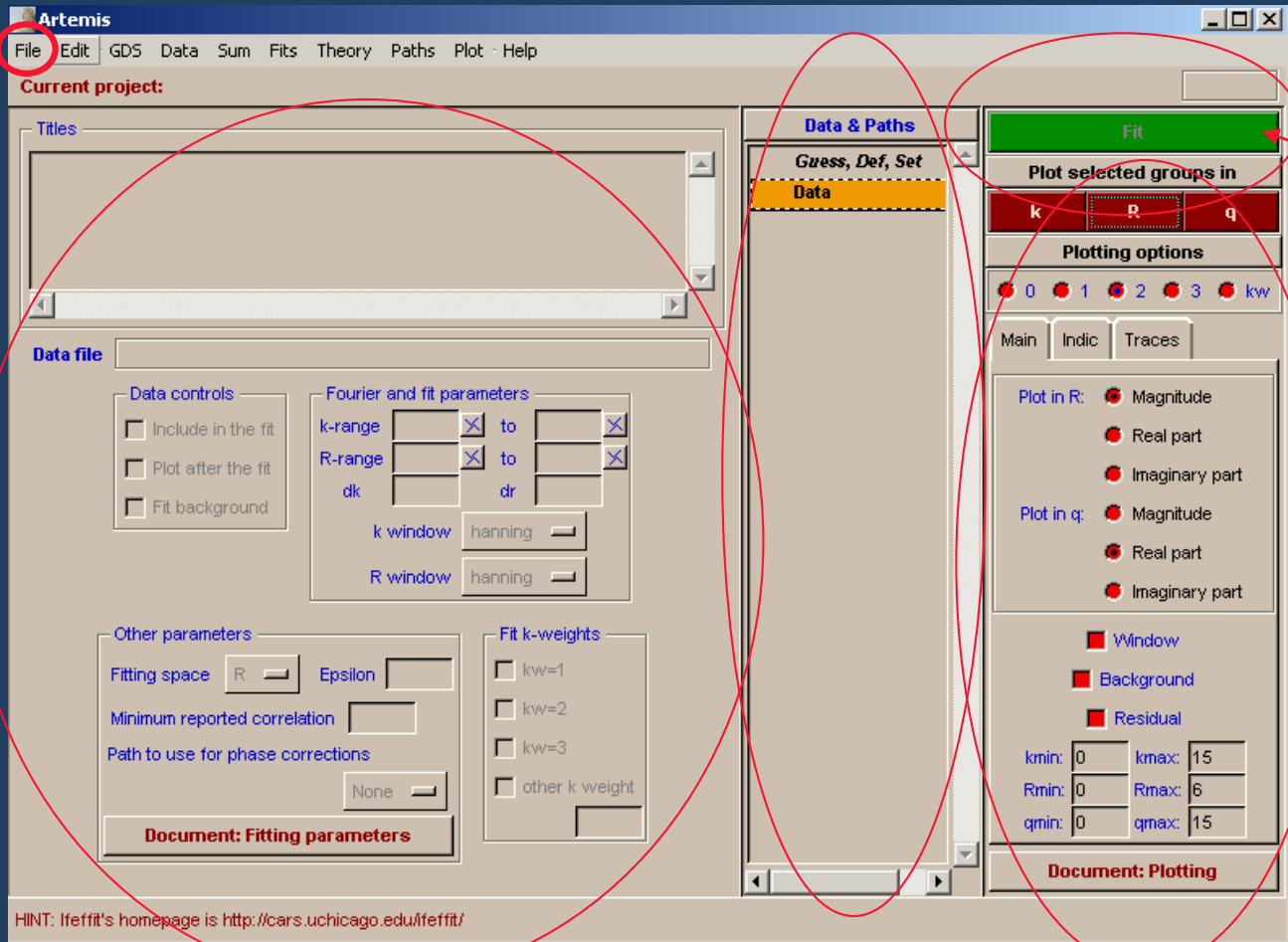


Structural model & Data refinement

Start ARTEMIS program

Open Cu.inp file from the Cu directory

Start the refinement



Depends on what is highlighted in the Data & Paths panel

Controls for plotting

Artemis

File Edit - GDS Data Sum Fits Theory Paths Plot - Help

Current project: modified

Atoms feff.inp Interpretation

Titles

name: copper
formula: Cu
sites: Cu1

Space group f m 3 m

	Core	EI	X	Y	Z	
A	1		Cu	0.00000	0.00000	0.00000
B						
C						
Alpha				90.00000		
Beta						
Gamma						
Cluster size				6.00000		
Edge				K		
Shift vector				0	0	0

Edit selected site

Element: Tag: Define

Z: New

Run Atoms Document: Atoms

Importing crystallography data done!

Data & Paths

Guess, Def, Set

Data

FEFF0

Fit

Plot selected groups in

k R q

Plotting options

0 1 2 3 kw

Main Indic Traces

Plot in R: Magnitude
 Real part
 Imaginary part

Plot in q: Magnitude
 Real part
 Imaginary part

Window
 Background
 Residual

kmin: 0 kmax: 15
Rmin: 0 Rmax: 6
qmin: 0 qmax: 15

Document: Plotting

Artemis

File Edit - GDS Data Sum Fits Theory Paths Plot - Help

Current project:

Atoms feff.inp Interpretation

Data & Paths

Guess, Def, Set

Data

FEFF0

```
* This feff6 input file was generated by Artemis 0.
* Atoms written by and copyright (c) Bruce Ravel, 1
*
* --- * --- * --- * --- * --- * --- * --- * --- * --- *
* total mu*x=1:    4.06 microns, unit edge step
* specific gravity = 8.971
*
* Normalization correction:  0.00046 ang^2
*
* -----
* The following crystallographic data were used:
*
* ti
* ti
* ti
* ti
* ti
* ti
* ti
* sp
* a
* al
```

Artemis: Question...

How many feff paths do you want to import right now?

No paths Just the first The first 10 All paths

Run Feff Document: Feff and its input file

Running atoms ... done!

It builds the cluster

2

Sh	R	N	$R_{Cu}(A)$
I:	$a/\sqrt{2}$	12	2.553
II:	a	6	3.610
III:	$a \cdot \sqrt{1.5}$	24	4.421
IV:	$a \cdot \sqrt{2}$	12	5.105
V:	$a \cdot \sqrt{2.5}$	24	5.708
....			

Atoms feff.inp Interpretation

```
* this list contains 79 atom
```

y	z	ipot	tag	dis
000	0.00000	0.00000	0 Cu1	0.00000
500	1.80500	0.00000	1 Cu1_1	2.55266
500	1.80500	0.00000	1 Cu1_1	2.55266
500	-1.80500	0.00000	1 Cu1_1	2.55266
500	-1.80500	0.00000	1 Cu1_1	2.55266
500	0.00000	1.80500	1 Cu1_1	2.55266
500	0.00000	1.80500	1 Cu1_1	2.55266
000	1.80500	1.80500	1 Cu1_1	2.55266
000	-1.80500	1.80500	1 Cu1_1	2.55266
500	0.00000	-1.80500	1 Cu1_1	2.55266
500	0.00000	-1.80500	1 Cu1_1	2.55266
000	1.80500	-1.80500	1 Cu1_1	2.55266
000	-1.80500	-1.80500	1 Cu1_1	2.55266
000	0.00000	0.00000	1 Cu1_2	3.61000
000	0.00000	0.00000	1 Cu1_2	3.61000
000	3.61000	0.00000	1 Cu1_2	3.61000
000	-3.61000	0.00000	1 Cu1_2	3.61000
000	0.00000	3.61000	1 Cu1_2	3.61000
000	0.00000	-3.61000	1 Cu1_2	3.61000
000	1.80500	1.80500	1 Cu1_3	4.42133
000	1.80500	1.80500	1 Cu1_3	4.42133
500	3.61000	1.80500	1 Cu1_3	4.42133
500	3.61000	1.80500	1 Cu1_3	4.42133

4

Artemis: Question...

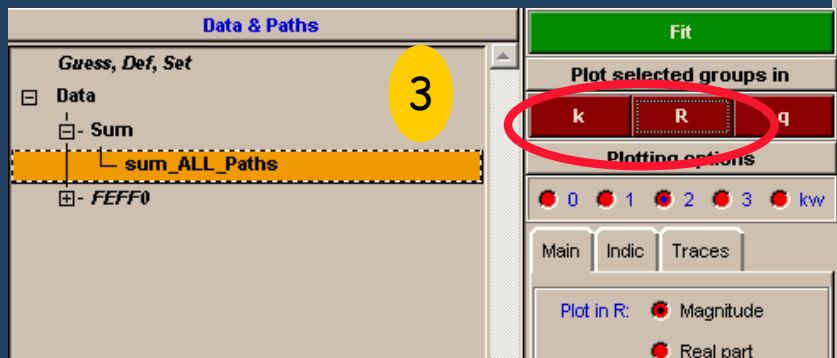
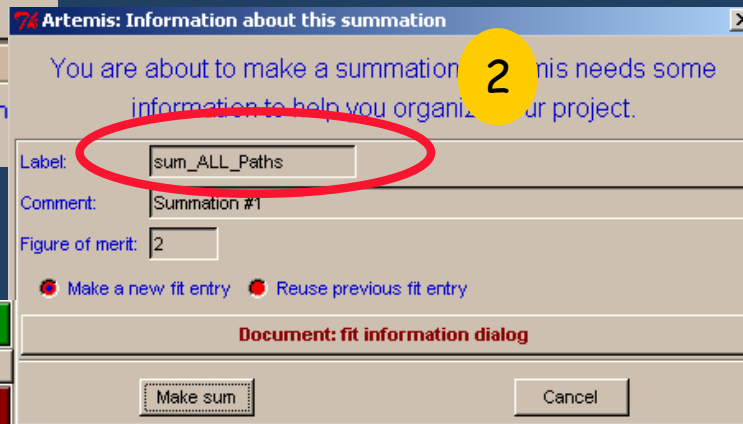
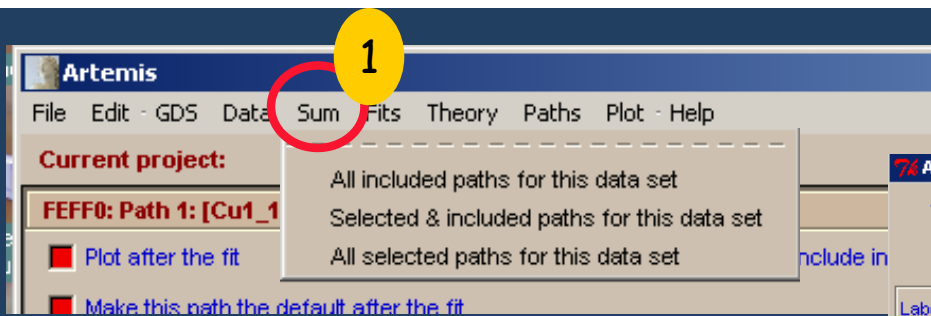
How many feff paths do you want to import right now?

No paths Just the first The first 10 All paths

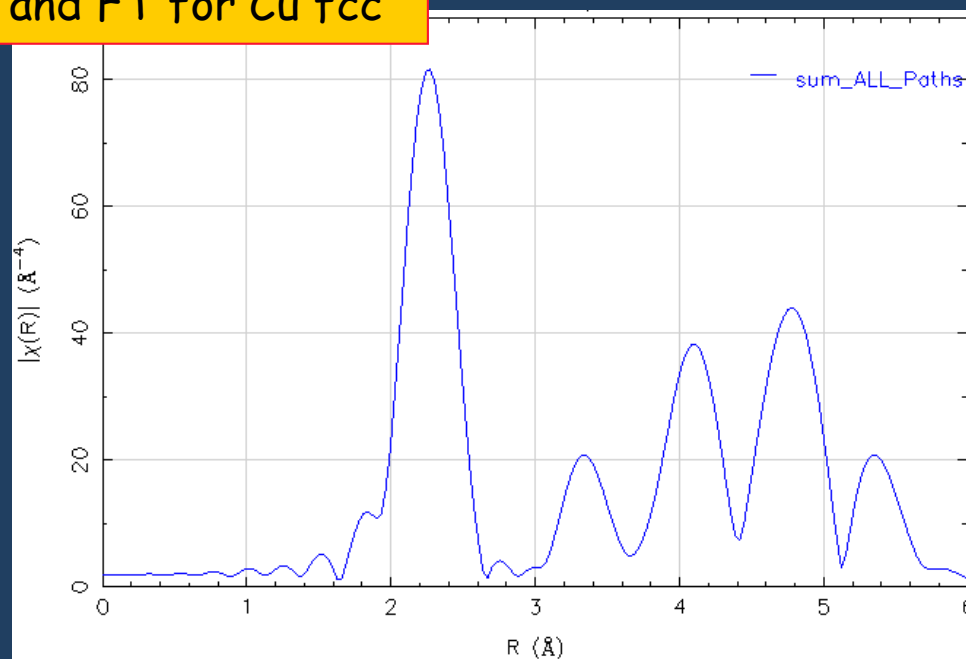
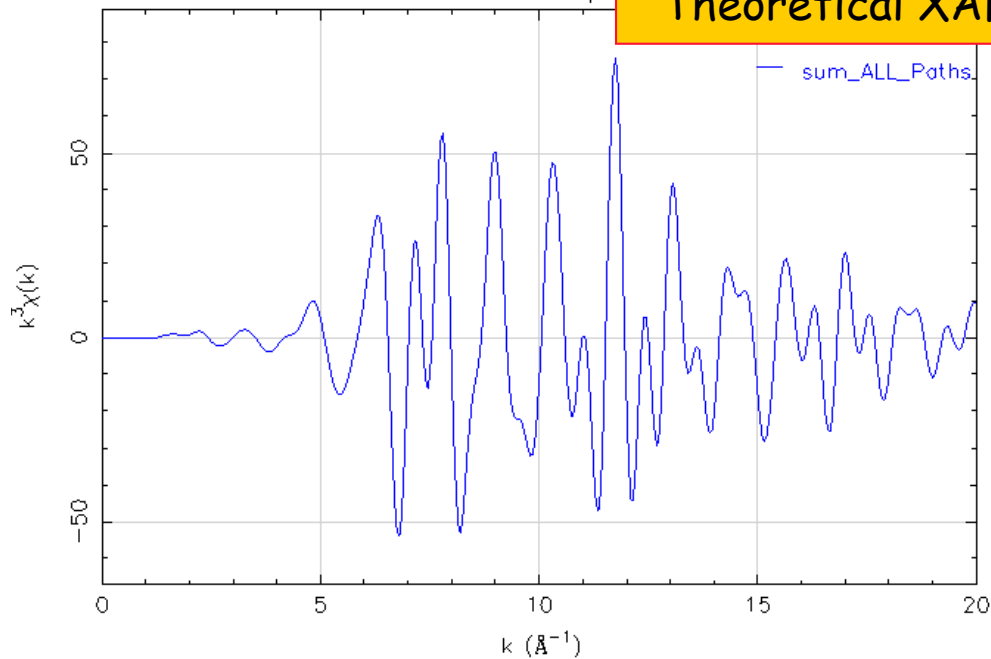
5

FEFF0

- Path 1: [Cu1_1]
- Path 2: [Cu1_2]
- Path 3: [Cu1_1 Cu1_4]
- Path 4: [Cu1_2 Cu1_1]
- Path 5: [Cu1_3]
- Path 6: [Cu1_1 Cu1_1]
- Path 7: [Cu1_3 Cu1_1]
- Path 8: [Cu1_4]
- Path 9: [Cu1_1 Cu1_1]
- Path 10: [Cu1_4 Cu1_1]
- Path 11: [Cu1_1 [+] Cu1_1]
- Path 12: [Cu1_1 [+] Cu1_1]
- Path 14: [Cu1_1 Cu1_4 Cu1_1]
- Path 15: [Cu1_1 Cu1_1 Cu1_1]
- Path 18: [Cu1_3 Cu1_1]



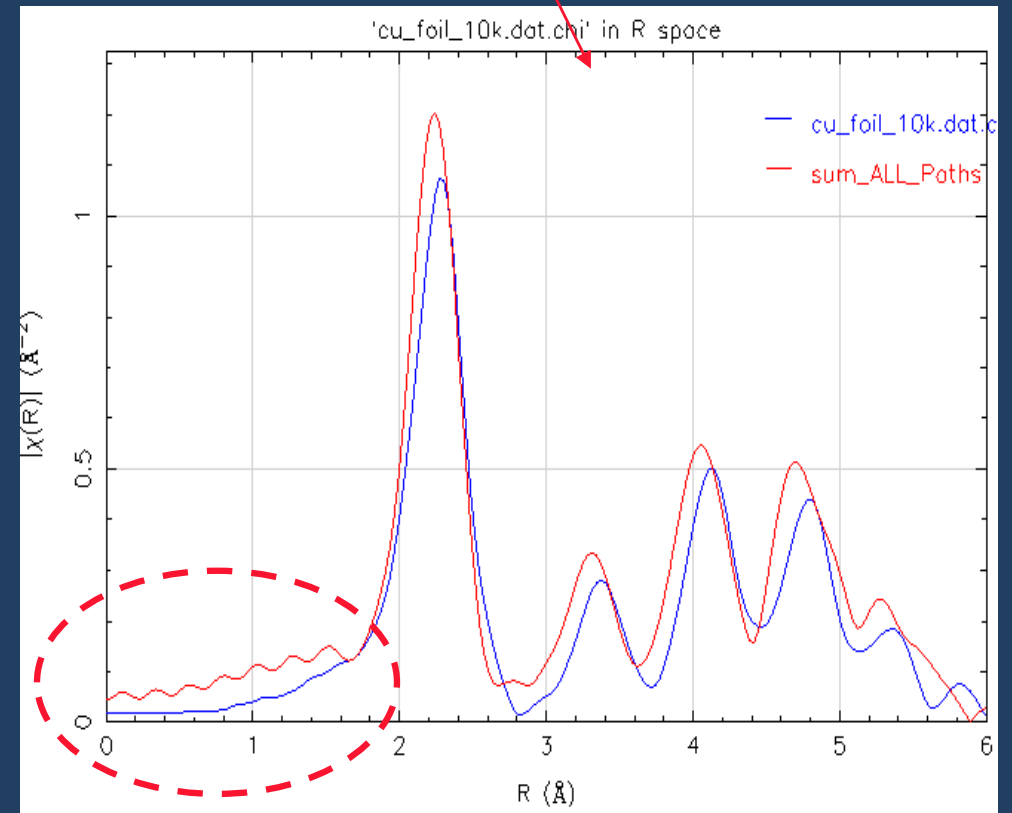
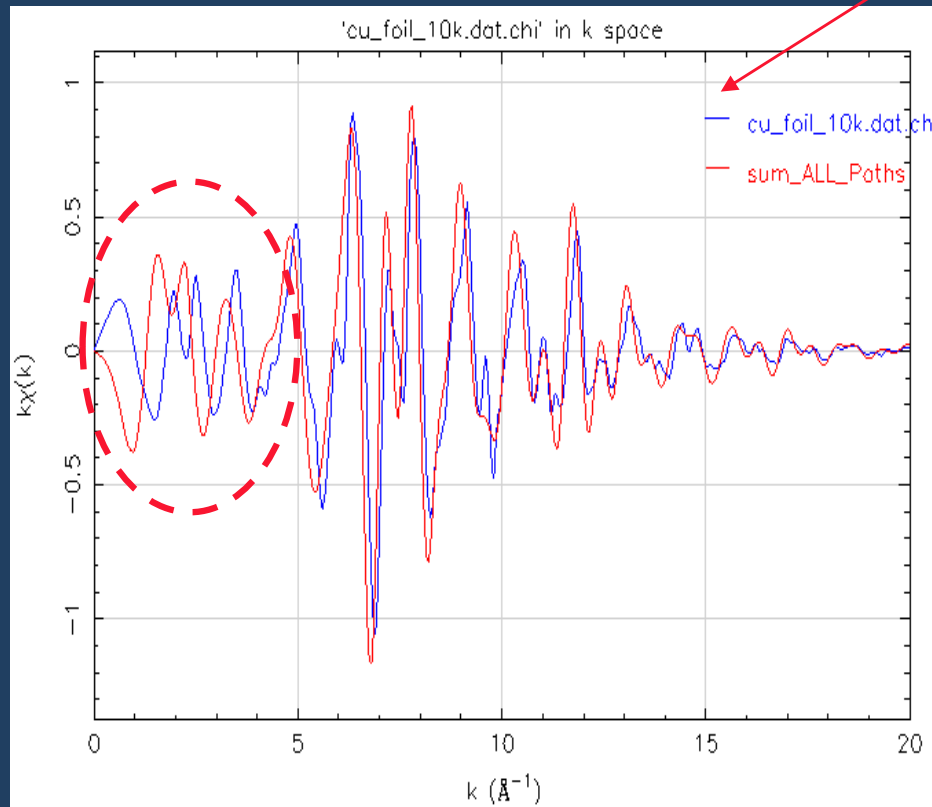
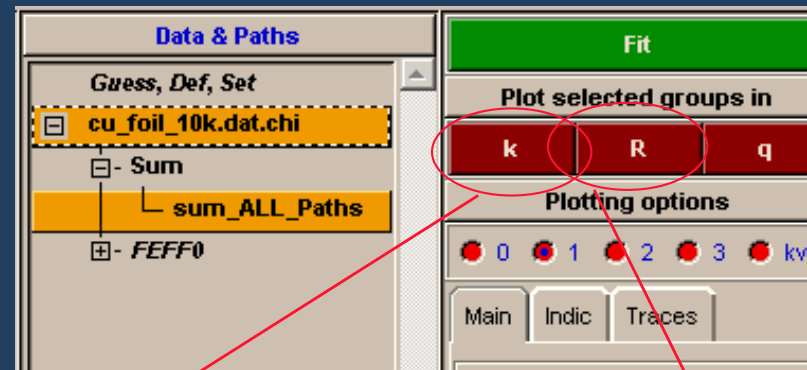
Theoretical XAFS and FT for Cu fcc



Compare model and experimental data

Open Cu010k.chi

Using CTRL key
select groups
for plot



1st shell analysis

remove all paths or
restart ARTEMIS

Right click

The screenshot shows the ARTEMIS software interface. On the left, a tree view under 'Data & Paths' shows a folder 'cu_foil_10k.d' containing 'Sum', 'sum_', and 'FEFF0'. A yellow box labeled 'Right click' points to 'FEFF0'. A context menu is open over 'FEFF0', listing options like 'View this feffNNNN.dat file', 'Show this path', 'Save this path as ...', 'Add math expression to each path', 'Clear math expression for each path', 'Include paths for fitting', 'Discard paths', 'Clone this feff path', 'Rename this path', 'Export these paths parameters ...', 'Add a feff path', and 'Extended path parameters'. The 'Discard paths' option is expanded, showing a sub-menu with 'Discard this path', 'For this feff calculation ...' (circled in red), and 'Discard selected paths'. The 'For this feff calculation ...' sub-menu includes 'discard all paths' (circled in red), 'discard all paths after current', 'discard all paths with more than N legs', 'discard all paths longer than R', and 'discard all paths with amplitude smaller than A'.

add 1st shell path to the list

select and Right click

The screenshot shows a table of scattering paths in the ARTEMIS software. The table has columns: '#', 'Deg.', 'Reff', 'amp.', 'fs', and 'Scattering Path'. The first four rows are highlighted in yellow. A context menu is open over the first row, listing options: 'Add feff0001.dat to the path list', 'Add and jump to feff0001.dat', 'Show geometry for', and 'View'.

#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00	[+]	Cu1_1 [+]
2	6	3.610	22.98	[+]	Cu1_2 [+]
3	48	3.829	10.59	[+]	Cu1_1 Cu1_1 [+]
4	48	4.358	8.65	[+]	Cu1_2 Cu1_1 [+]
5	84	4.401	55.41	[+]	Cu1_2 [+]

The screenshot shows the 'Data & Paths' panel in the ARTEMIS software. It displays a tree view under 'Guess, Def, Set' containing a folder 'cu_foil_10k.dat.chi' with sub-items 'Sum', 'sum_ALL_Paths', 'FEFF0', and 'Path 1: [Cu1_1]' (circled in red).

FEFF0: Path 1: [Cu1_1]

- Plot after the fit
- Make this path the default after the fit
- Include in the fit

[+] Cu1_1 [+]

```

2 legs Reff=2.5527 amp=100.000 degen=12
leg 1:  0.00000  -1.80500  1.80500  1  Cu
        rleg=2.5527  beta=180.000
leg 2:  0.00000   0.00000   0.00000  0  Cu
        rleg=2.5527  beta=180.000

```

Path parameter math expressions

label: _____ Path label

N: 12 X S02 amp S_0^2

delE0: enot ← Energy shift

delR: delr ← Distance correction

sigma^2: ss ← Debye Waller factor

Ei: _____

3rd: _____

Data & Paths

```

Guess, Def, Set
cu_foil_10k.dat.chi
├─ Sum
│  └─ sum_ALL_Paths
└─ FEFF0
    └─ Path 1: [Cu1_1]

```

Name Math Expression

#	Name	Math Expression
1	g: amp	1
2	g: enot	0
3	g: delr	0
4	g: ss	0.003

Data & Paths

```

Guess, Def, Set
cu_foil_10k.dat.chi
├─ Sum
│  └─ sum_ALL_Paths
└─ FEFF0
    └─ Path 1: [Cu1_1]

```

guess: optimized in the refinement

def: math expressions updated during the fit

set: numbers or expressions evaluated once at the fit beginning and not updated

Edit selected parameter

amp =

Guess Def Set Skip Restrain After

Undo edit New Grab Discard Hide

Document: Guess, Def, Set

Current project: E:\Duino_ago09\Examples\Cu_10K\artemis.apj

Titles

0

Data file cu_foil_10k.dat.chi

Data controls

- Include in the fit
- Plot after the fit
- Fit background

Fourier and fit parameters

k-range 3 to 18

R-range 1 to 3

dk 1 cr 0.0

k window Hanning

R window Hanning

Other parameters

Fitting space R Epsilon 0

Minimum reported correlation 0.25

Path to use for phase corrections None

Document: Fitting parameters

Fit k-weights

- kw=1
- kw=2
- kw=3
- other k weight

Data & Paths

```

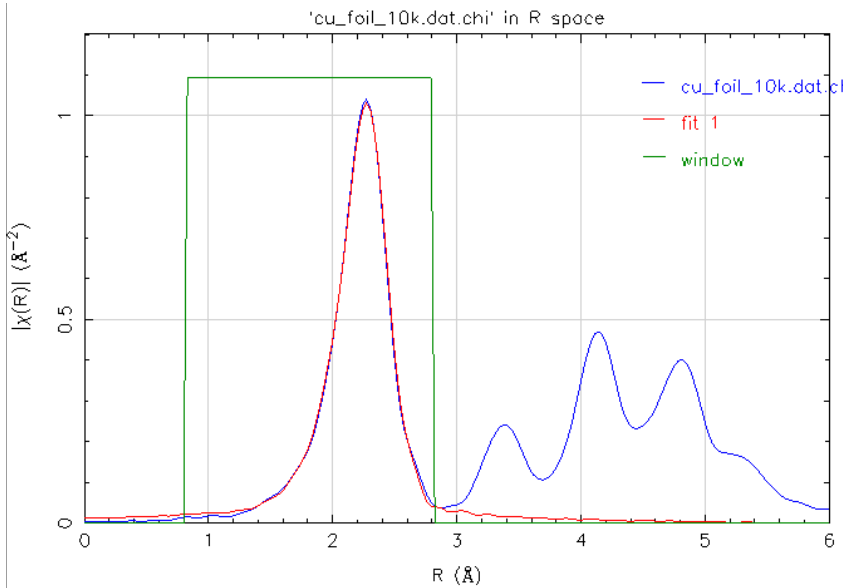
Guess, Def, Set
cu_foil_10k.dat.chi
├─ Sum
│  └─ sum_ALL_Paths
└─ FEFF0
    └─ Path 1: [Cu1_1]

```

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

The Data screen allow defining the fitting strategy and parameters





Examine log files

Current fit: fit 1

Choose a parameter: enot

Get parameters from Guess, Def, Set list

Parameter report

Calculations:

- Compute the average value
- Fit Einstein temp. to sigma*2 values
- Absorber: Scatterer:
- Prefer R-factor
- Prefer reduced chi-square
- Show y=0 in plot

Quick summaries of selected fits

Select all

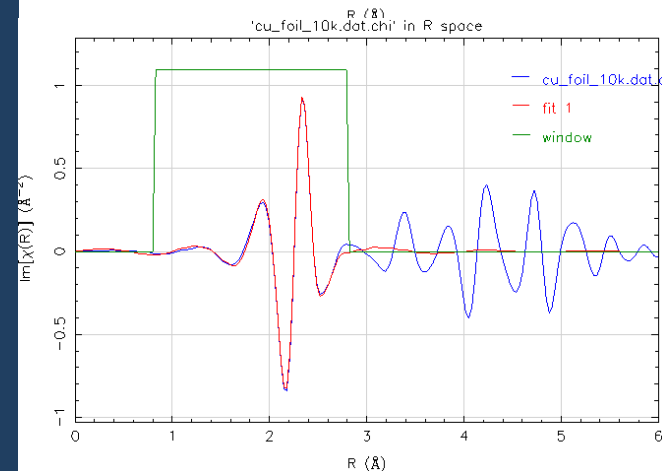
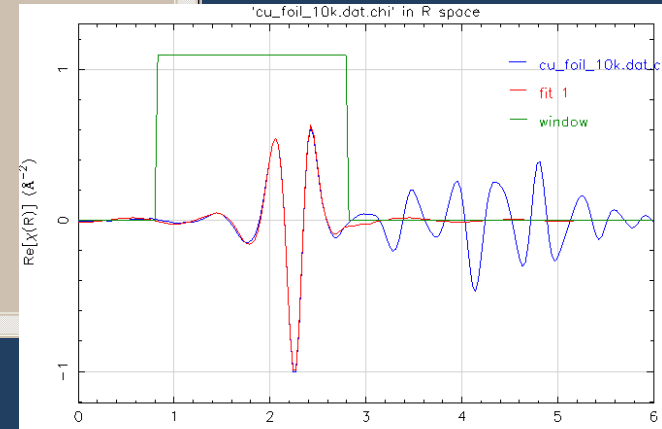
Clear selection

Document: Log viewer

Data & Paths

Guess, Def, Set

- cu_foil_10k.dot.chi
 - Fit
 - fit 1
 - FEFF0
 - Path 1: [Cu1_1]



$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left((\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right)$$

$$\chi_{\nu}^2 = \frac{\chi^2}{\nu}$$

$$\nu = N_{ind} - N_{var}$$

The refinement is performed on the Real and Imaginary parts of the FT

$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right]}{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i)))^2 \right]}$$

Absolute misfit between experimental data and theory

Structural results

Edit GDS Data Sum

- Write lfeffit script
- Display lfeffit buffer Ctrl-1
- Display fit results Ctrl-2
- View files Ctrl-3
- View messages Ctrl-4
- Display echo buffer Ctrl-5
- Write in journal Ctrl-6
- Edit project properties Ctrl-7
- Compact project
- Edit preferences

Artemis palettes

lfeffit Results Files Messages Echo Journal Properties

Results from the last fit

Raw log file Save

Independent points	=	18.687500000
Number of variables	=	4.000000000
Chi-square	=	92.986879023
Reduced Chi-square	=	6.331021550
R-factor	=	0.000735237
Measurement uncertainty (k)	=	0.001028657
Measurement uncertainty (R)	=	0.004036509
Number of data sets	=	1.000000000

Guess parameters +/- uncertainties (initial guess):

amp	=	0.9199910	+/-	0.0211700	(1.0000)
enot	=	5.4482800	+/-	0.2569030	(0.0000)
delr	=	-0.0046610	+/-	0.0015030	(0.0000)
ss	=	0.0035760	+/-	0.0001700	(0.0030)

Correlations between variables:

amp and ss	-->	0.8753
enot and delr	-->	0.8699

All other correlations are below 0.25

==== Data set >>cu_foil_10k.dat.chi<< =====

#	Name	Math Expression
1	g: amp	1
2	g: enot	0
3	g: delr	0
4	g: ss	00.003

right click

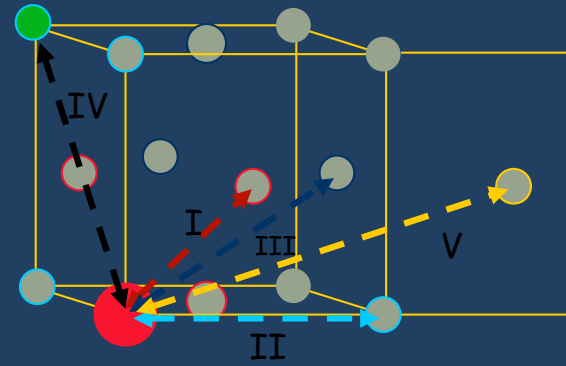
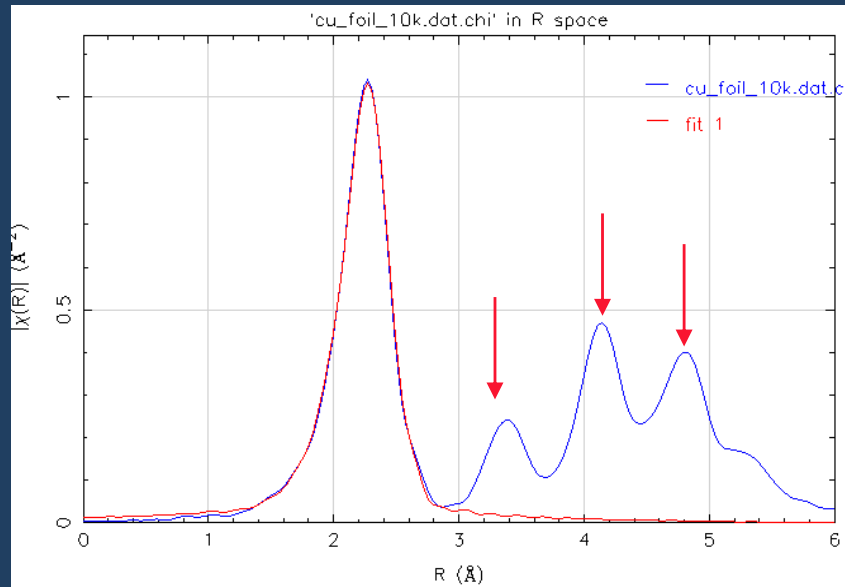
- Make "amp" ...
- Move "amp" ...
- Insert separator ...
- Copy "amp"
- Build restraint from "amp"
- Annotate "amp"
- Grab best fit for "amp"
- Find where "amp" is used
- Change name of "amp" globally
- Discard "amp"

1	g: amp	0.919991 (0.021170)
2	g: enot	0
3	g: delr	0
4	g: ss	00.003

$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left((\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right)$$

$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i) - \Re\tilde{\chi}^{th}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i) - \Im\tilde{\chi}^{th}(r_i)))^2 \right]}{\sum_{i=1}^{N_{pts}} \left[(\Re(\tilde{\chi}^{exp}(r_i)))^2 + (\Im(\tilde{\chi}^{exp}(r_i)))^2 \right]}$$

Add new contributions



Atoms feff.inp Interpretation

Interpretation of the FEFF Calculation

TITLE name: copper
 # TITLE formula: Cu
 # TITLE sites: Cu1
 # TITLE refer1: Kittel, ISSP
 # TITLE refer2:

#	Deg.	Ref	amp.	fs	Scattering Path
1	12	2.553	100.00		[+] Cu1_1 [+]
2	6	3.610	22.98		[+] Cu1_2 [+]
3	48	3.829	10.59		[+] Cu1_1 Cu1_1 [+]
4	48	4.358	8.65		[+] Cu1_2 Cu1_1 [+]
5	24	4.421	55.41		[+] Cu1_3 [+]
6	48	4.763	10.63		[+] Cu1_1 Cu1_1 [+]
7	96	4.763	21.81		[+] Cu1_3 Cu1_1 [+]
8	12	5.105	18.94		[+] Cu1_4 [+]
9	12	5.105	8.46		[+] Cu1_1 Cu1_1 [+]
10	24	5.105	43.71	1	[+] Cu1_4 Cu1_1 [+]
11	12	5.105	8.21	1	[+] Cu1_1 [+] Cu1_1 [+]
12	12	5.105	3.57		[+] Cu1_1 [+] Cu1_1 [+]

Document: Feff interpretation

Single Scattering

MS + Focusing



Data & Paths

Guess, Def, Set

cu_foil_10k.dat.chi

Fit

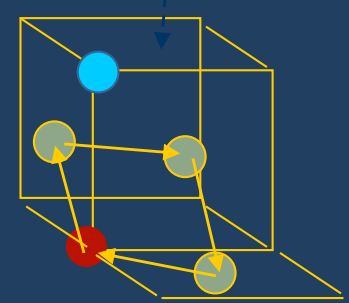
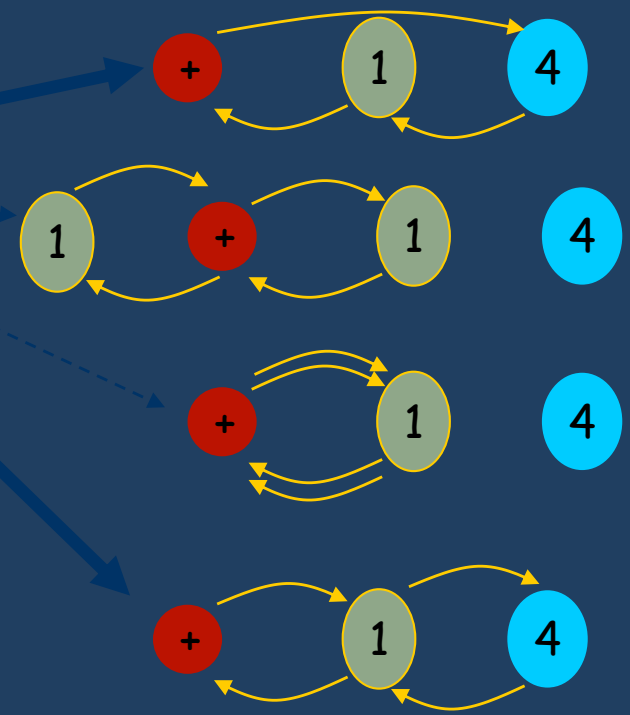
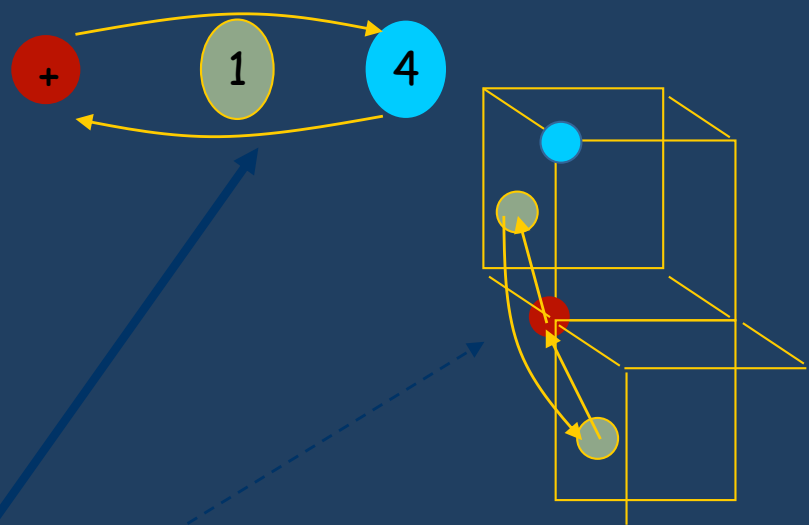
- fit K^1 wgt
- fit K^3 wgt
- fit K^3 wgt-multishel

FEFF0

- Path 1: [Cu1_1]
- Path 2: [Cu1_2]
- Path 5: [Cu1_3]
- Path 8: [Cu1_4]
- Path 10: [Cu1_4 Cu1_1]
- Path 11: [Cu1_1 [+] Cu1_1]
- Path 14: [Cu1_1 Cu1_4 Cu1_1]

MS paths

8	12	5.105	18.94	[+]	Cu1_4	[+]			
9	12	5.105	8.46	[+]	Cu1_1	Cu1_1	[+]		
10	24	5.105	43.71	1	[+]	Cu1_4	Cu1_1	[+]	
11	12	5.105	8.21	1	[+]	Cu1_1	[+]	Cu1_1	[+]
12	12	5.105	3.57	[+]	Cu1_1	[+]	Cu1_1	[+]	
14	12	5.105	32.80	2	[+]	Cu1_1	Cu1_4	Cu1_1	[+]
15	48	5.105	3.26	[+]	Cu1_1	Cu1_1	Cu1_1	[+]	



Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: E:/Duino_ago09/Examples/Cu_10K/Artemis.apj

FEFF0: Path 2: [Cu1_2]

Plot after the fit Include in the fit

Make this path the default after the fit

[+] Cu1_2 [+]

```

2 legs Reff=3.6100 amp=22.980 degen=6

leg 1: -3.61000 0.00000 0.00000 1 Cu
      rleg=3.6100 beta=180.000
leg 2: 0.00000 0.00000 0.00000 0 Cu
      rleg=3.6100 beta=180.000
  
```

Path parameter math expressions

label:

N: 6 S02: amp

delE0: enot

delR: delr2

sigma^2: ss2

Ei:

3rd:

4th:

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Fit
 - fit K^1wgt
 - fit K^3 wgt
 - FEFF0
 - Path 1: [Cu1_1]
 - Path 2: [Cu1_2]**
 - Path 5: [Cu1_3]
 - Path 8: [Cu1_4]

Document: Paths and path parameters

#	Name	Math Expression
1	s: amp	0.919991 (0.021170)
2	g: enot	5.448280 (0.256903)
3	g: delr	-0.004661 (0.001503)
4	g: delr2	-0.004661
5	g: delr3	-0.004661
6	g: delr4	-0.004661
7	g: ss	0.003576 (0.000170)
8	g: ss2	0.004
9	g: ss3	0.004
10	g: ss4	0.004

Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
 - Fit
 - fit K^1wgt
 - fit K^3 wgt
 - FEFF0
 - Path 1: [Cu1_1]
 - Path 2: [Cu1_2]
 - Path 5: [Cu1_3]
 - Path 8: [Cu1_4]

Fourier and fit parameters

k-range 3 to 18

R-range 0.8 to 2.8

dk 1 dr 0.0

k window Hanning

R window Hanning

In principle the same for each shell

In principle different for each shell

The used path must be inside the fit range

#	Name	Math Expression
1	s: amp	0.919991
2	g: enot	5.448280
3	g: delr	-0.004
4	g: delr2	-0.004661
5	g: delr3	-0.004
6	g: delr4	-.004
7	g: ss	0.003596 (0.000283)
8	g: ss2	0.005123 (0.001735)
9	g: ss3	0.004593 (0.000671)
10	g: ss4	0.028058 (0.043714)
11	g: ss5	0.004597 (0.000968)
12	g: ss6	0.006

```

Independent points      = 44.382812500
Number of variables    = 12.000000000
Chi-square             = 1816.763460636
Reduced Chi-square     = 56.102707590
R-factor               = 0.011517825
Measurement uncertainty (k) = 0.001028657
Measurement uncertainty (R) = 0.004036509
Number of data sets   = 1.000000000

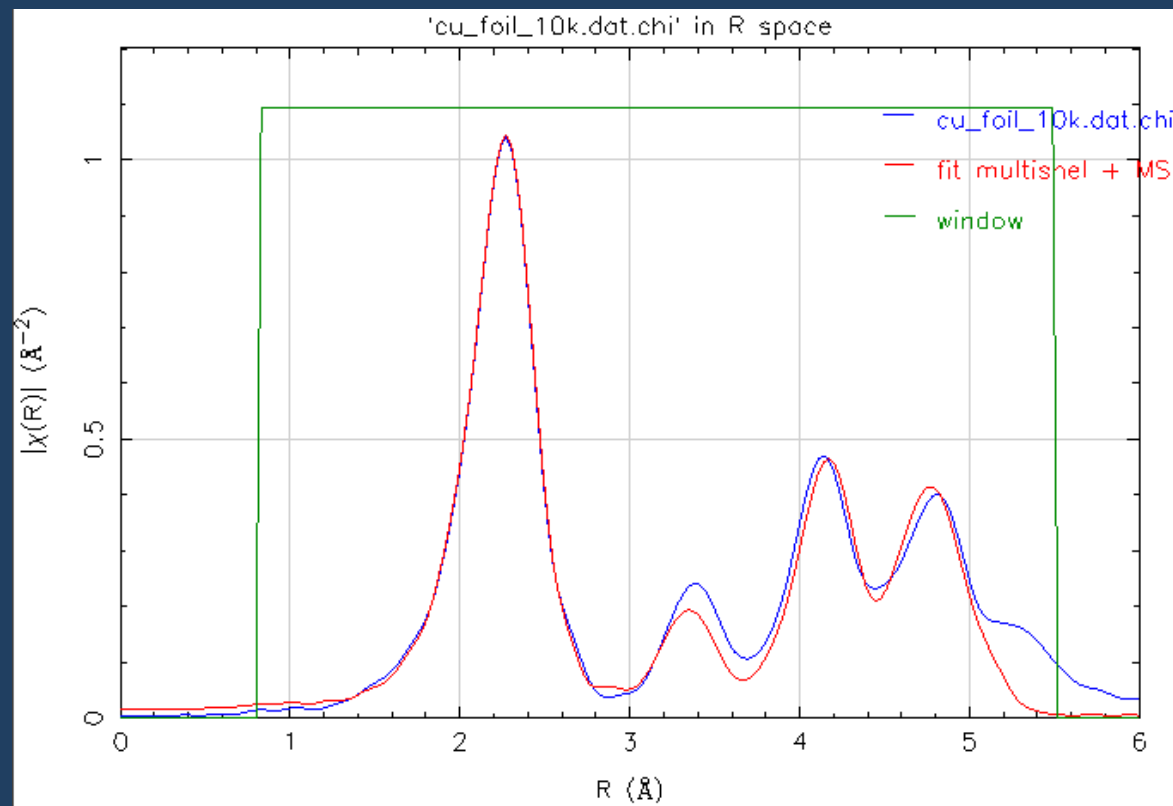
Guess parameters +/- uncertainties (initial guess):
enot      = 5.1036410 +/- 0.6089100
delr      = -0.0063660 +/- 0.0037480
delr2     = -0.0235000 +/- 0.0122330
delr3     = 0.0189970 +/- 0.0075140
delr4     = -0.0359130 +/- 0.0098410
ss        = 0.0035890 +/- 0.0002440
ss2       = 0.0044530 +/- 0.0013020
ss3       = 0.0045820 +/- 0.0005800
ss4       = 0.3097740 +/- 132.3316580
ss5       = 0.0151180 +/- 0.0062090
ss6       = -0.0003130 +/- 0.0019450
ss7       = 0.0073710 +/- 0.0022950

```

Correlations between variables:

ss6 and ss7	-->	-0.8579
enot and delr	-->	0.8206
delr4 and ss5	-->	-0.6973
enot and delr3	-->	0.6923
delr and delr3	-->	0.5675
enot and ss5	-->	0.4211
enot and delr2	-->	0.3650
delr and ss5	-->	0.3464
delr3 and delr4	-->	0.3298
delr and delr2	-->	0.2970
delr4 and ss6	-->	-0.2649
enot and ss7	-->	0.2521

All other correlations are below 0.25



#	Name	Math Expression
1	s: amp	0.919991
2	g: enot	5.448280
3	d: delr	delr2/sqrt(2)
4	g: delr2	-0.004661
5	d: delr3	delr2*sqrt(1.5)
6	d: delr4	delr2*sqrt(2)
7	g: ss	0.003596 (0.000283)
8	g: ss2	0.005123 (0.001735)
9	g: ss3	0.004593 (0.000671)
10	g: ss4	0.028058 (0.043714)
11	g: ss5	0.004597 (0.000968)
12	g: ss6	0.006
13	g: ss7	0.006964 (0.006210)

```

Independent points      =      44.382812500
Number of variables    =      9.000000000
Chi-square             =      3499.926965502
Reduced Chi-square     =      98.916019339
R-factor               =      0.022188660
Measurement uncertainty (k) =      0.001028657
Measurement uncertainty (R) =      0.004036509
Number of data sets    =      1.000000000

```

```

Correlations between variables:
ss6 and ss7      --> -0.9544
enot and delr2   -->  0.8598
ss4 and ss5      -->  0.6684
ss5 and ss7      -->  0.6517
ss4 and ss7      -->  0.6019
ss5 and ss6      --> -0.5675
ss4 and ss6      --> -0.4966

```

```

Guess parameters +/- uncertainties (initial guess):
enot      =      4.5727030 +/-      0.7133360
delr2     =      -0.0051830 +/-      0.0061960
ss        =      0.0036500 +/-      0.0003280
ss2       =      0.0046410 +/-      0.0018030
ss3       =      0.0047920 +/-      0.0007880
ss4       =      0.0239730 +/-      0.0373920
ss5       =      0.0057660 +/-      0.0014520
ss6       =      0.0010460 +/-      0.0058090
ss7       =      0.0060830 +/-      0.0044900

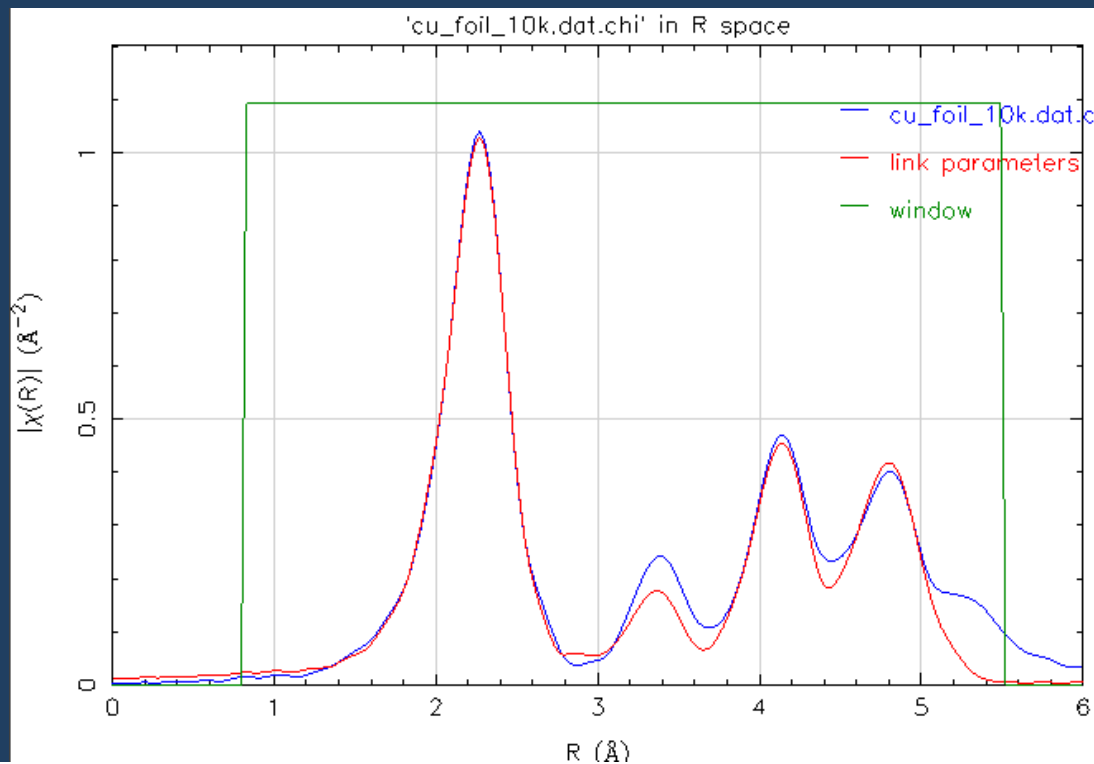
```

Edit selected parameter

delr3 = delr2*sqrt(1.5)

Guess
 Def
 Set
 Skip
 Restrain
 After

Document: Guess, Def, Set



Data & Paths Current project: E:\Duino_ago09\Examples\Cu_10K\Cu_10

#	Name	Math Expression
1	g: amp	0.907810 (0.096404)
2	g: enot	5.448280
3	g: delr	0.0
4	g: delr2	-0.004661
5	d: delr3	delr2*sqrt(1.5)
6	d: delr4	delr2*sqrt(2)
7	d: delr5	delr2*sqrt(2.5)
8	g: ss	0.003596 (0.000283)
9	g: ss2	0.005123 (0.001735)
10	g: ss3	0.004593 (0.000671)
11	g: ss4	0.028058 (0.043714)
12	g: ss5	0.004597 (0.000968)
13	g: ss6	0.006
14	g: ss7	0.006964 (0.006210)
15	g: ss8	0.006964 (0.006210)

Independent points = 48.178710937
 Number of variables = 12.000000000
 Chi-square = 8110.229963402
 Reduced Chi-square = 224.171335939
 R-factor = 0.000045721
 Measurement uncertainty (k) = 0.000533874
 Measurement uncertainty (R) = 0.445387356
 Number of data sets = 1.000000000

Guess parameters +/- uncertainties (initial guess):

amp	=	0.9054050	+/-	0.0941340
enot	=	3.7197170	+/-	0.3651800
delr	=	-0.0094960	+/-	0.0028930
delr2	=	-0.0009550	+/-	0.0034220
ss	=	0.0034400	+/-	0.0004310
ss2	=	0.0048280	+/-	0.0005880
ss3	=	0.0048200	+/-	0.0004620
ss4	=	0.0355080	+/-	0.1148830
ss5	=	0.0047690	+/-	0.0009910
ss6	=	0.0022460	+/-	0.0040870
ss7	=	0.0078980	+/-	0.0043780
ss8	=	0.0052190	+/-	0.0006400

Data file cu_foil_10k.dat.chi

Data controls

Include in the fit
 Plot after the fit
 Fit background

Fourier and fit parameters

k-range: 3 to 18
 R-range: 0.8 to 5.9
 dk: 1 dr: 0.0
 k window: Hanning
 R window: Hanning

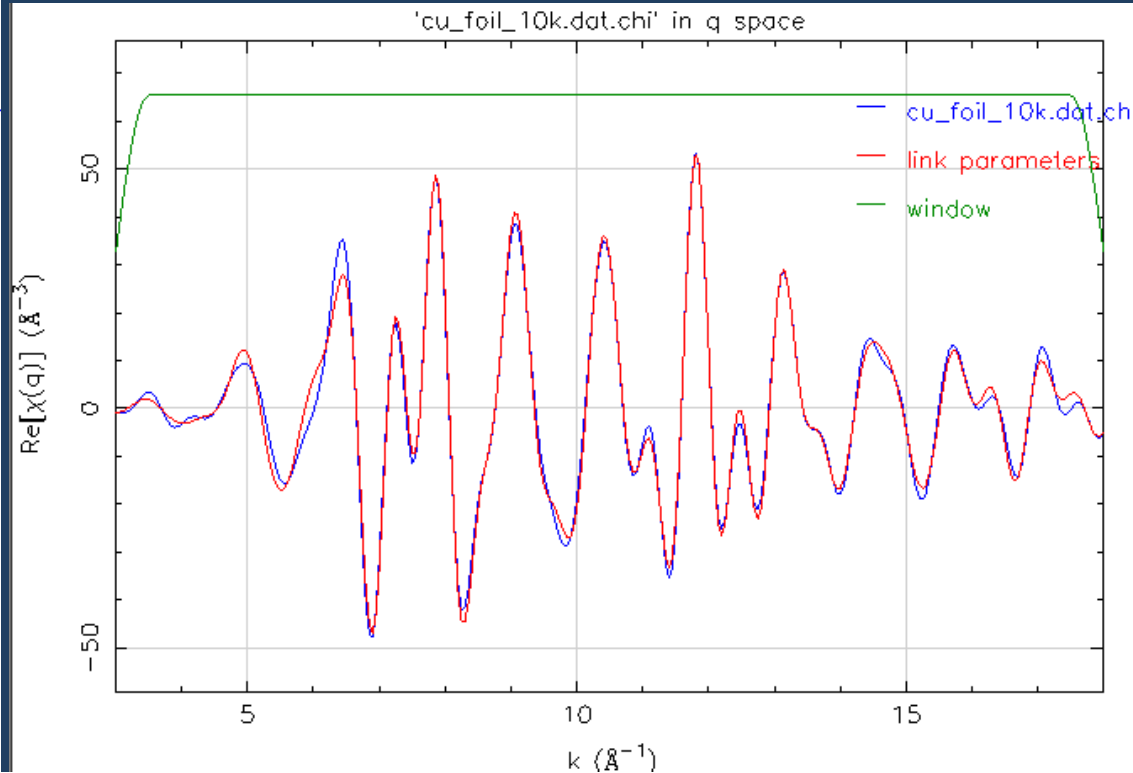
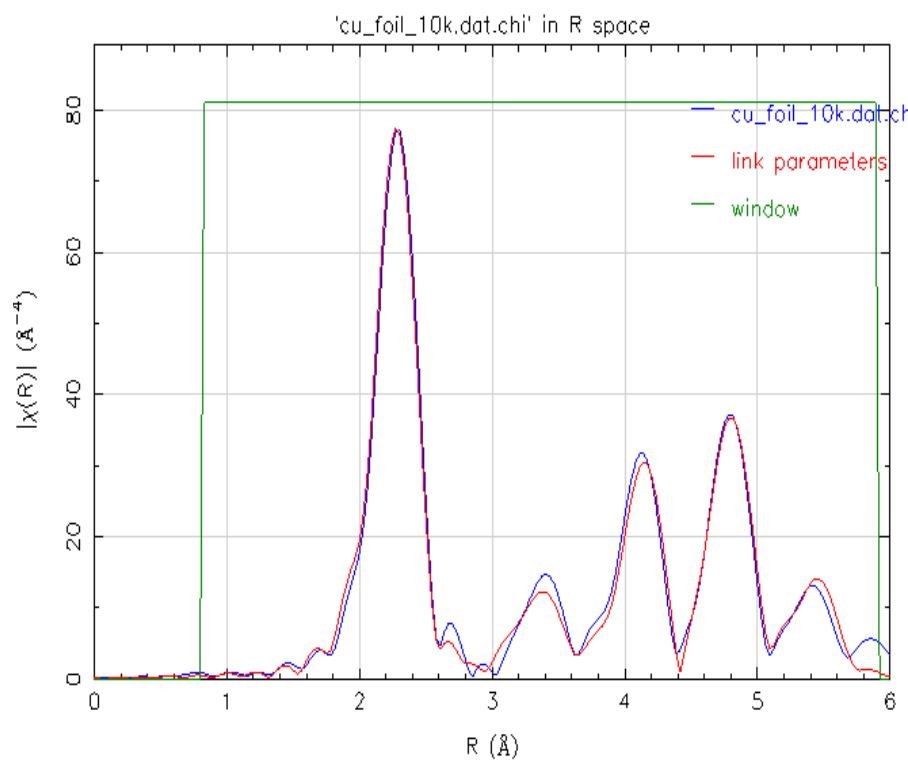
Other parameters

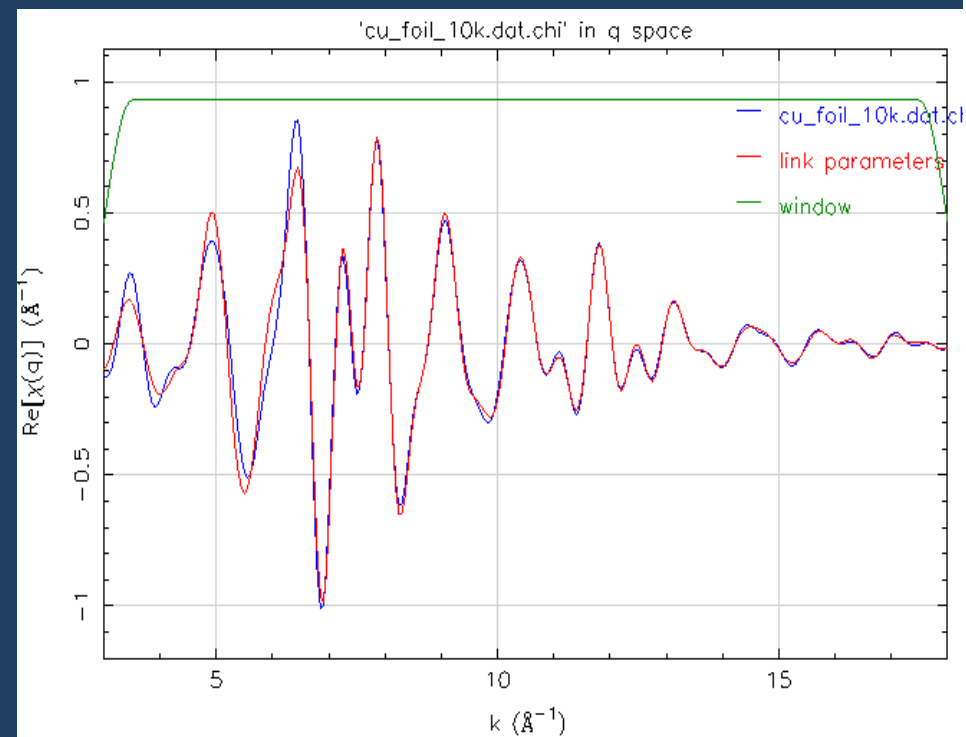
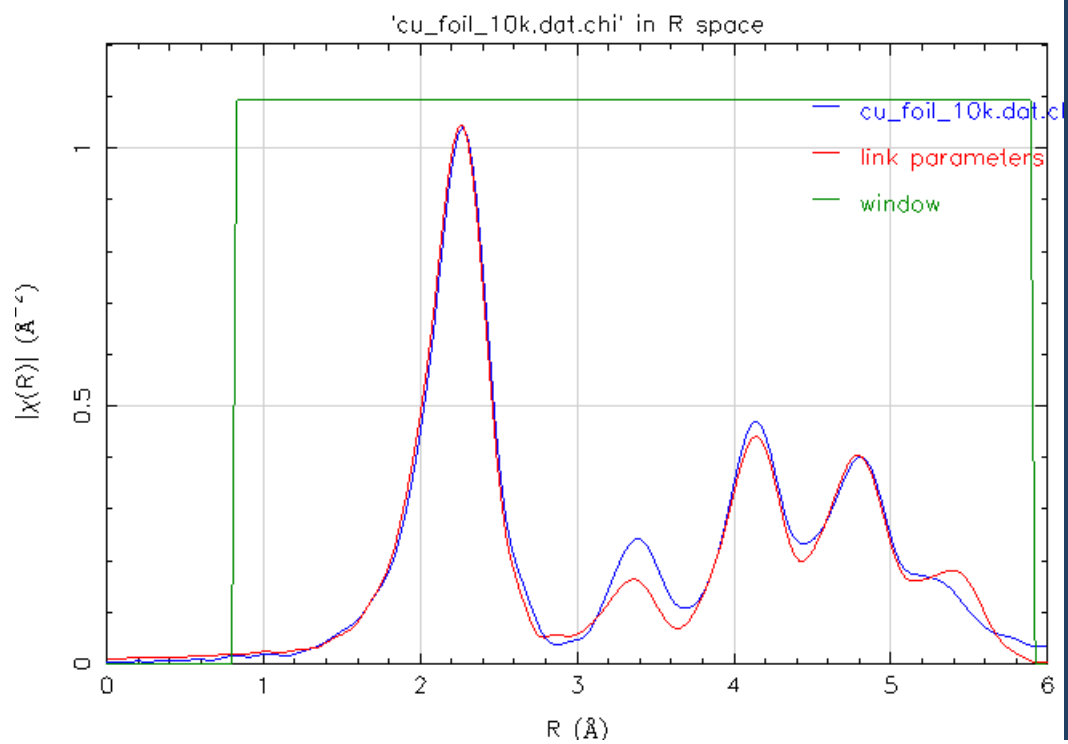
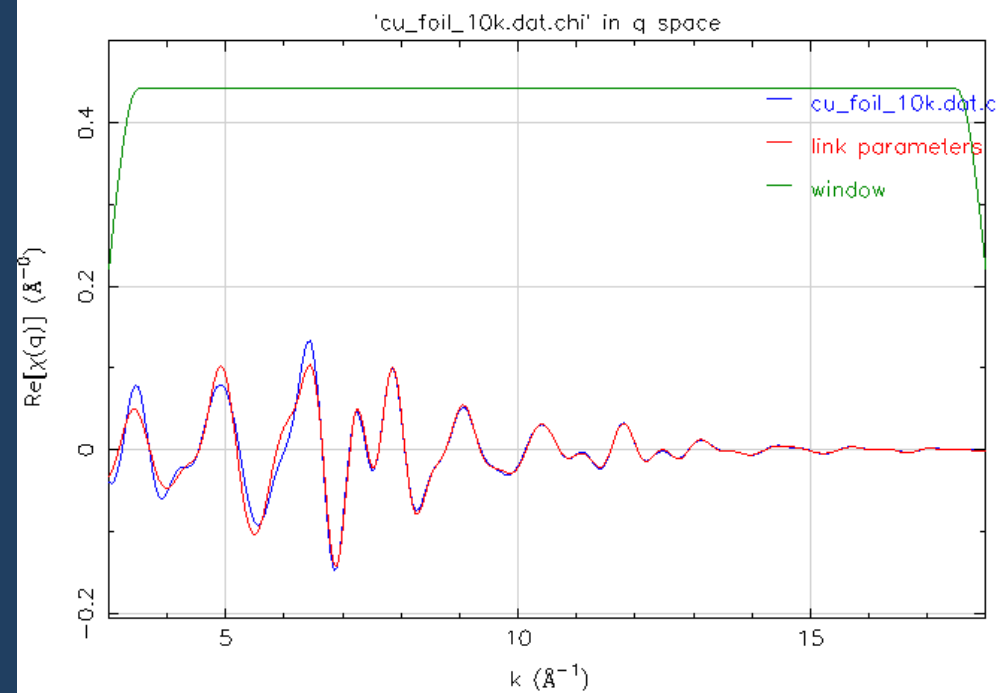
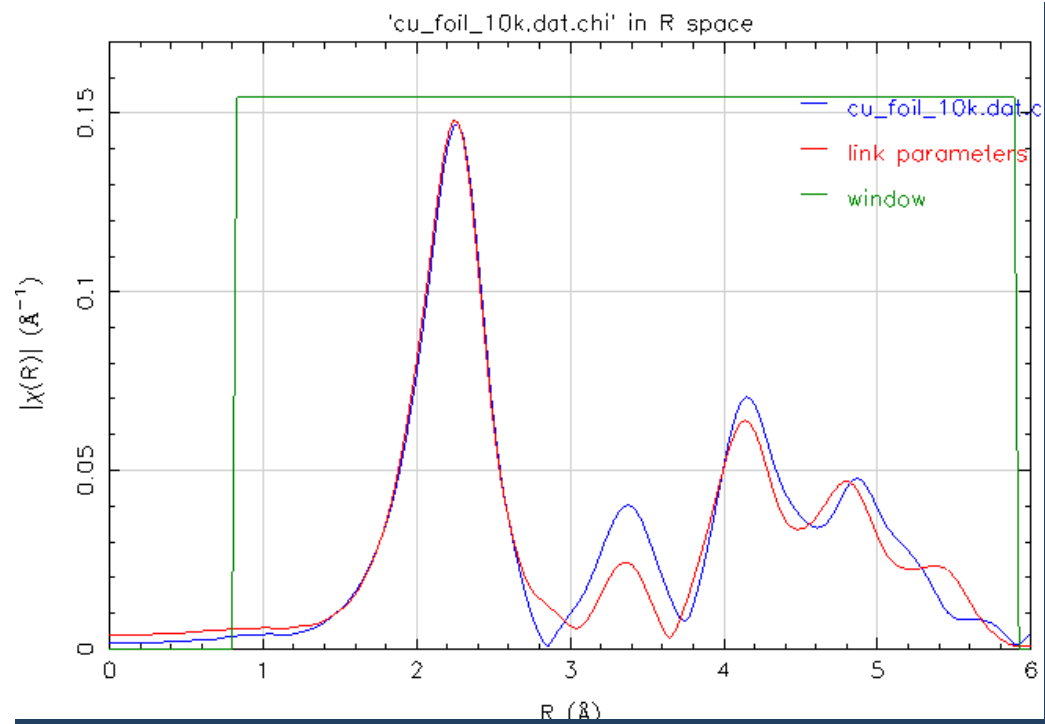
Fitting space: R Epsilon: 0
 Minimum reported correlation: 0.25
 Path to use for phase corrections: None

Fit k-weights

kw=1
 kw=2
 kw=3
 other kweight

Document: Fitting parameters





it's your work now!

a. amorphous Ge

b. GeO

c. Pt