The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2332-19

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

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XAS data analysis

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Introduction to the EXAFS data analysis

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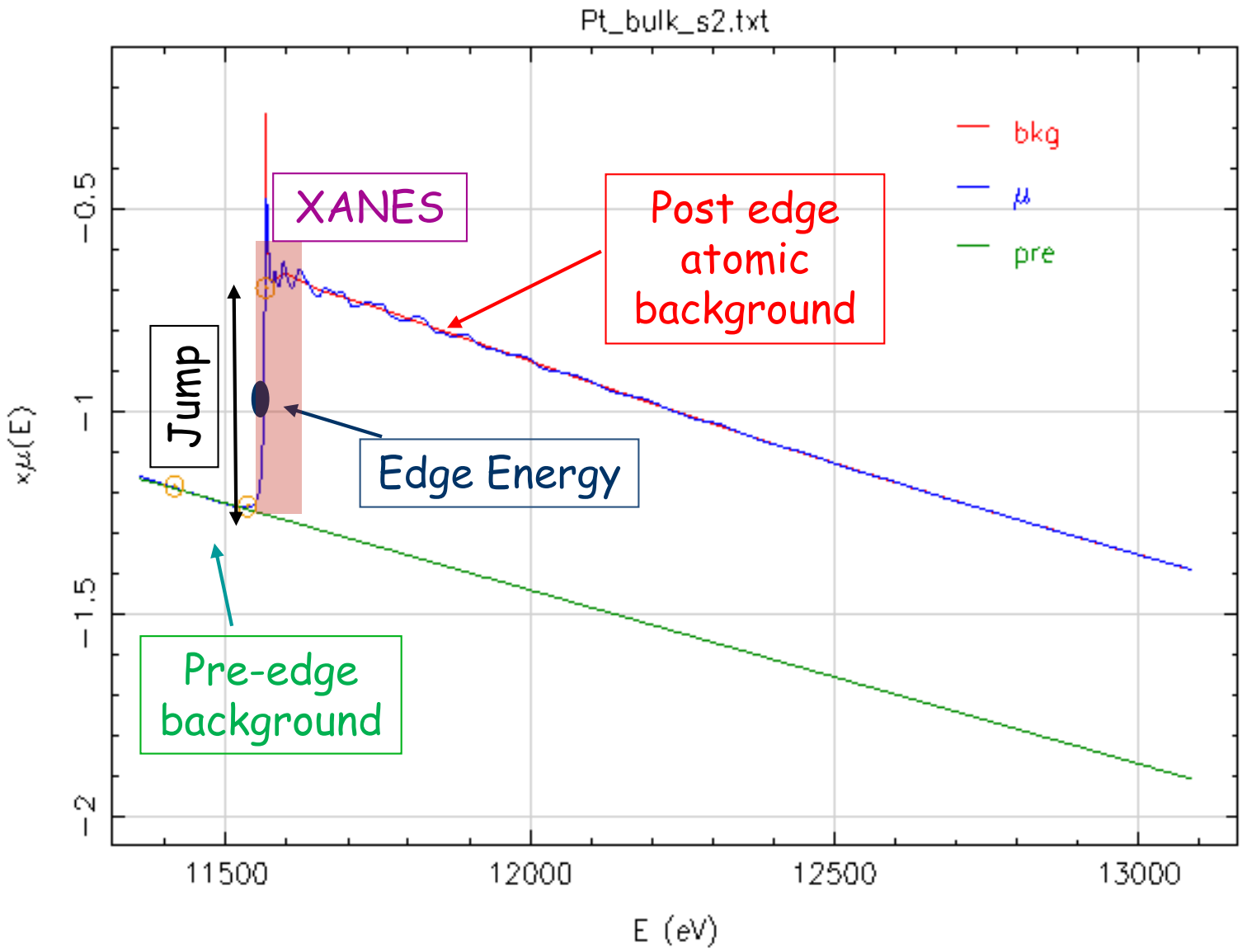
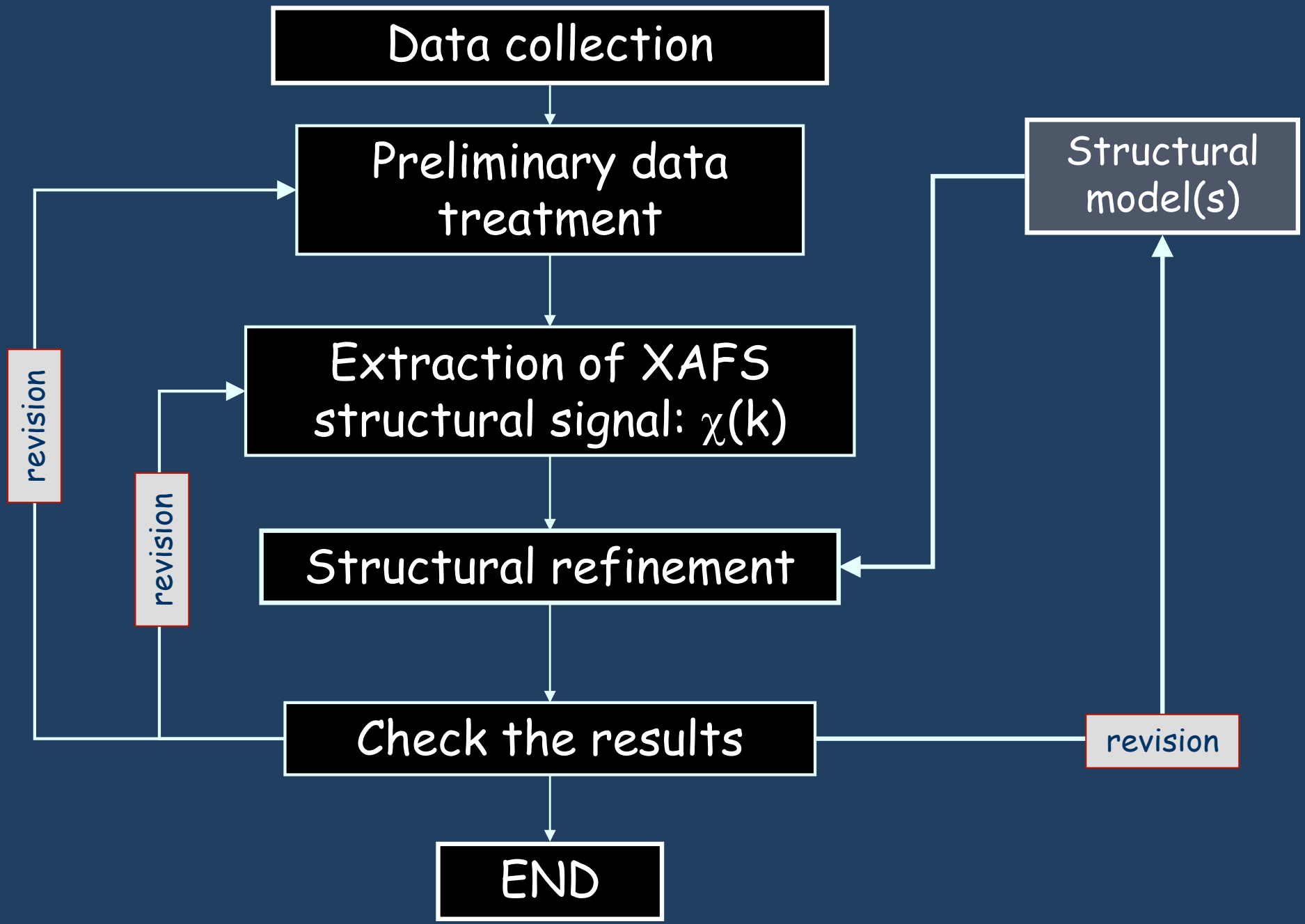
Material almost integrally taken from Carlo Meneghini: EXAFS tutorial at Synchrotron Radiation school of Duino 2011

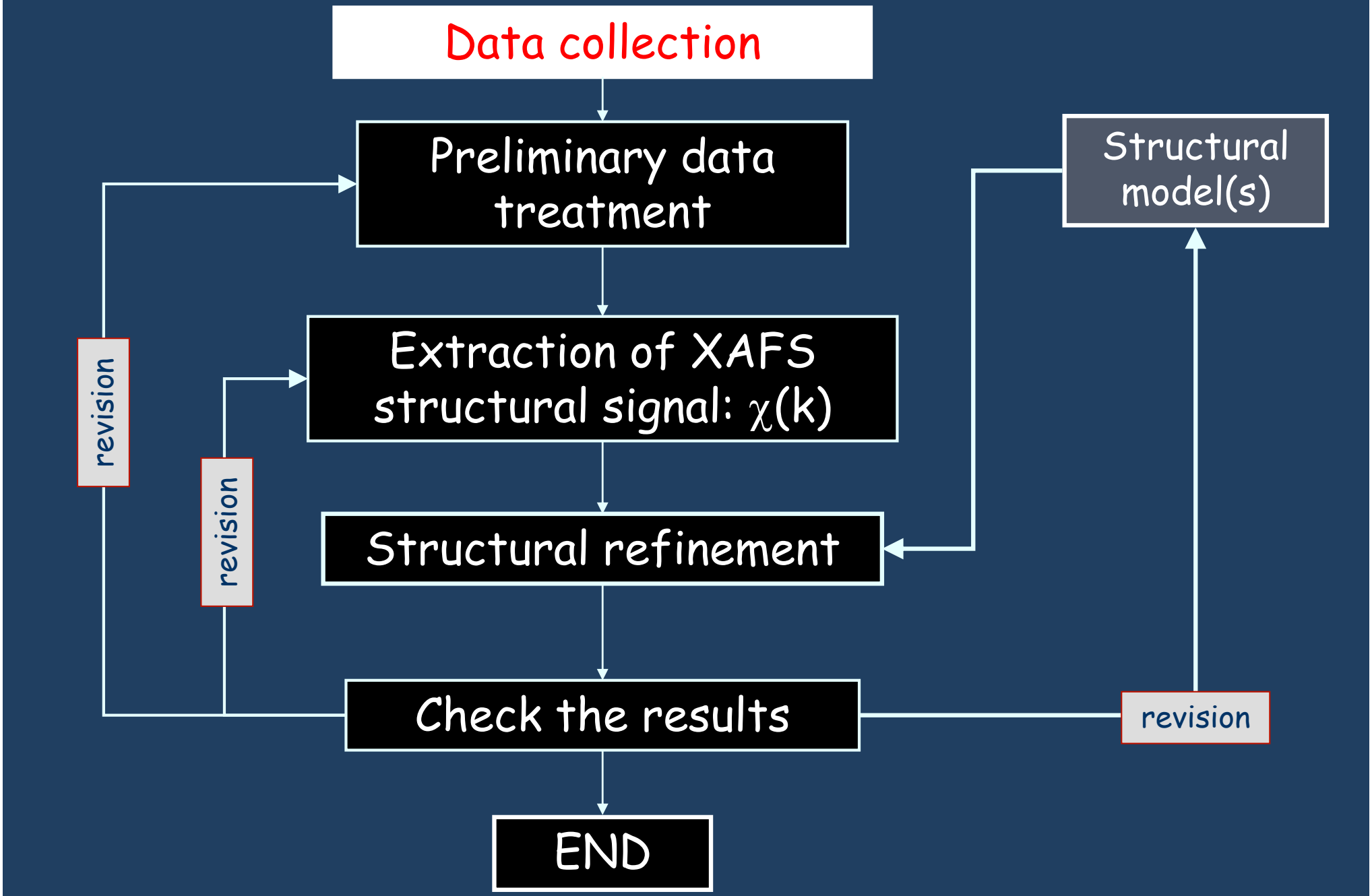
Characteristics of a XAS spectrum



XAFS study: from experiment to results



XAFS study: from experiment to results

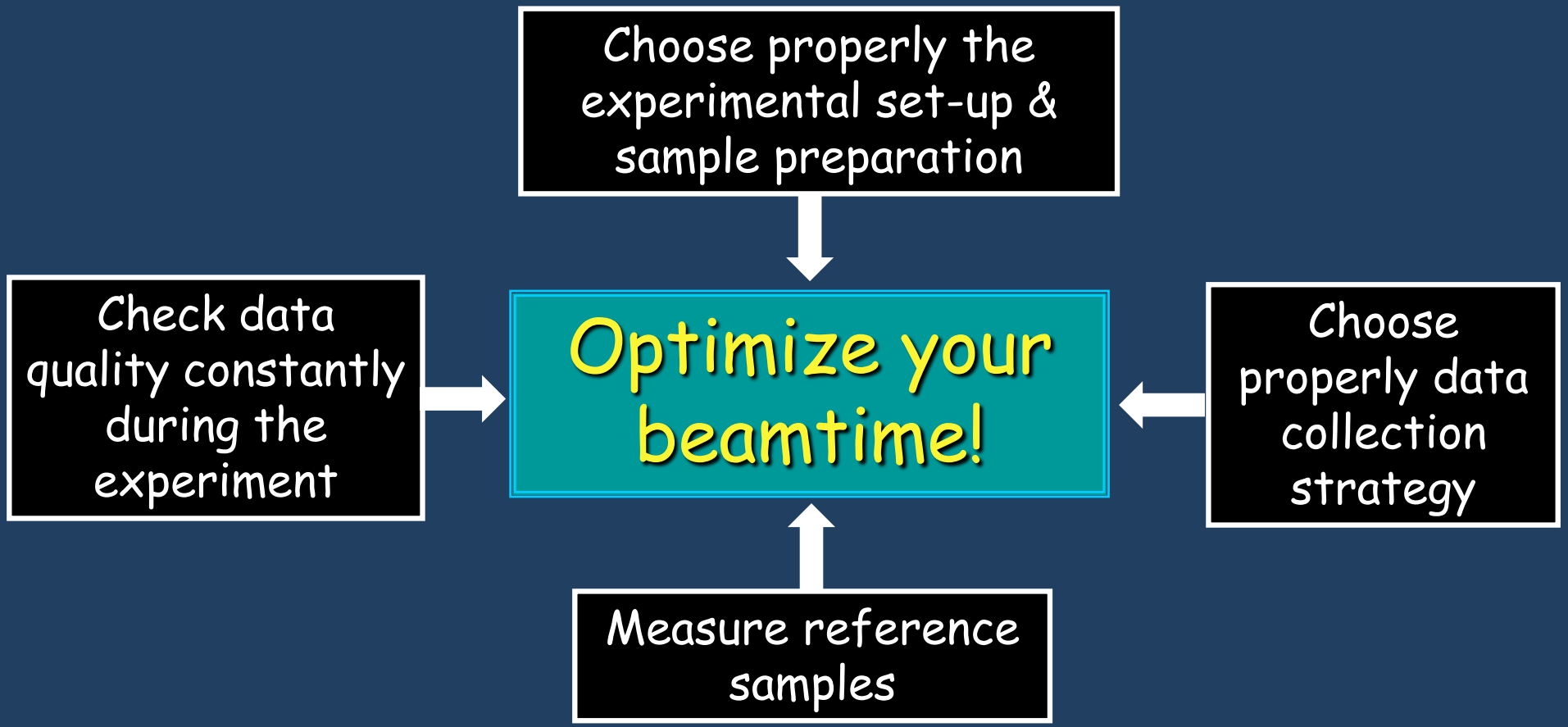


Data collection

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...

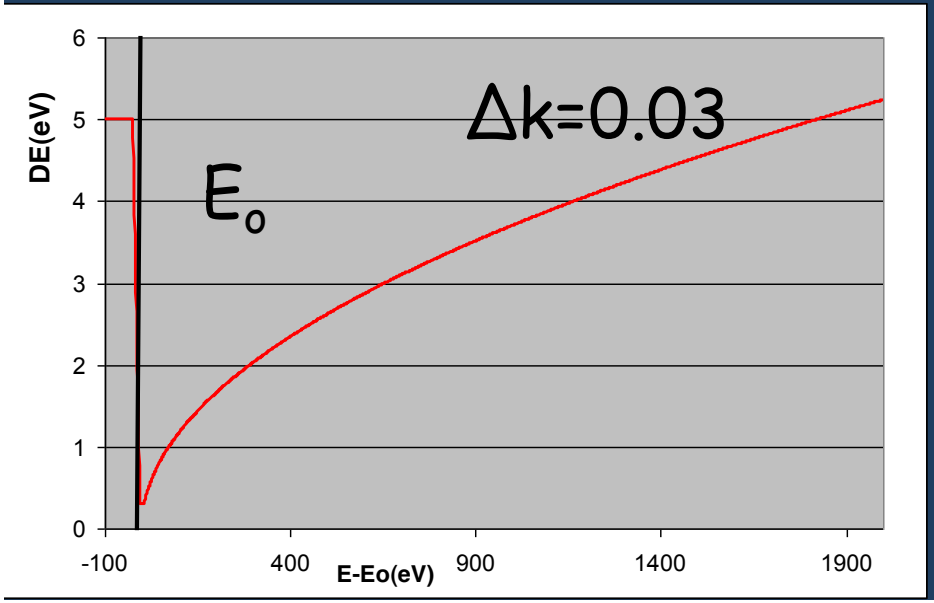
- For thin concentrated or thin diluted samples: **FLUORESCENCE**

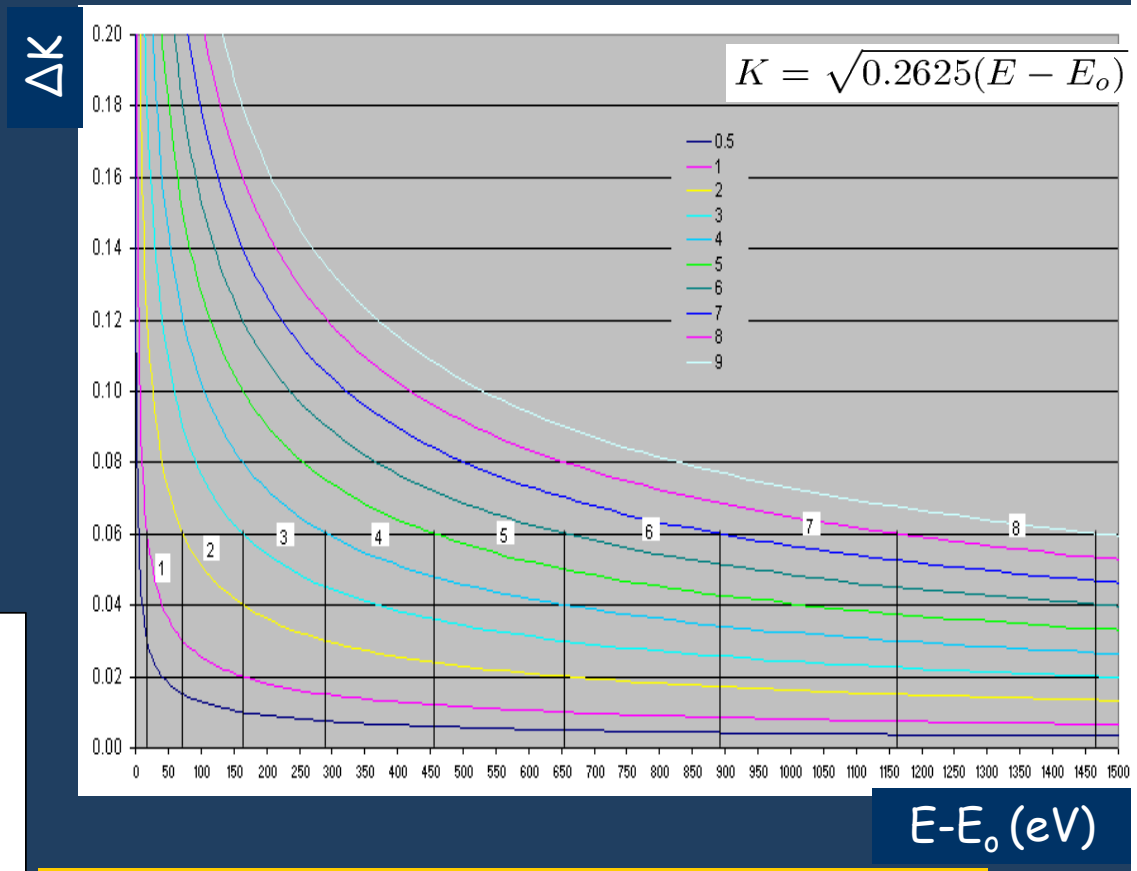
Self absorption, detector linearity, Bragg reflections

Data collection

Choose properly the data collection strategy

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



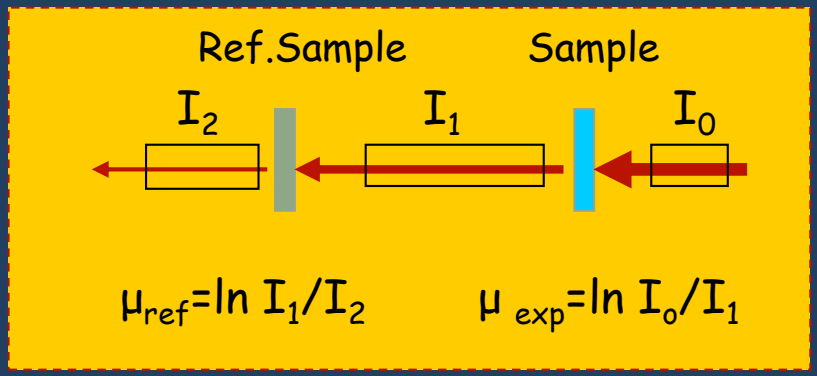


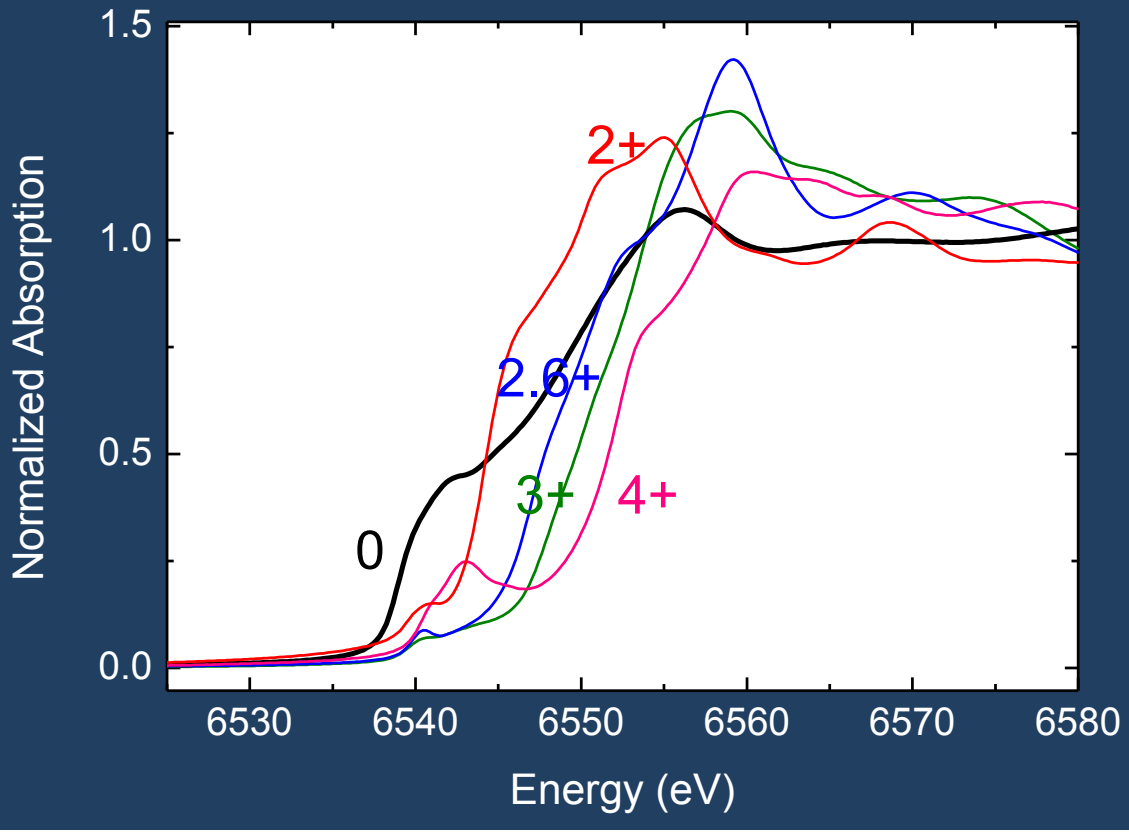
Constant Δk acquisition

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

Data collection

Measure reference samples

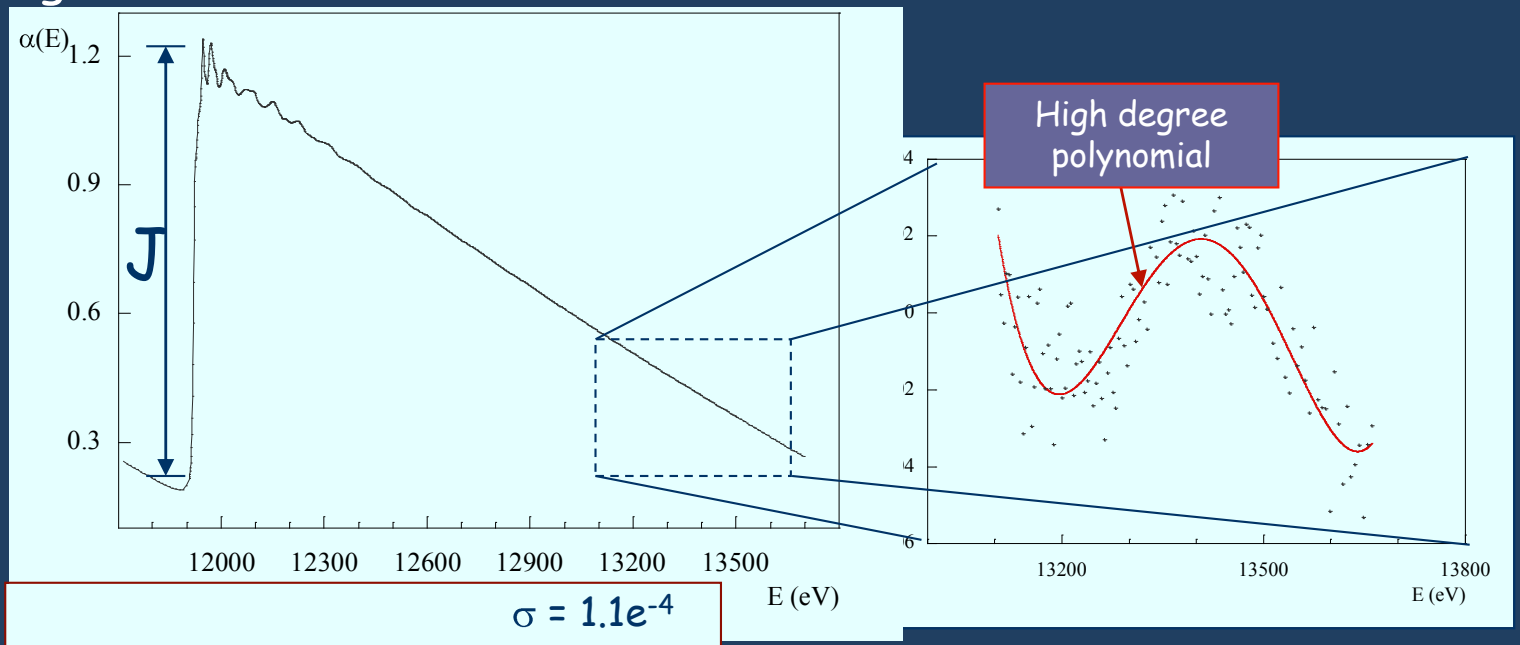


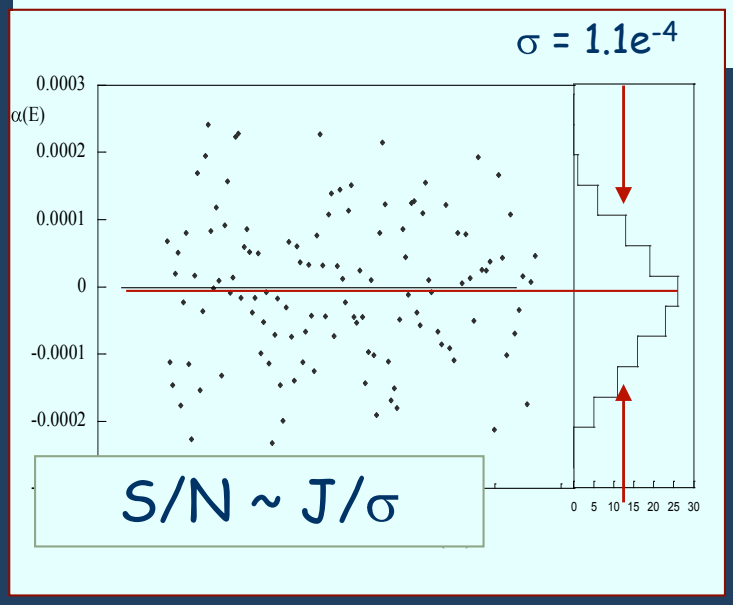


Data collection

Check data quality constantly during the experiment

- Evaluate signal/noise ratio





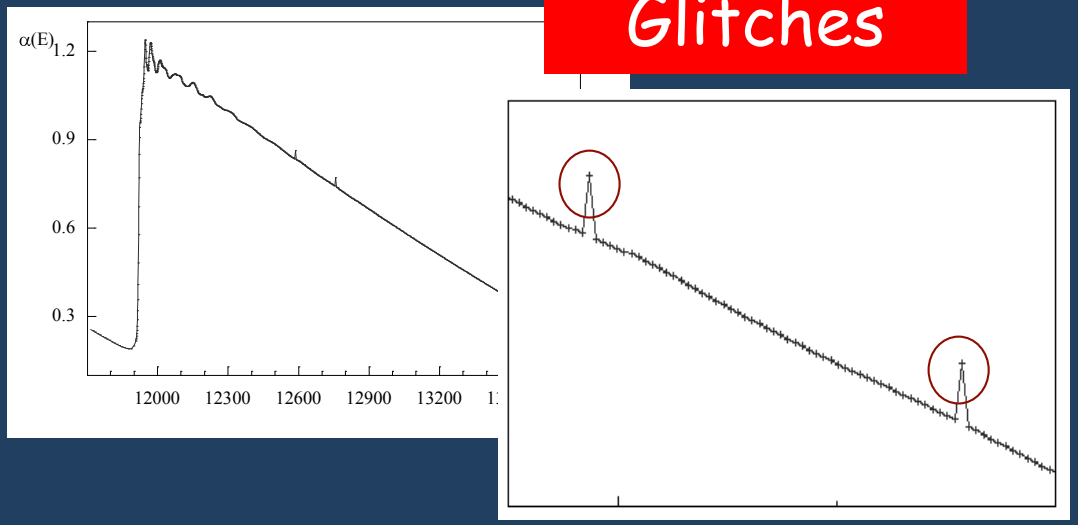
S/N ratio should be less than 10^{-3}

Data collection

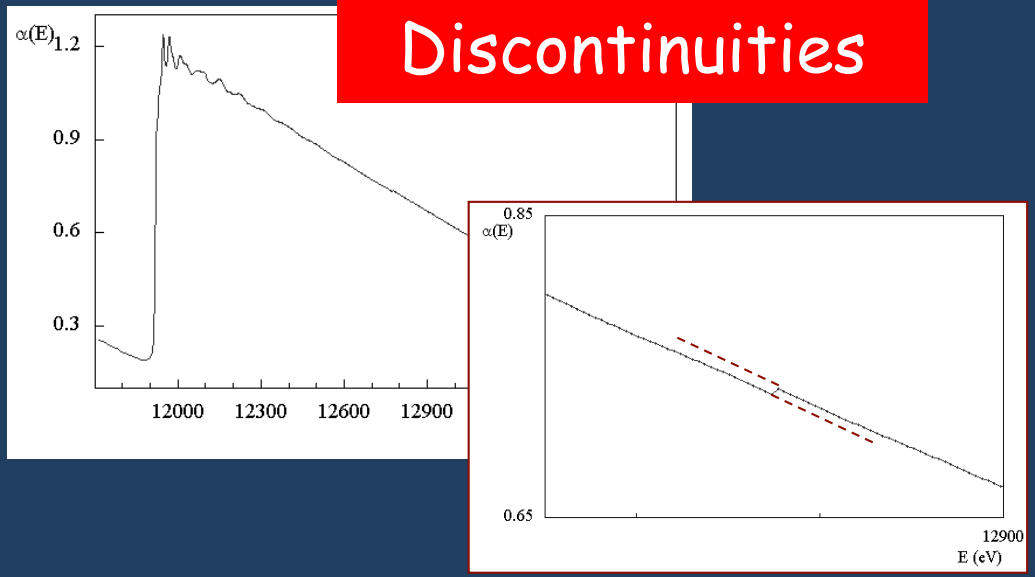
Check data quality constantly during the experiment

- Check for:

Glitches

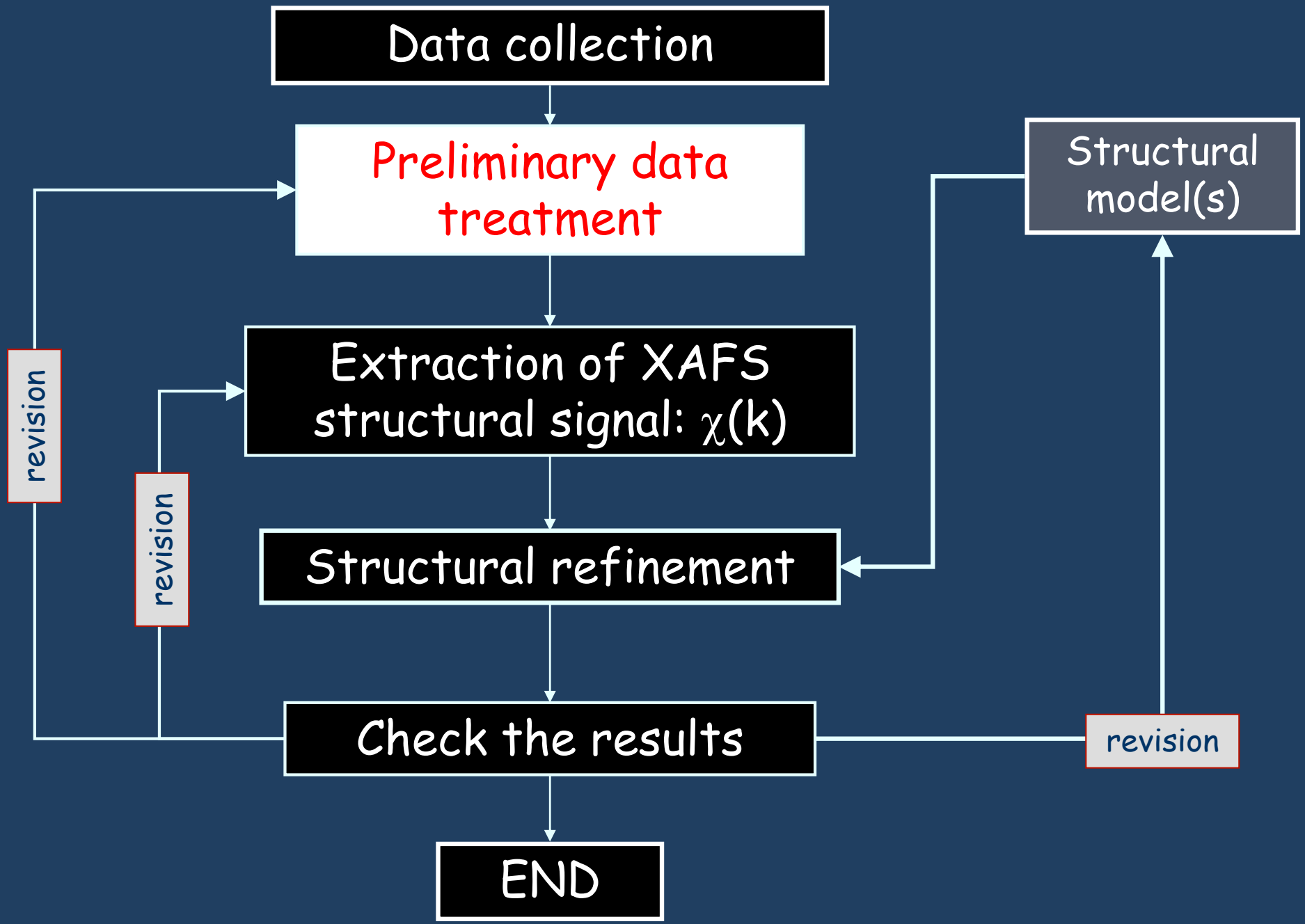


Discontinuities



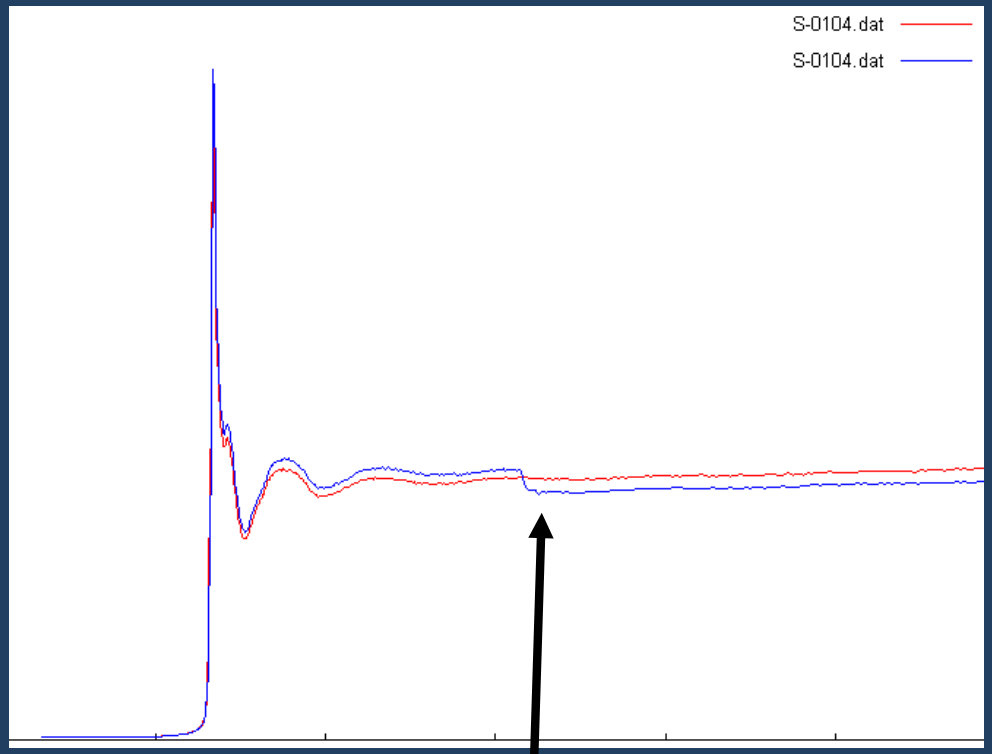
edge shift

XAFS analysis: from experiment to results

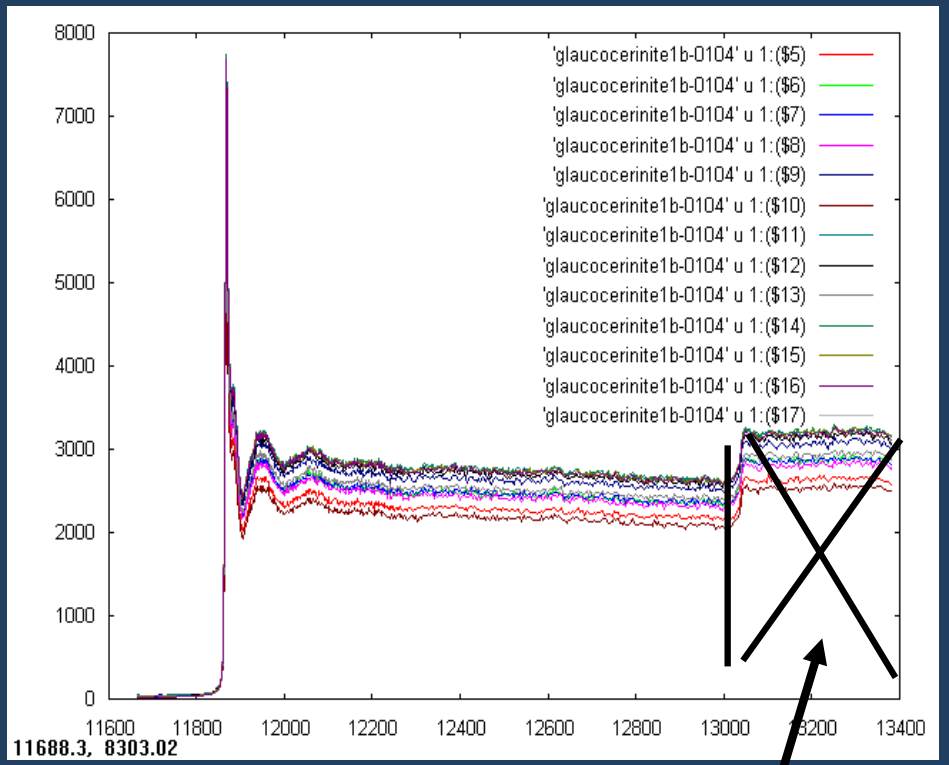


Preliminary data treatment

Choose the best spectra and useful data regions



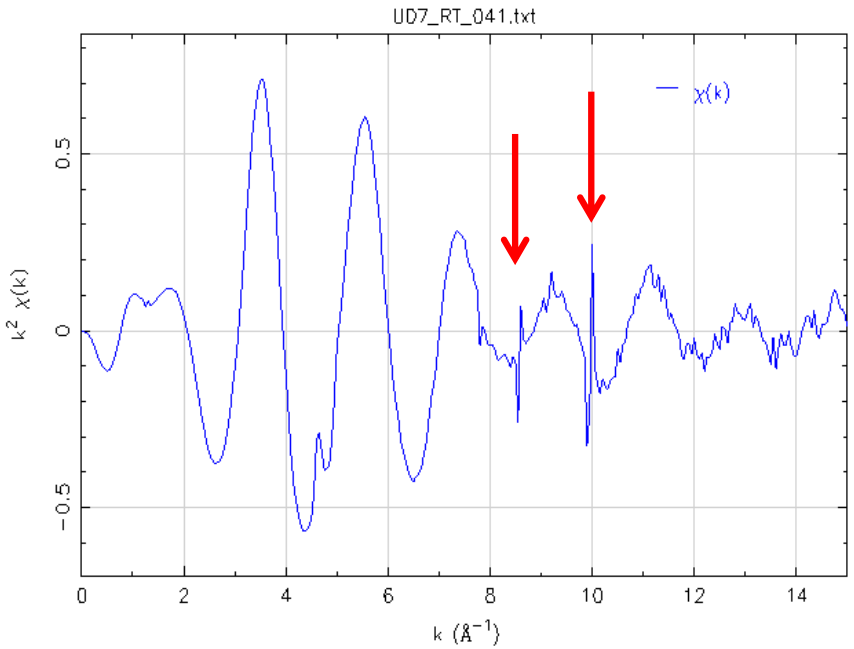
do not use the blue one!

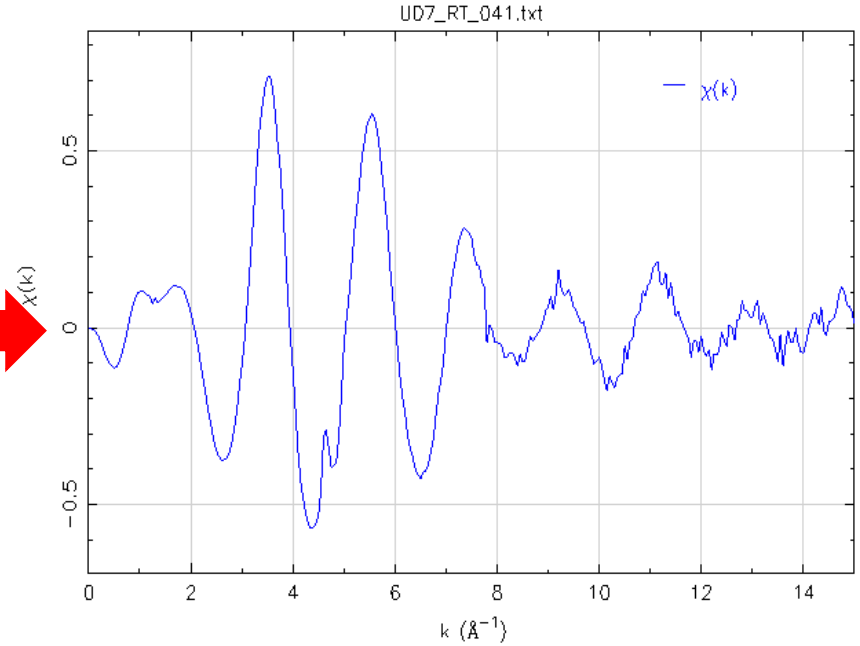


do not use data beyond 13000 eV !

Preliminary data treatment

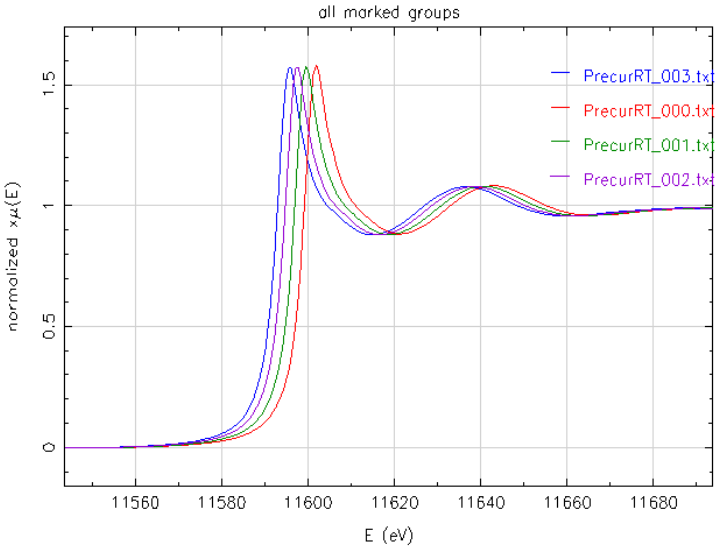
De-glitch

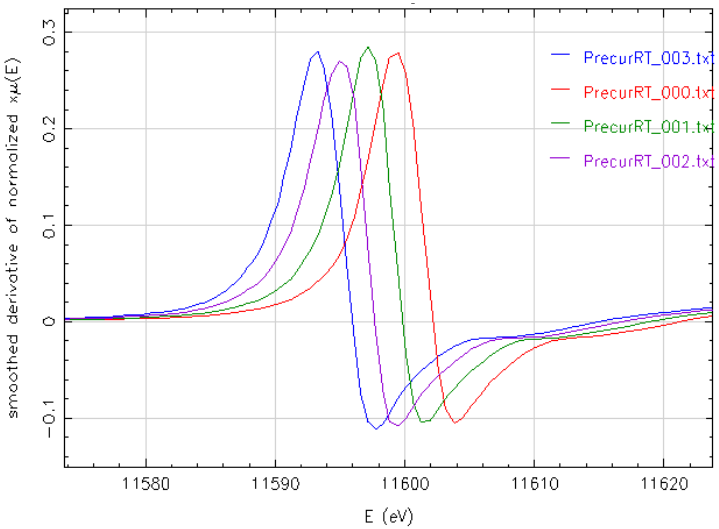


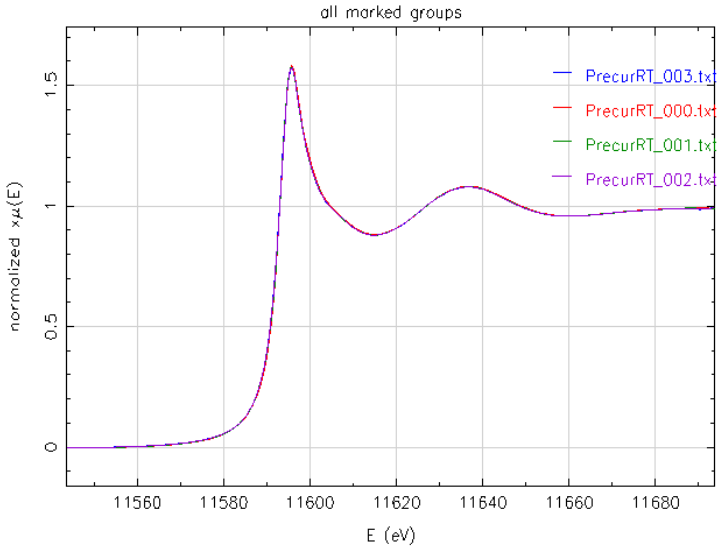


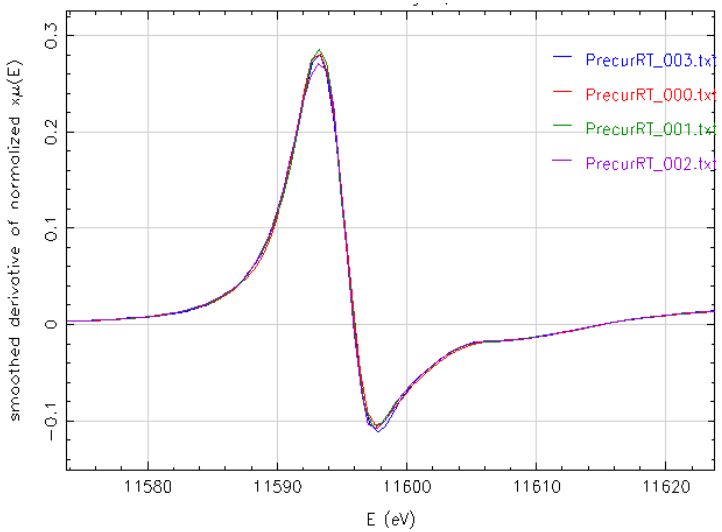
Preliminary data treatment

Align



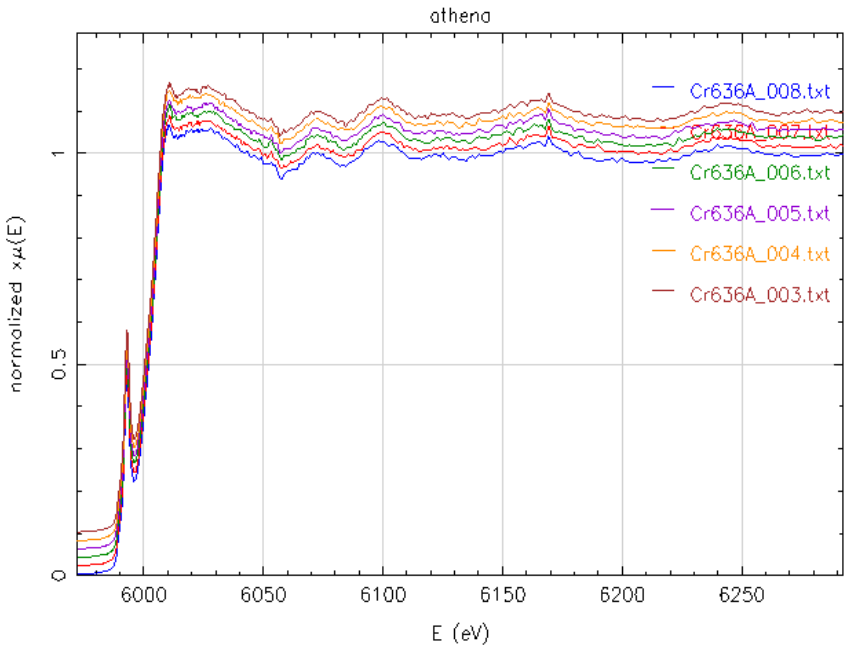


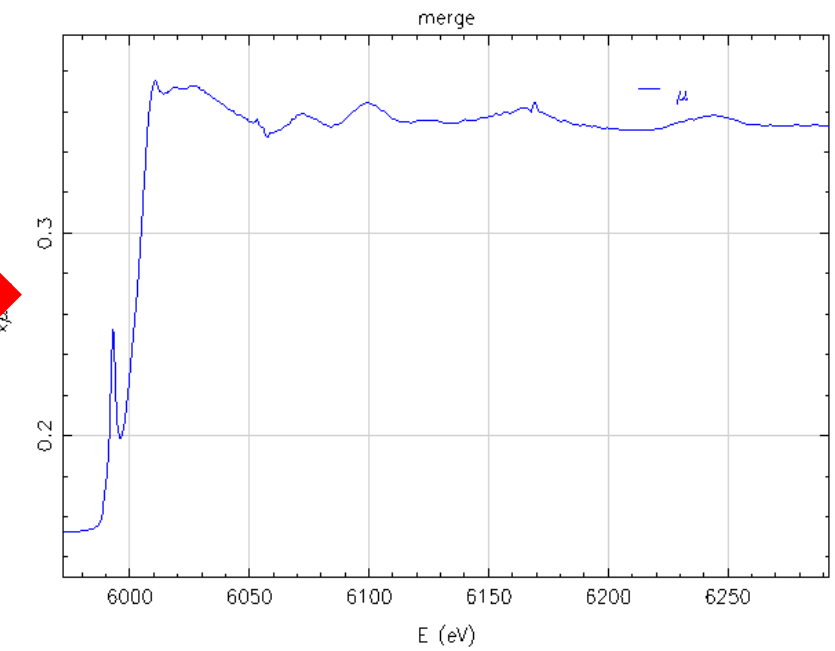




Preliminary data treatment

Average





Preliminary data treatment

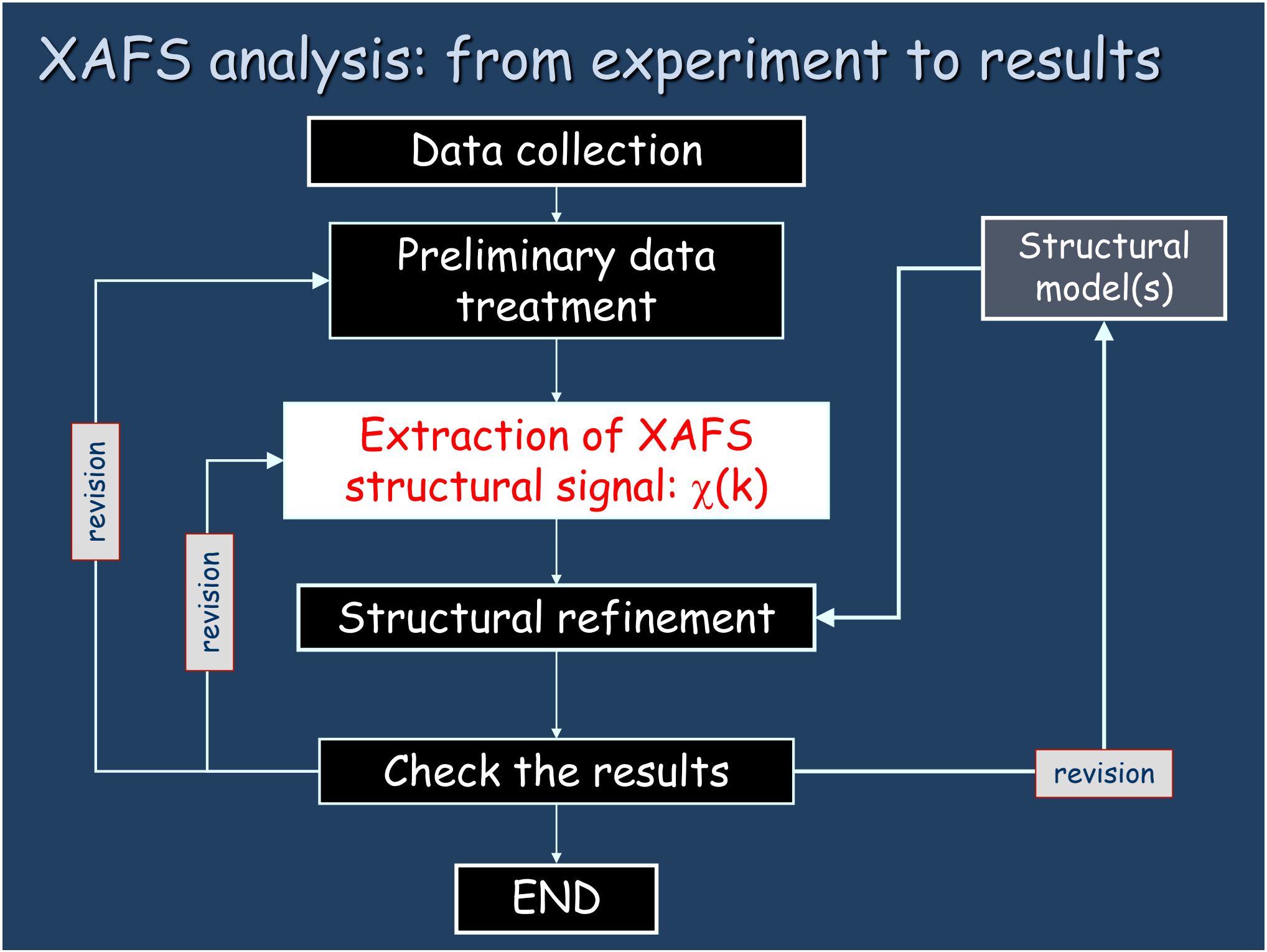
Preliminary data treatment is boring, it may be long…

While you are waiting for your data collection to finish…

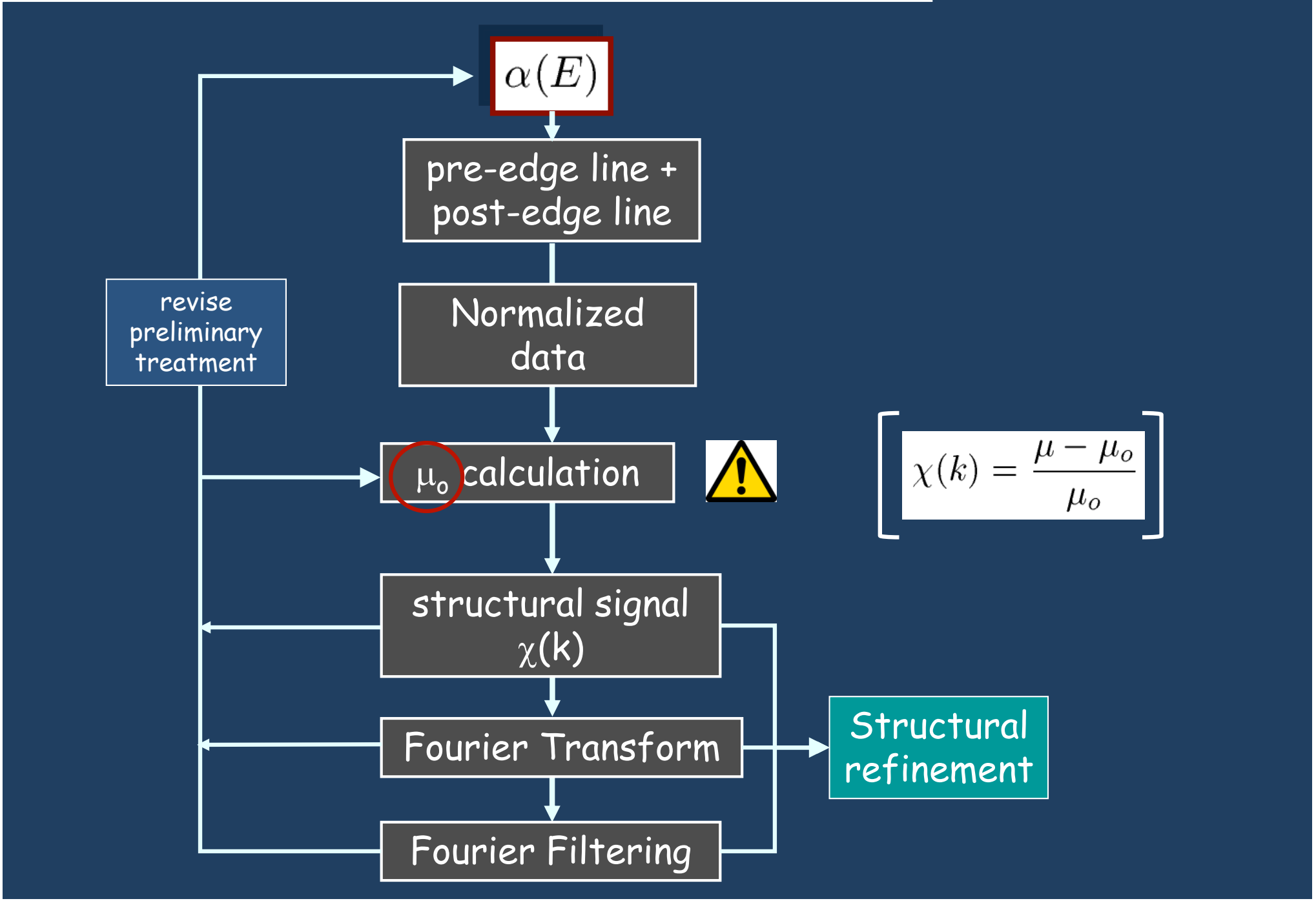
Do it on already collected data!!

You will save your time at home!!

XAFS analysis: from experiment to results



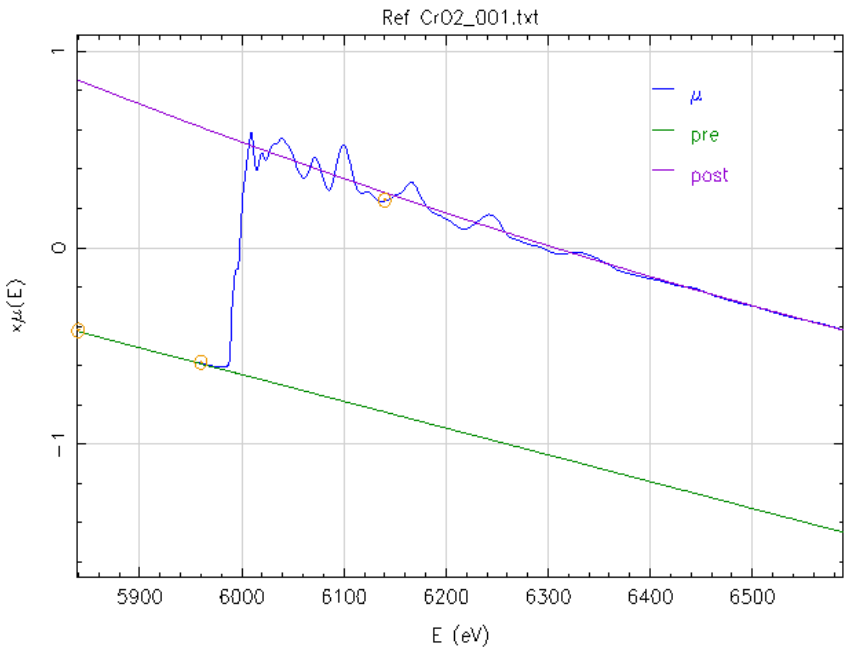
Extraction of the EXAFS signal

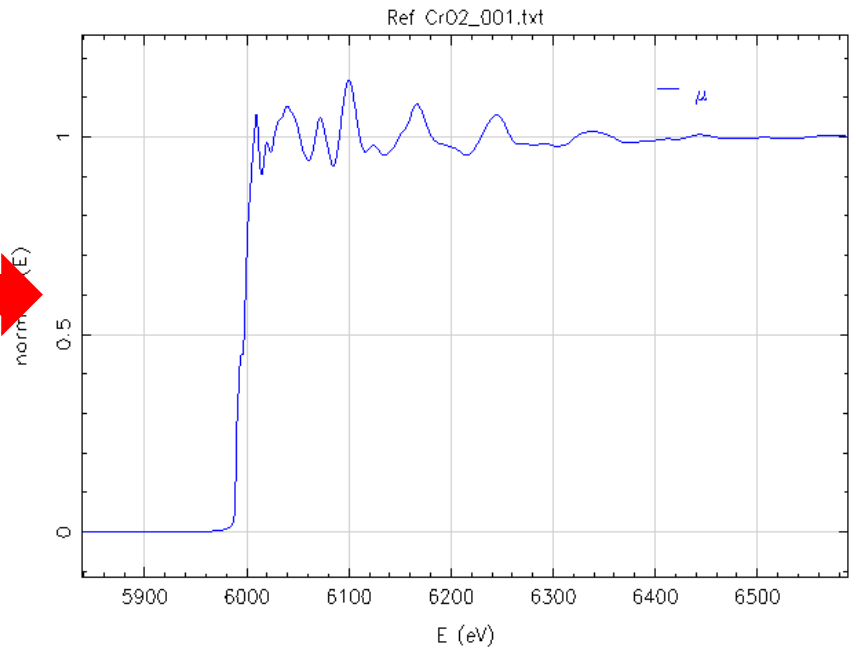


Extraction of the EXAFS signal

pre-edge line + post-edge line

Normalized data

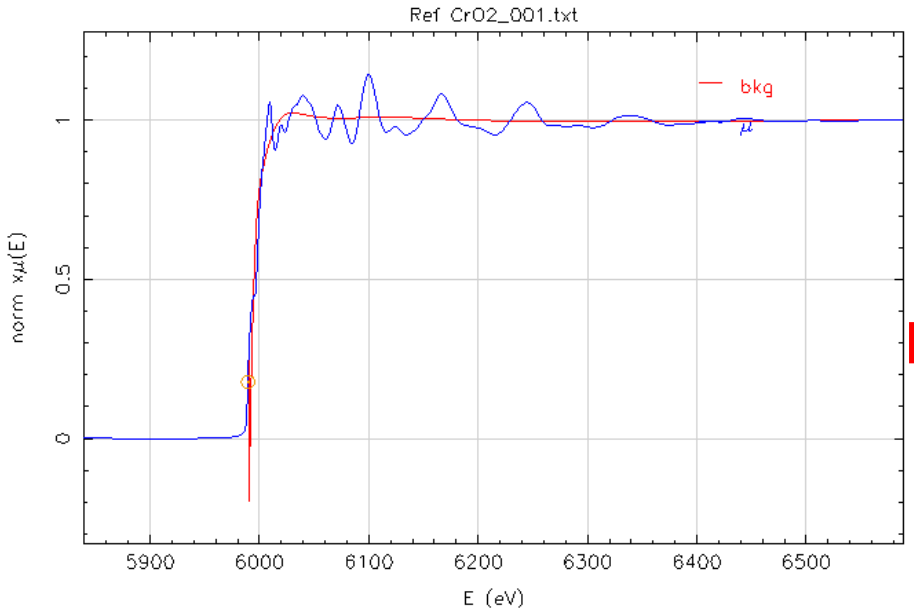


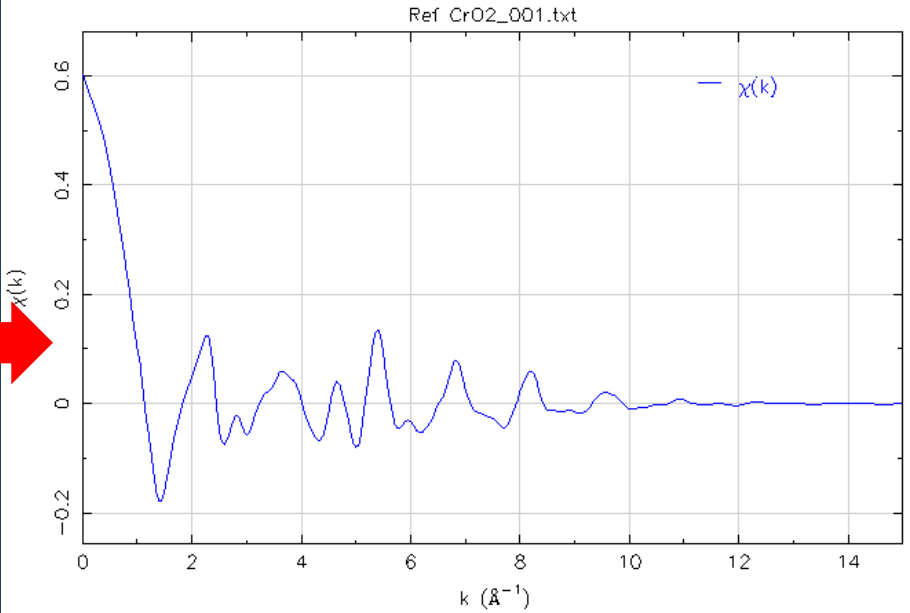


Extraction of the EXAFS signal

μ_o calculation

structural signal $\chi(k)$

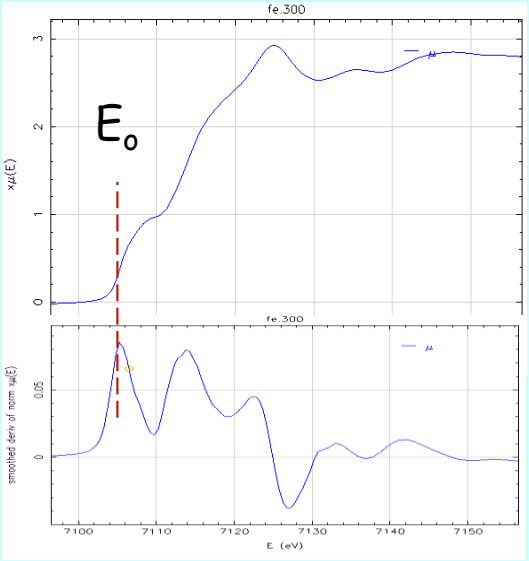




Extraction of the EXAFS signal

μ_0 calculation

1) Define E_0



E_0 will allow to set the starting point of χ(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.

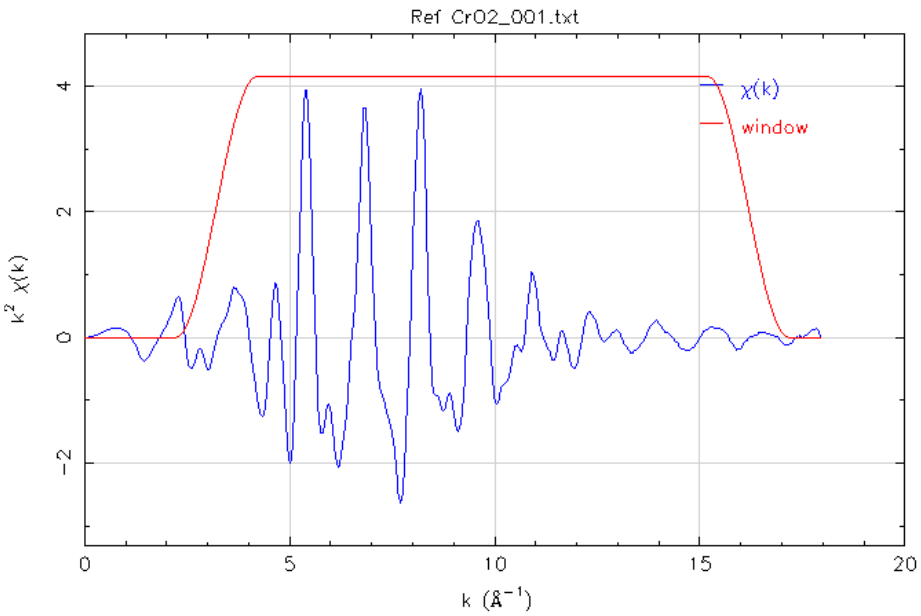
It is calculated **empirically as a smooth curve** across the data.

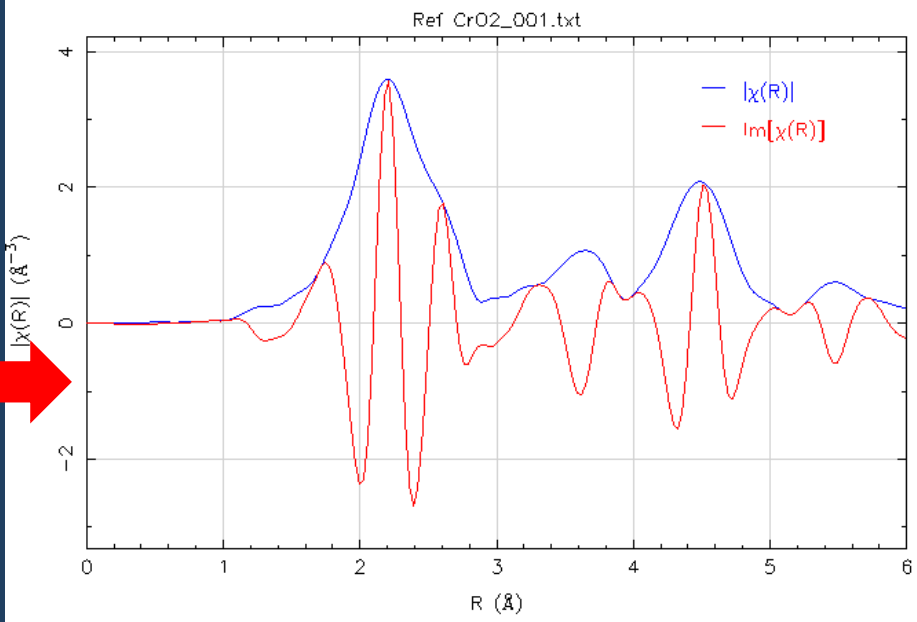
Different XAFS data analysis softwares apply different (equivalent) approaches

3) Subtract μ_0 from μ

Extraction of the EXAFS signal

Fourier Transform



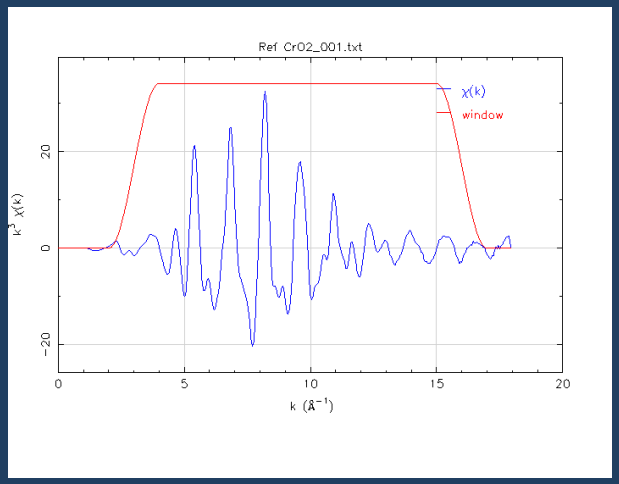


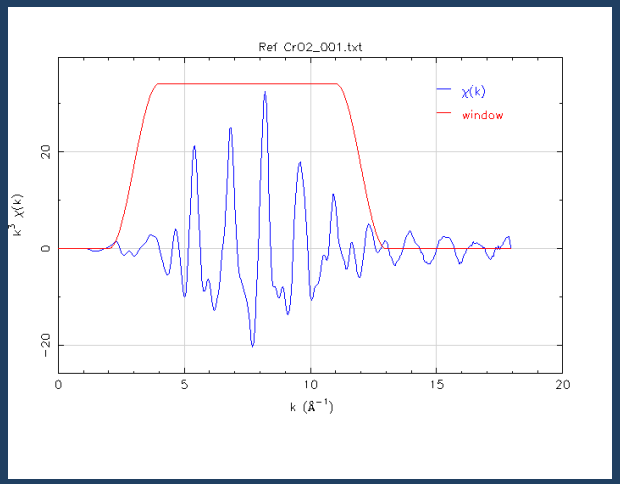
FT shows more intuitively the main structural features in the real space: the FT modulus represent a pseudo-radial distribution function (RDF)

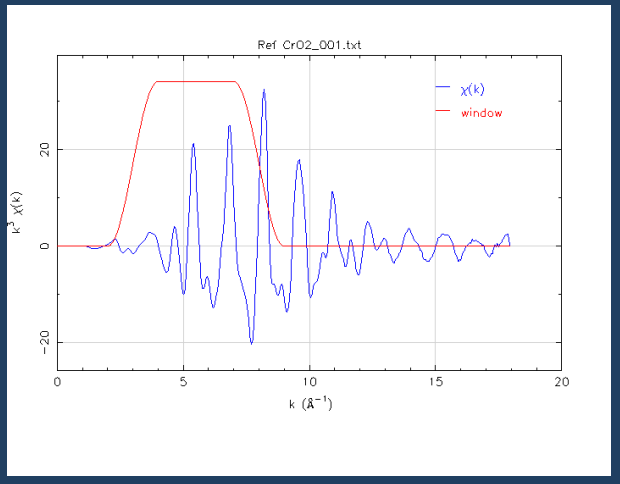
|FT| peaks represent interatomic correlation

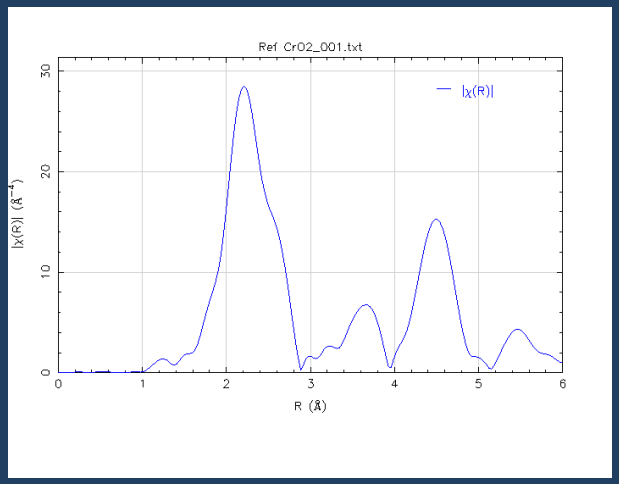
Peak position are not the true correlation distances due to the phase shift effect

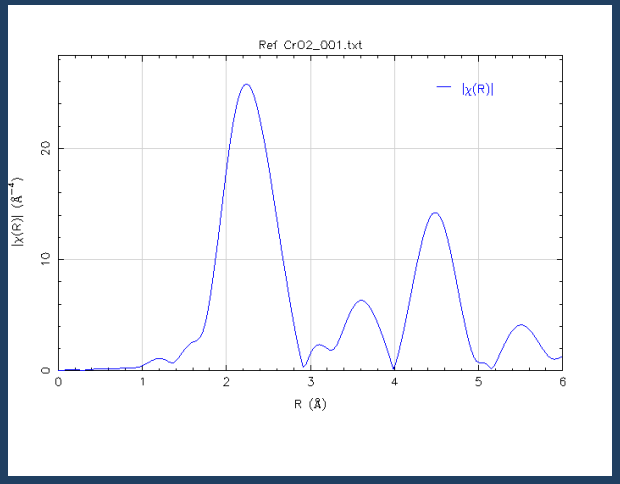
Fourier Transform – window size effect

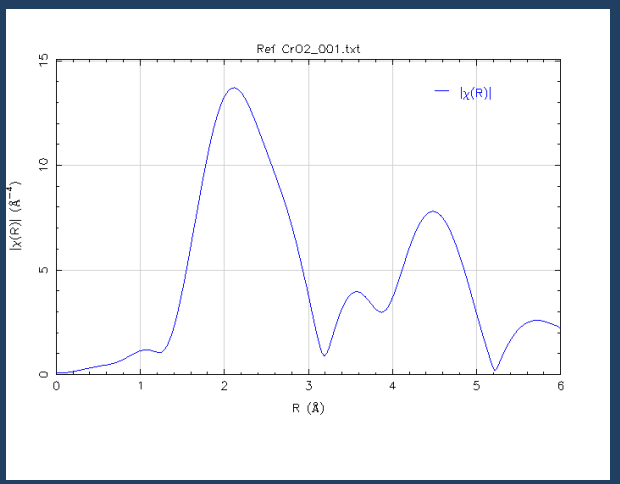








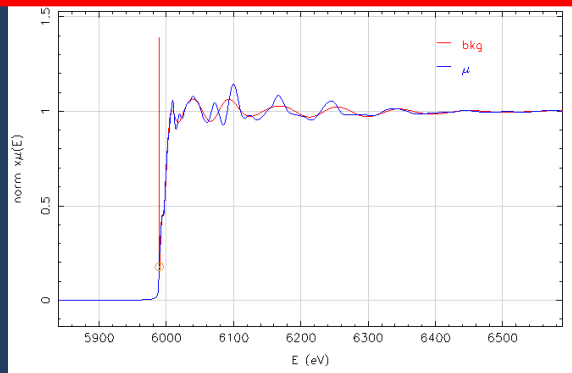


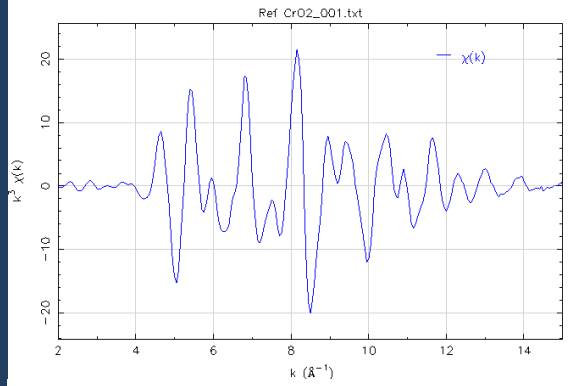


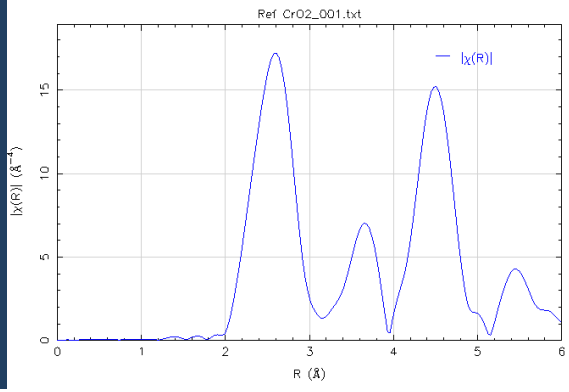
Minor effects are given by type of windows (Hanning, Kaiser-Bessel, Sine) and apodization

Extraction of the EXAFS signal

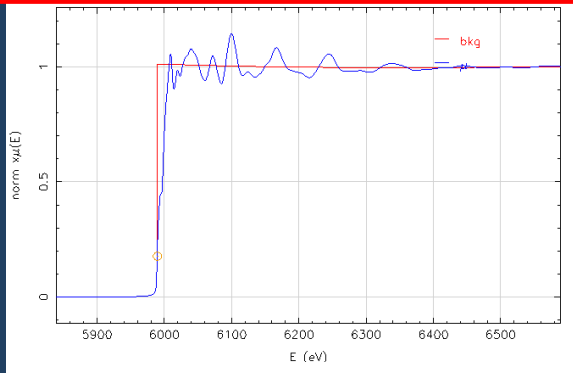
DO NOT REMOVE TRUE STRUCTURAL FEATURES

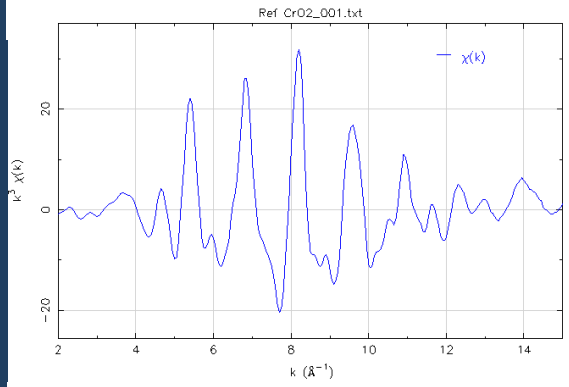


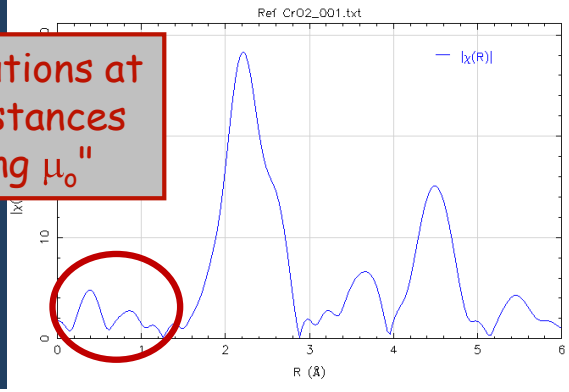




DO NOT DO THE OPPOSITE ERROR





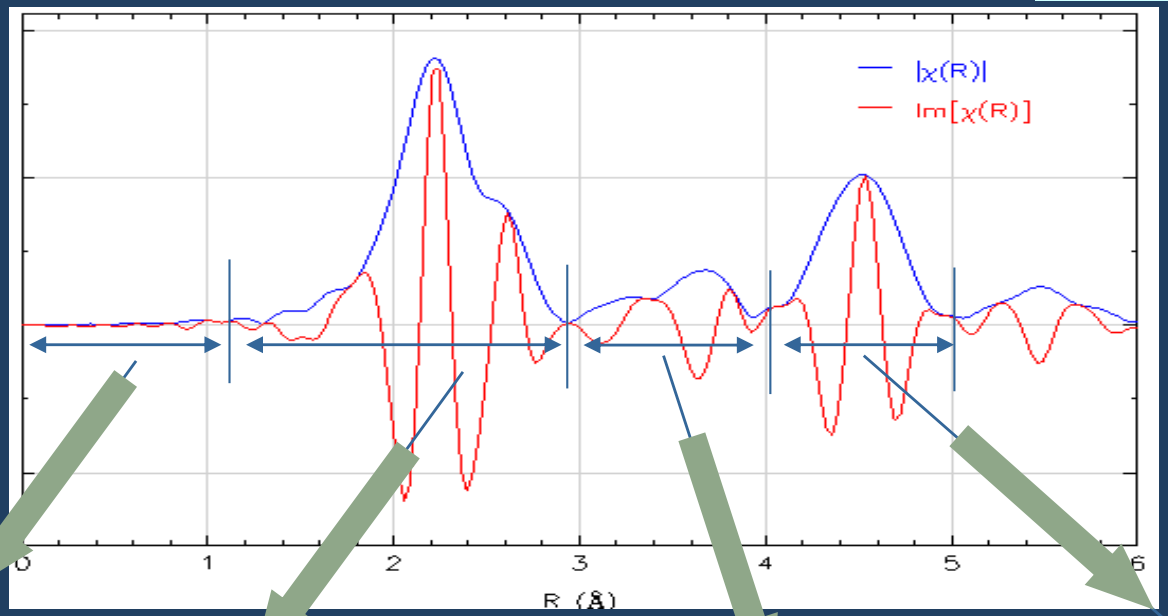


Large |FT| contributions at low (unphysical) distances may signify "wrong μ_0"

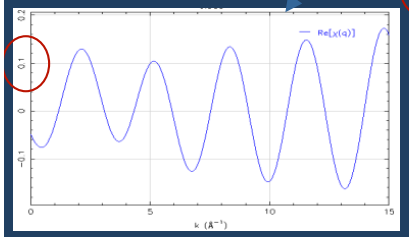
Extraction of the EXAFS signal

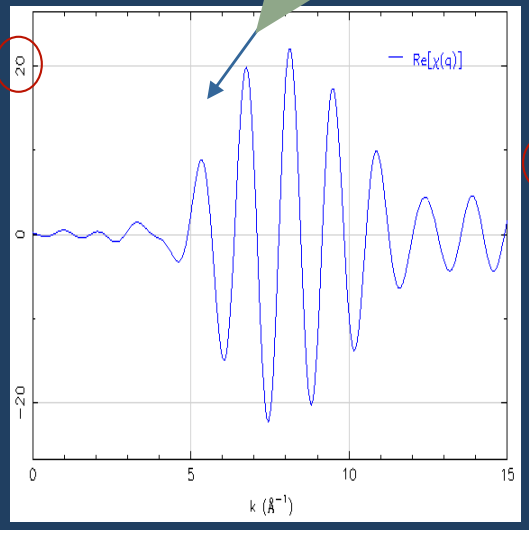
Fourier Filtering

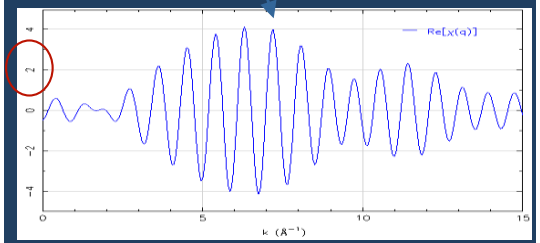
Fourier filtering allows isolating contributions of selected regions of the FT

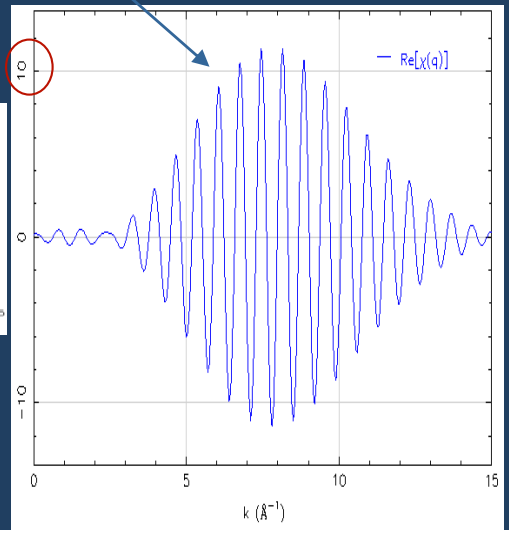


Background contribution

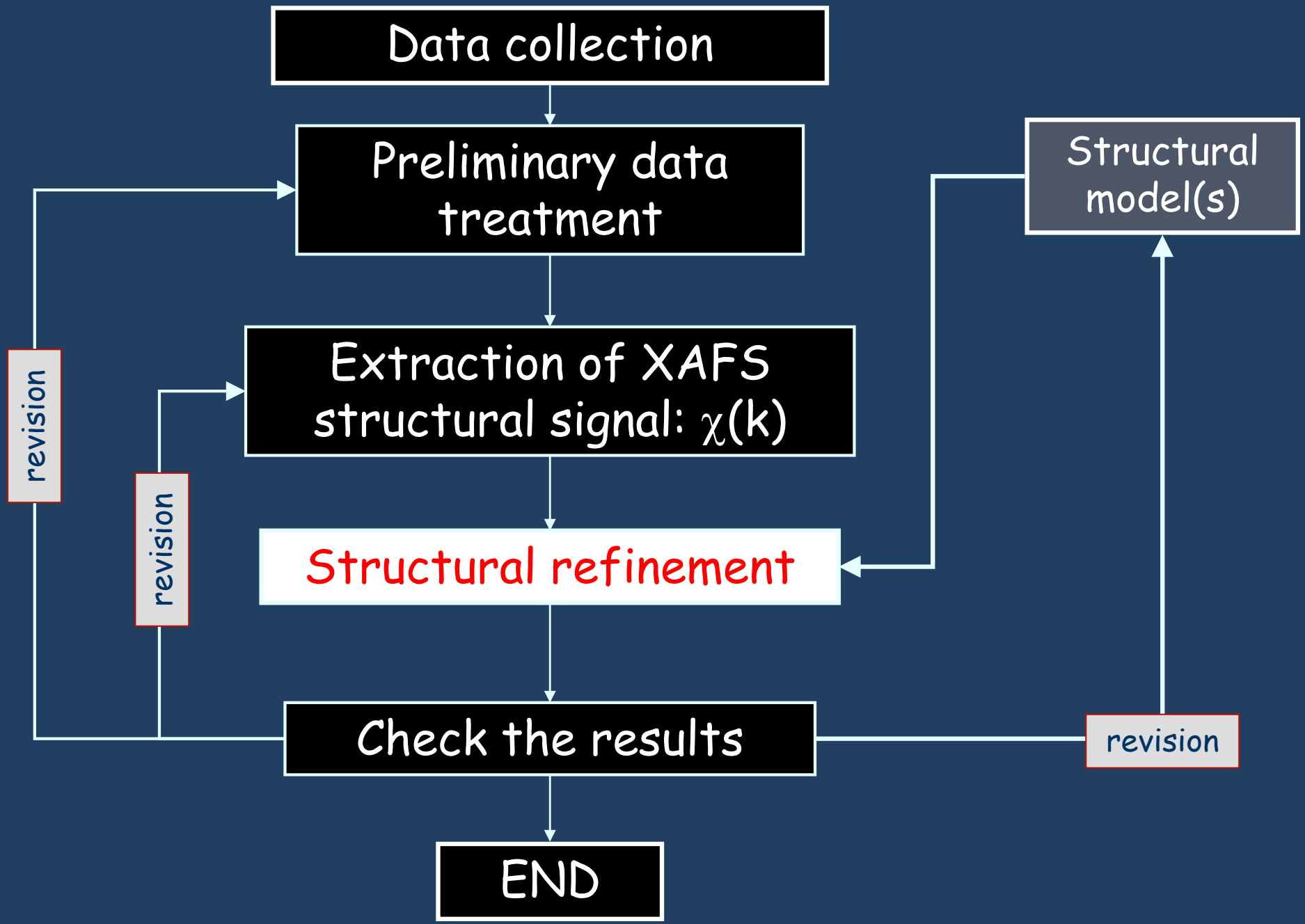








XAFS analysis: from experiment to results

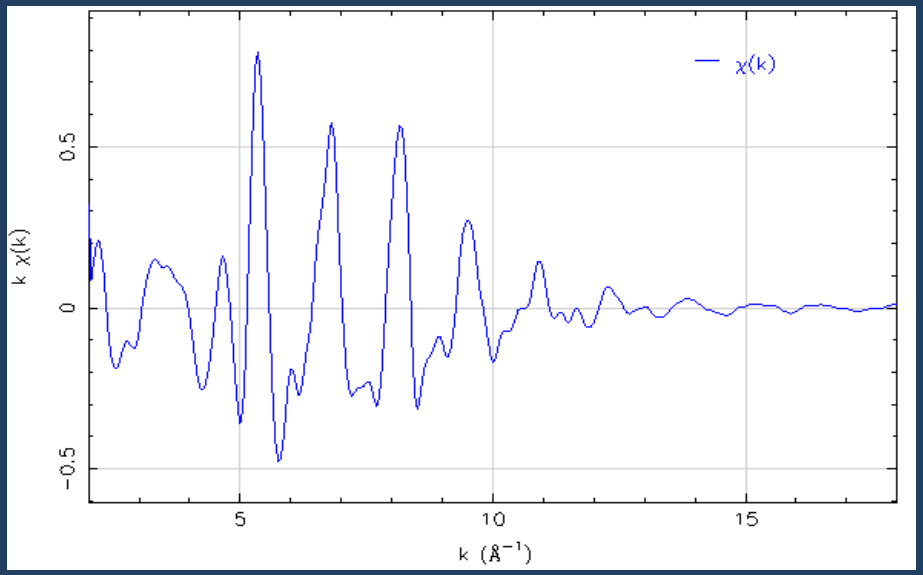


Structural refinement

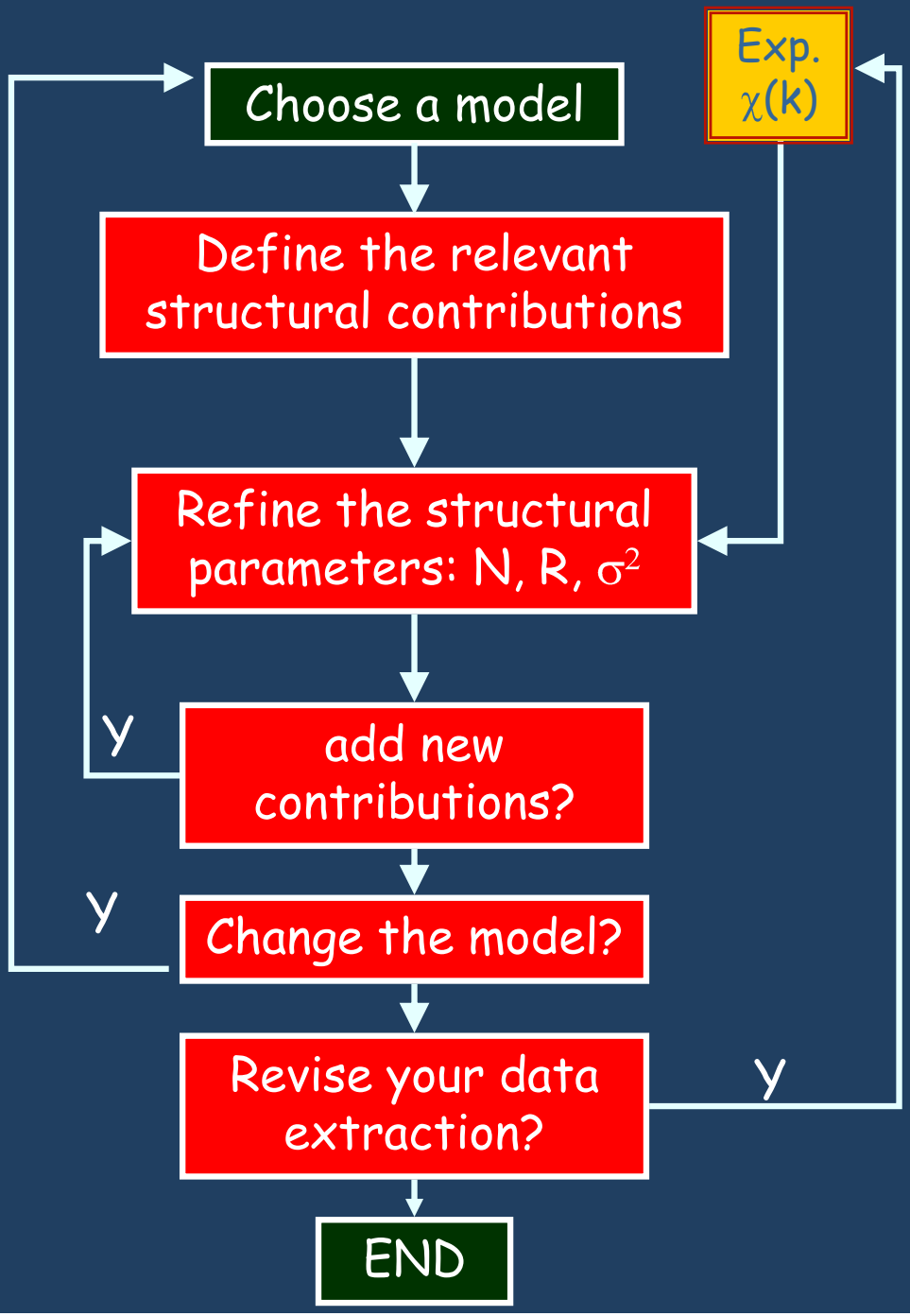
Theoretical $\chi(k)$

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

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

NEUTRONS FOR SCIENCE

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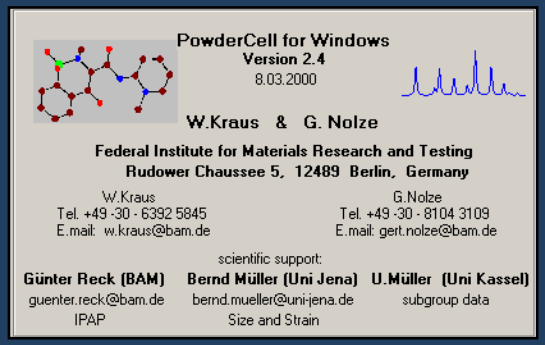
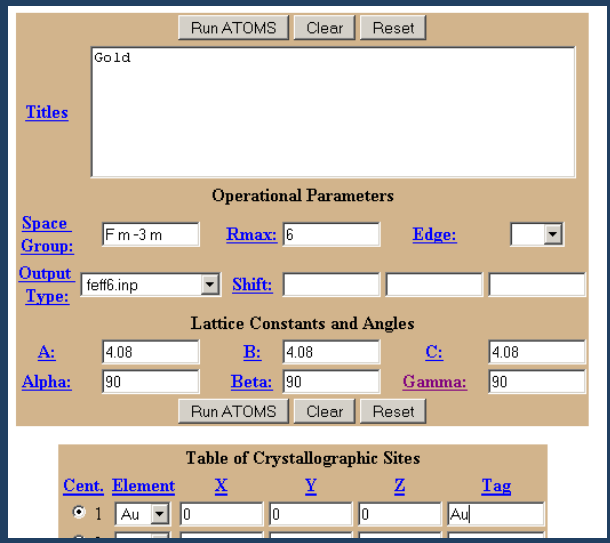
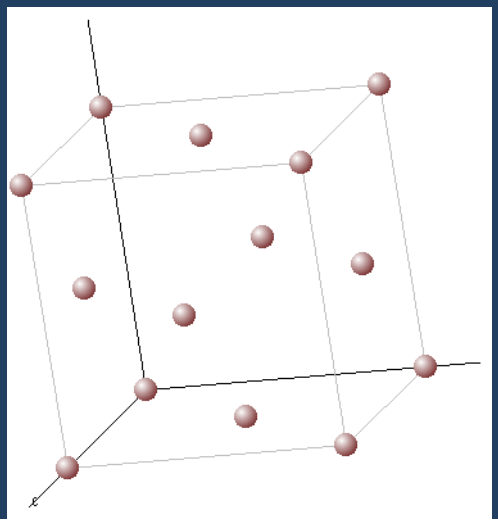


ATOMS on the Web

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

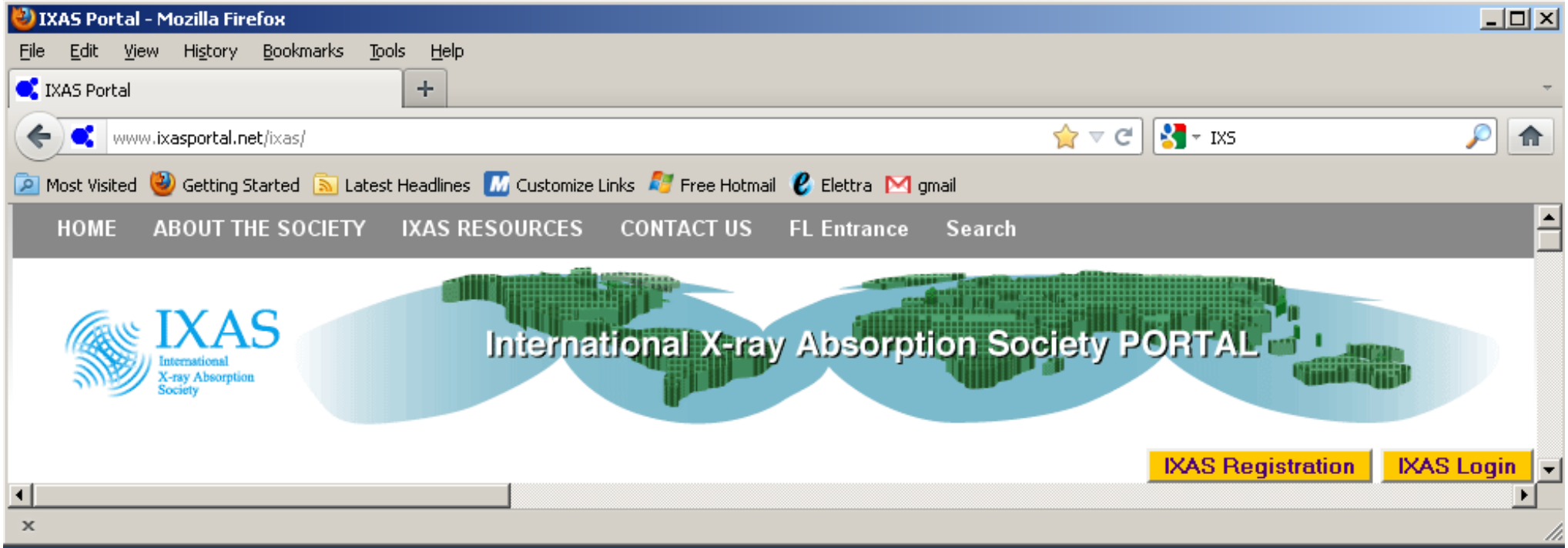


http://database.iem.ac.ru/mincryst/



ICSD database

XAFS data analysis softwares



http://www.xafs.org/

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

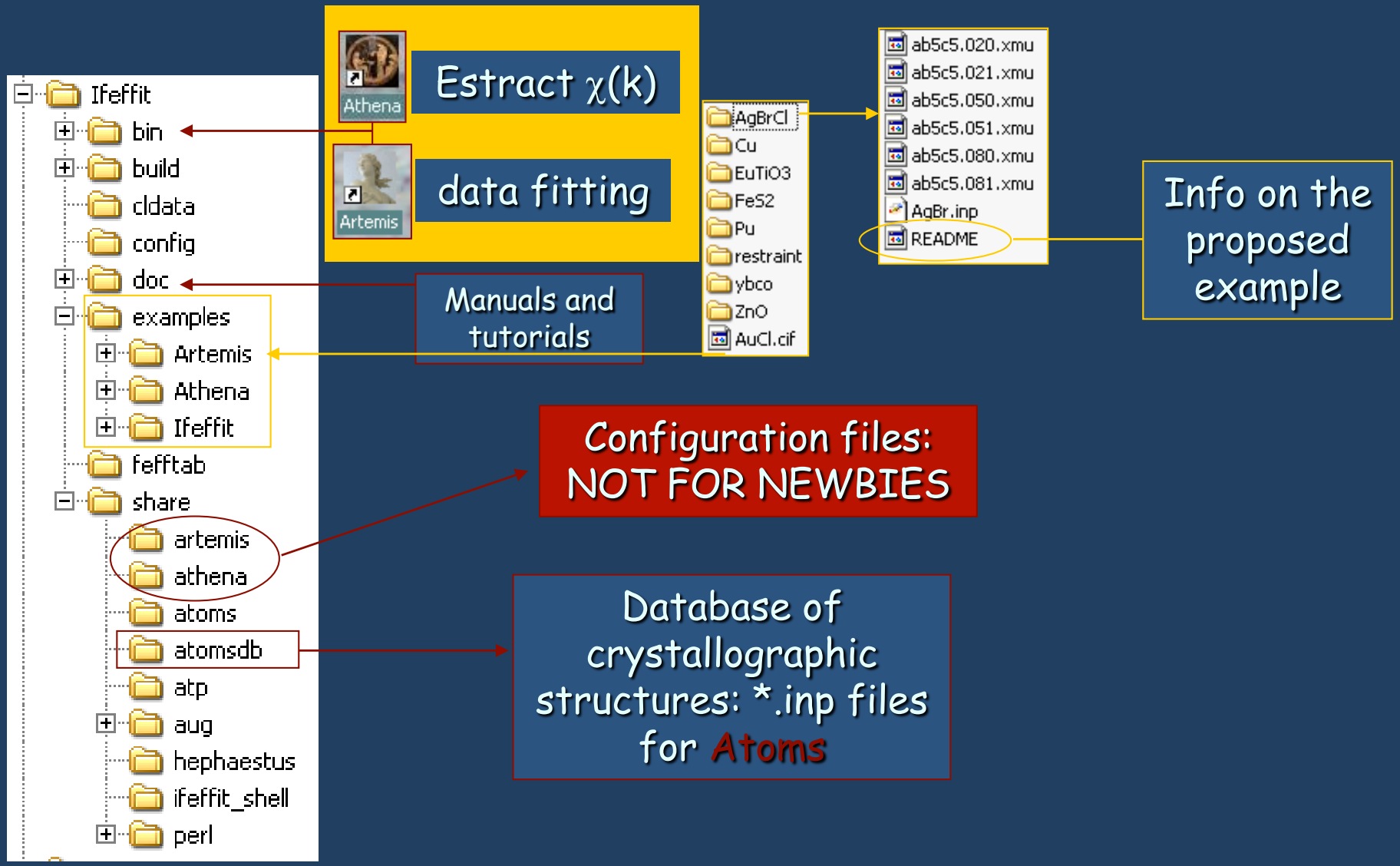
Click DOWNLOADS

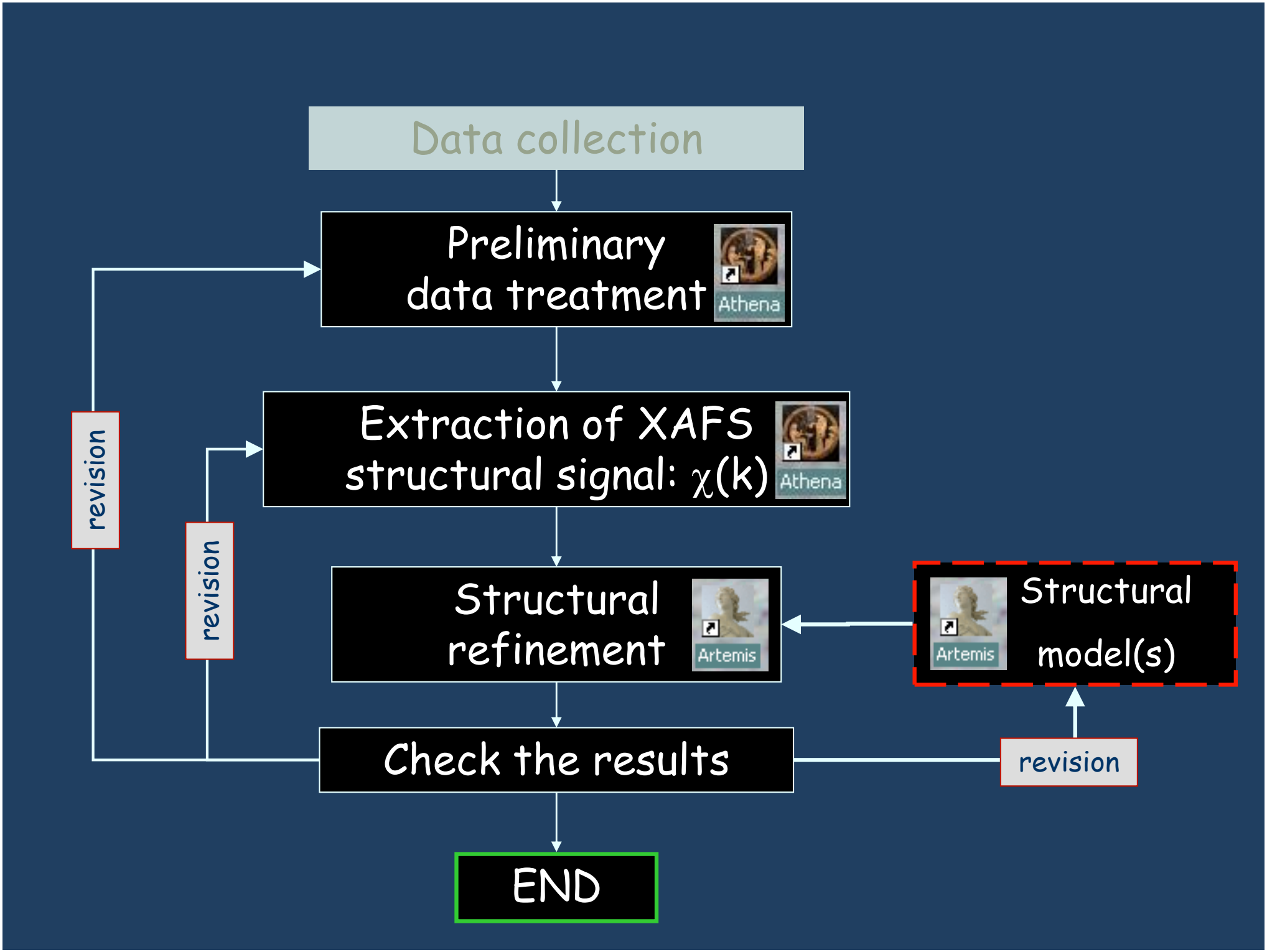
Click ifeffit-1.2.11.exe

Install Ifeffit.exe

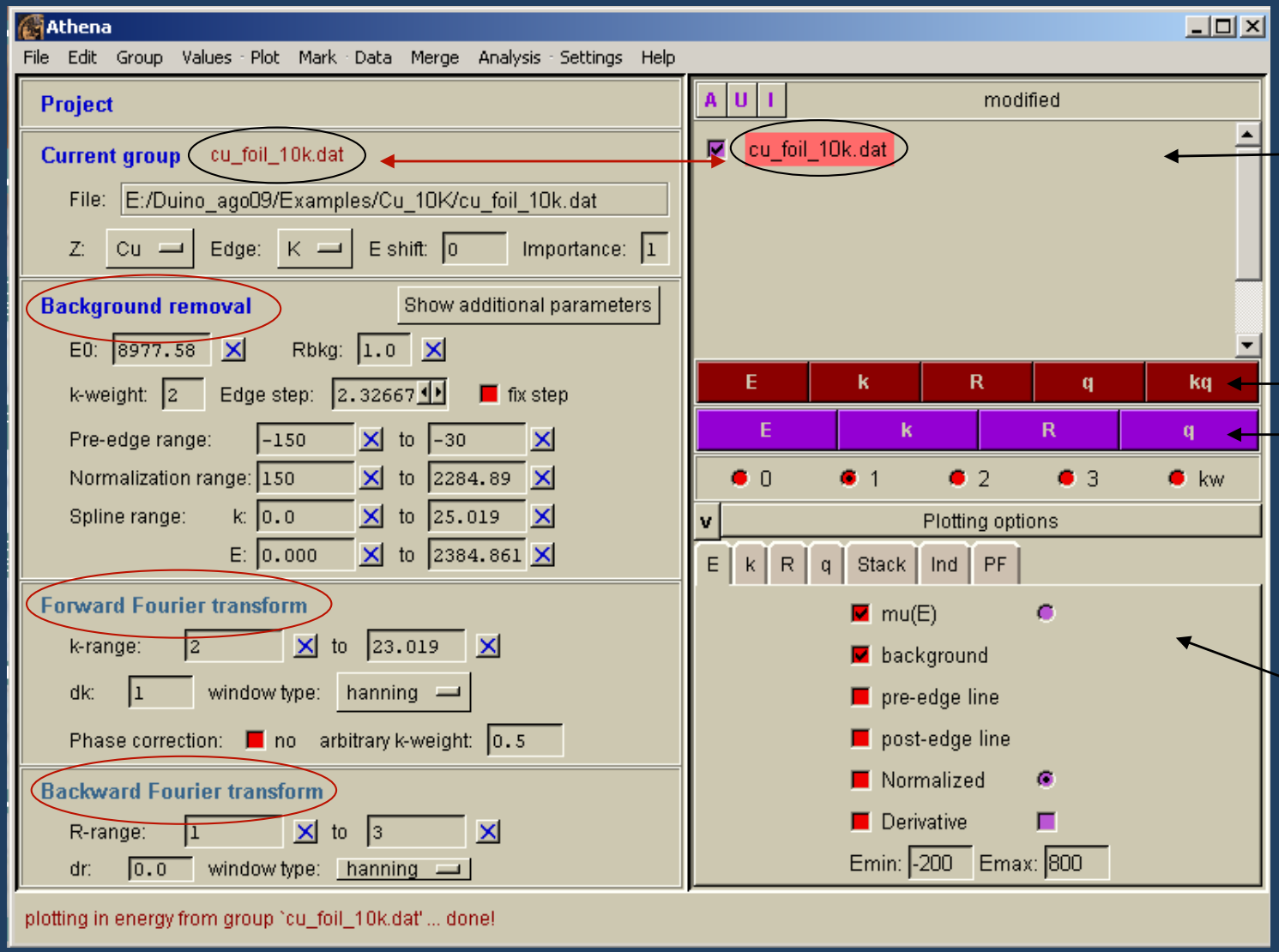
1.	athena	GUI for Data Processing with Ifeffit 
2.	artemis	GUI for XAFS Fitting with Ifeffit 
3.	hephaestus	GUI for general x-ray properties of the elements
4.	sixpack	GUI for XAFS Processing and Fitting with Ifeffit
5.	feff6	Stand-alone program for ab inito EXAFS calculations
6.	atoms	Stand-alone, command 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




Data collection
Preliminary data treatment
Athena
Extraction of XAFS structural signal: χ(k)
Athena
Structural refinement
Artemis
Structural model(s)
Artemis
Check the results
END
revision
revision
revision

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



List of files (group) opened into Athena

Plot highlighted files

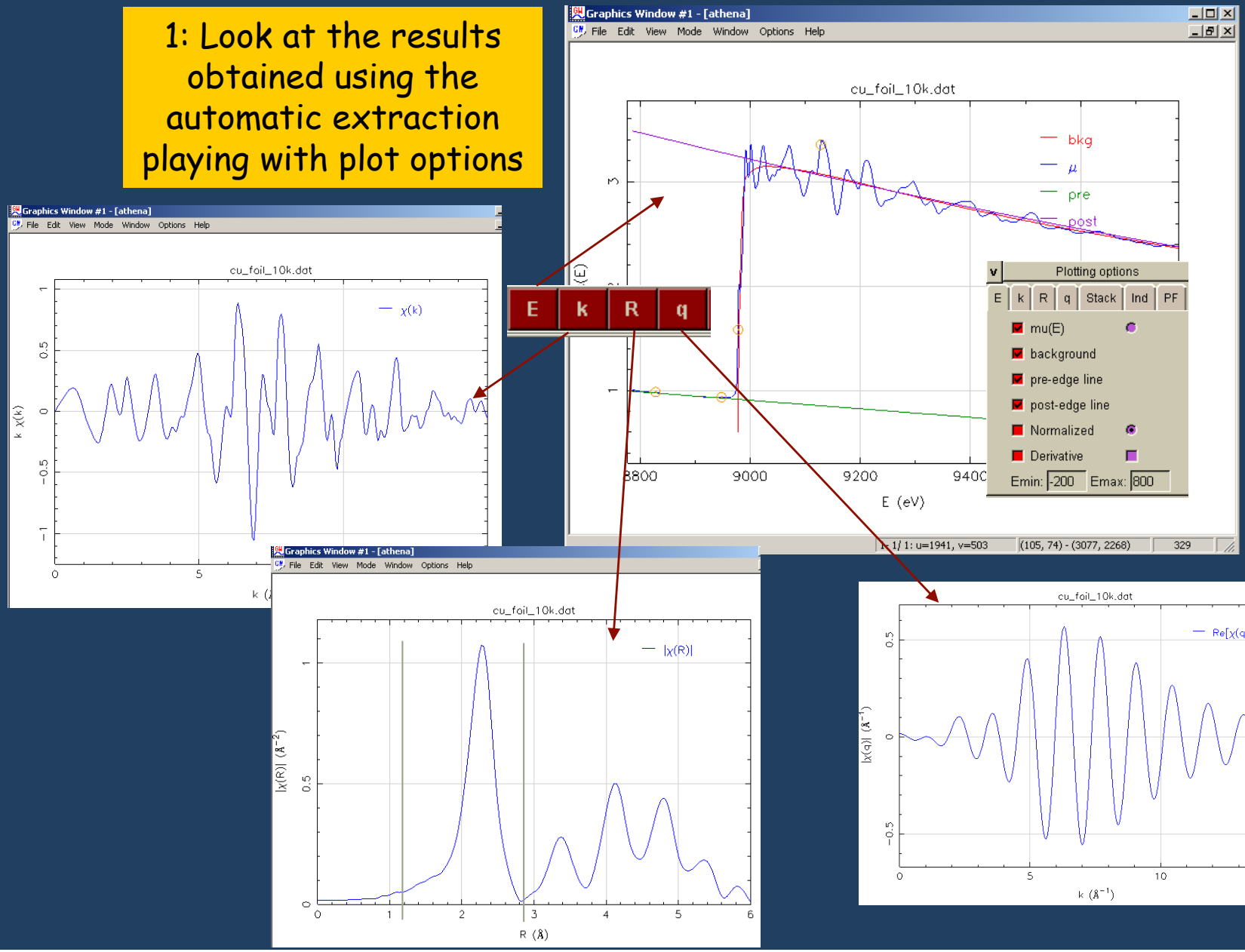
Plot (several) marked files

Options for plot

Example 1: Cu 10 K

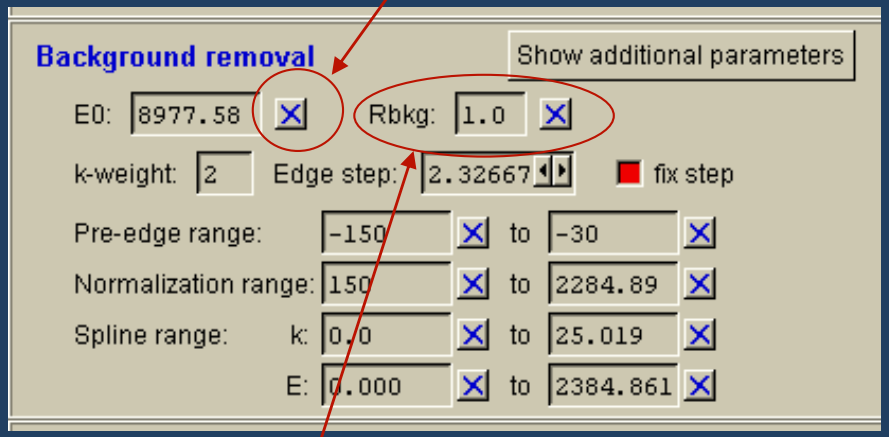
Open **cu010k.dat** into ATHENA

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



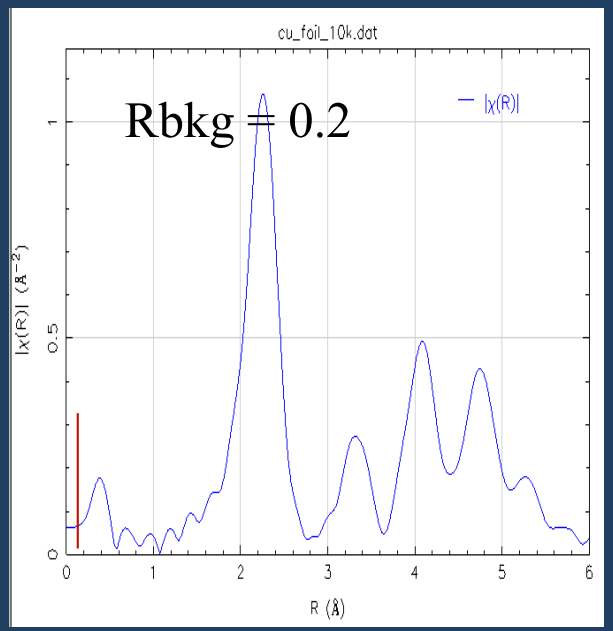
1: Look at the effects of changing background subtraction parameters

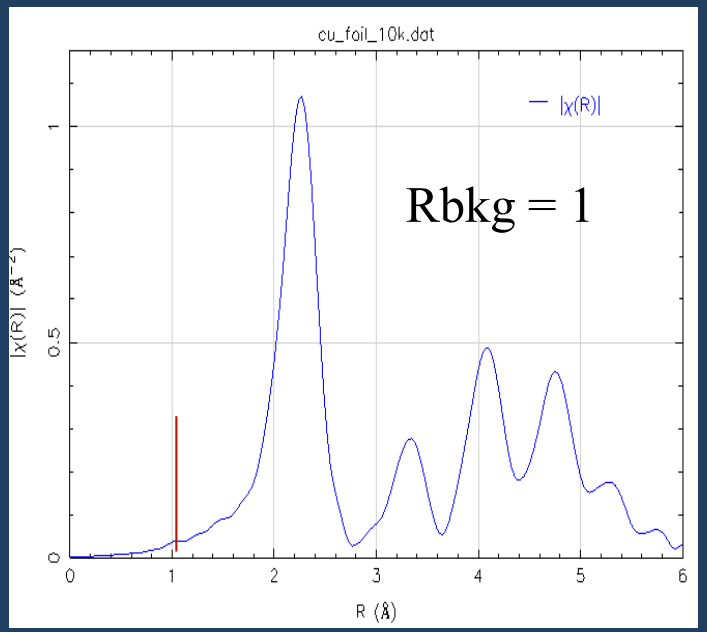
Takes the value from the cursor on the graph window

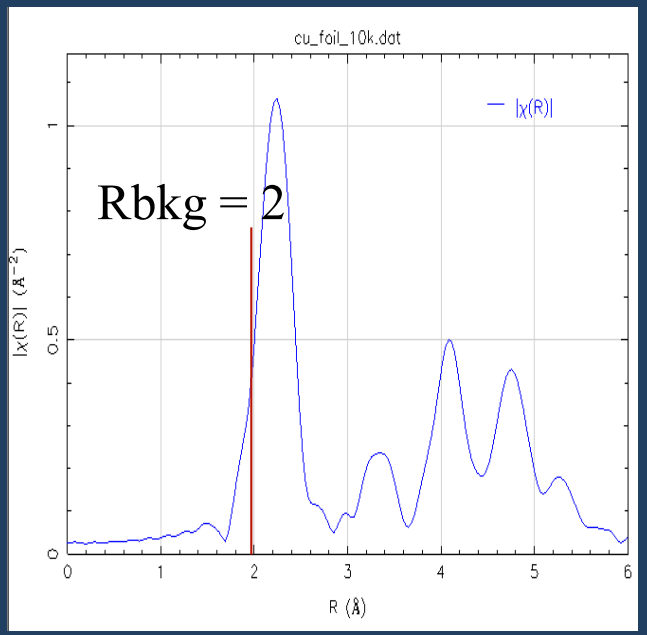


R cut off for automatic background calculation

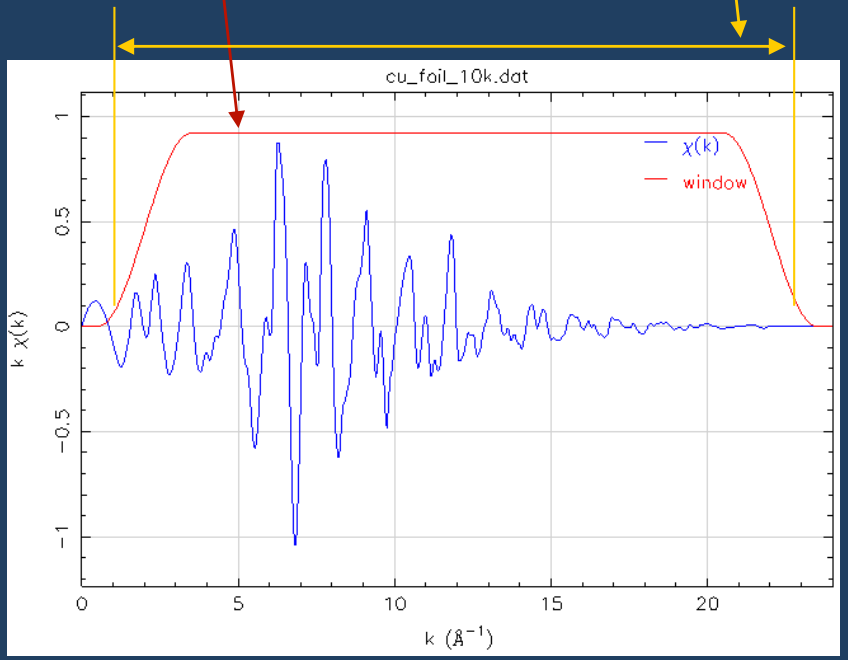
- Change Eo
- Change R_{bkg}
- ....



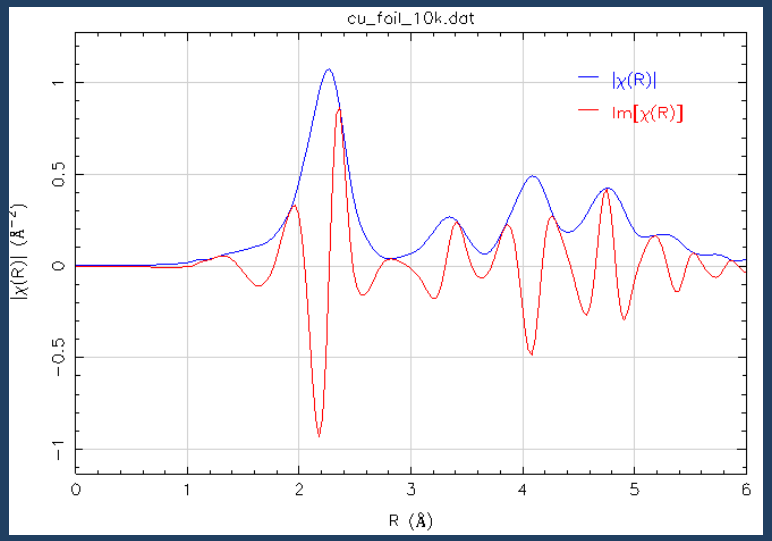


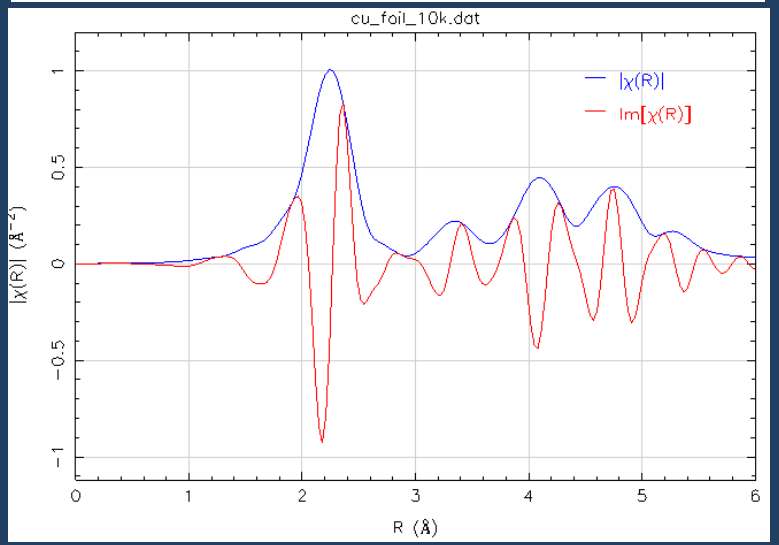


3: Look, in R space, at the effects of changing extraction and FT parameters



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



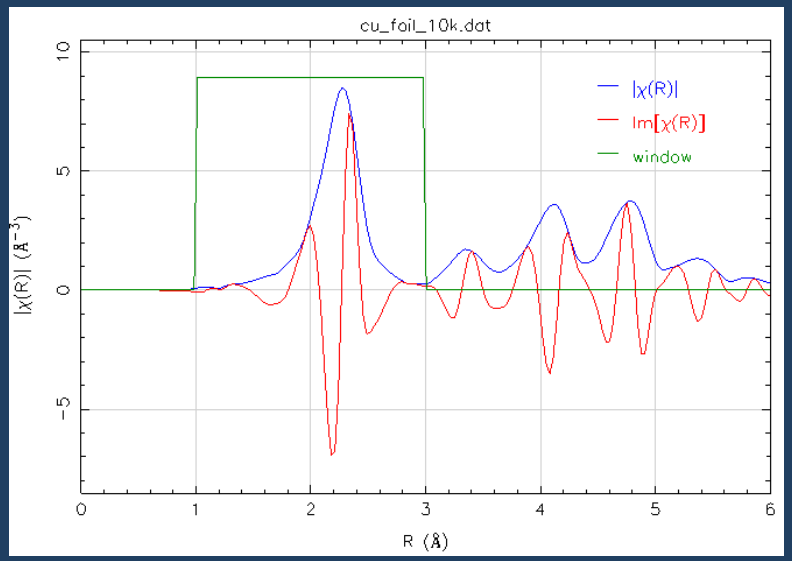


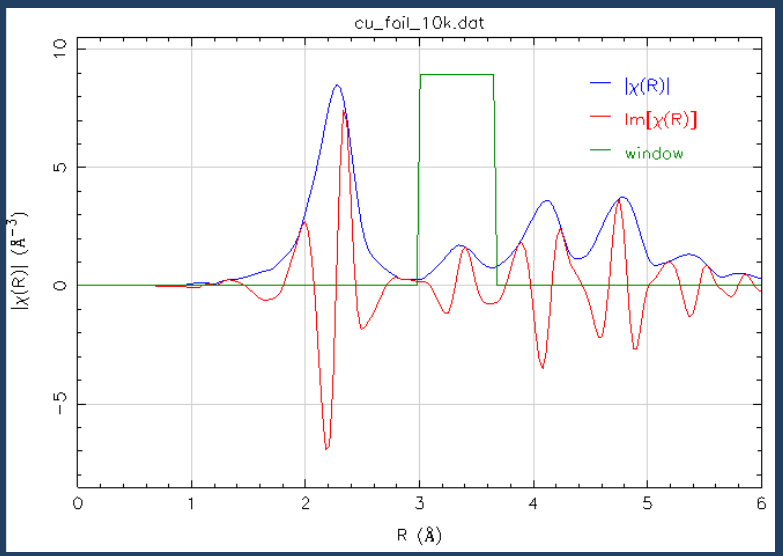
4: Look, in q (Back Fourier) space, at the effects of changing BF parameters

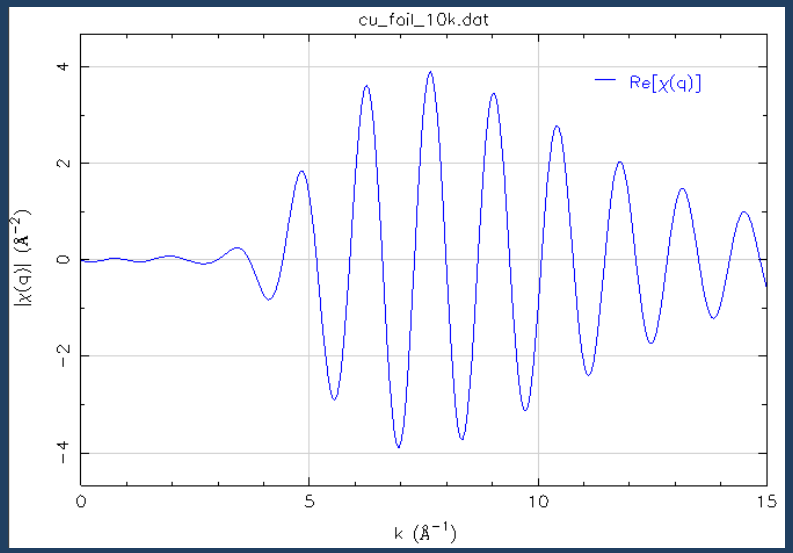
Backward Fourier transform

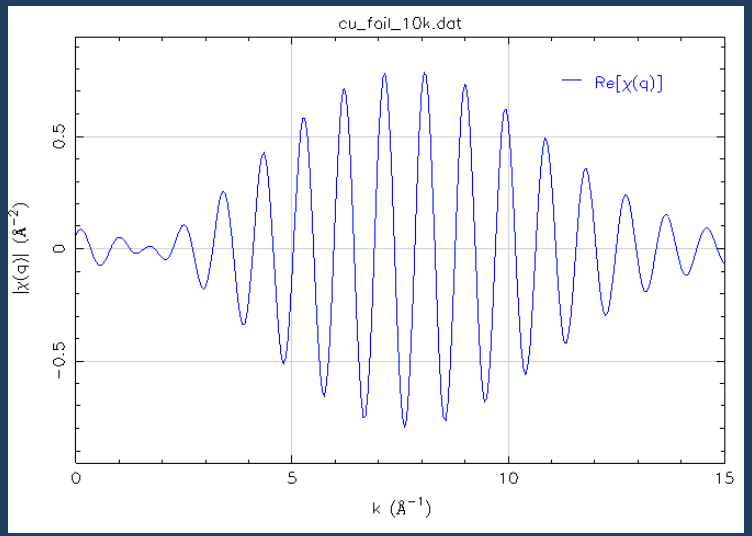
R-range: 1 to 3

dr: 0.0 window type: hanning

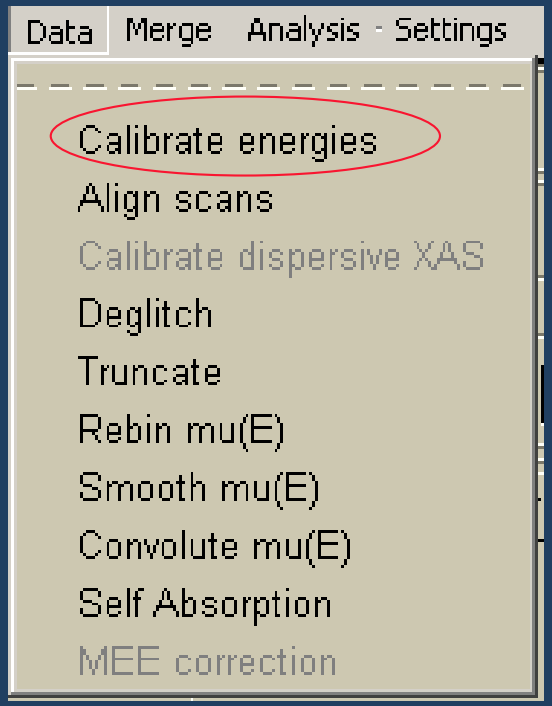


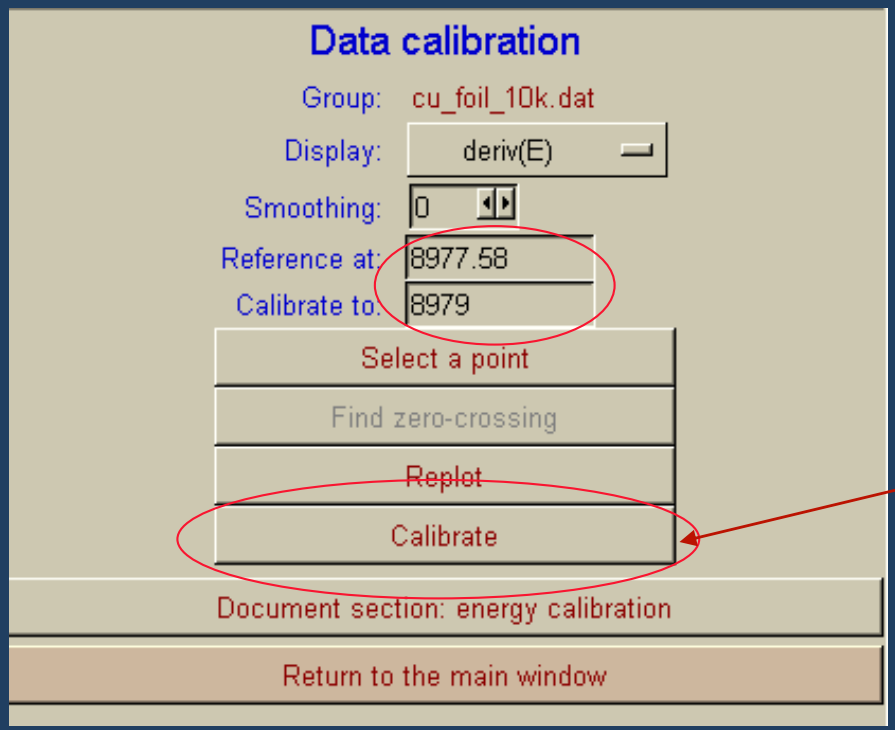


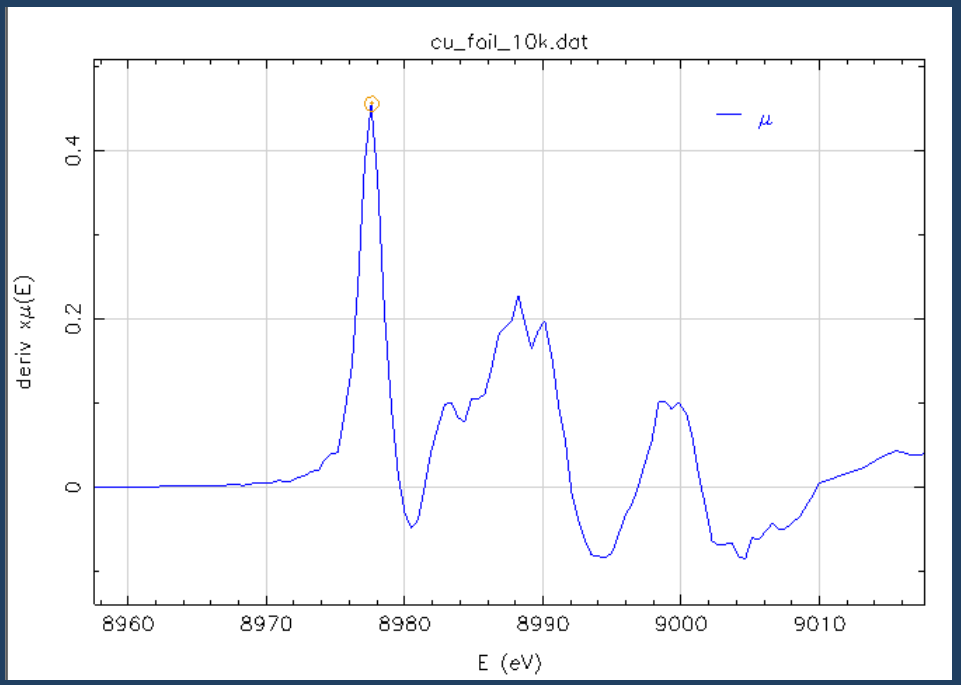


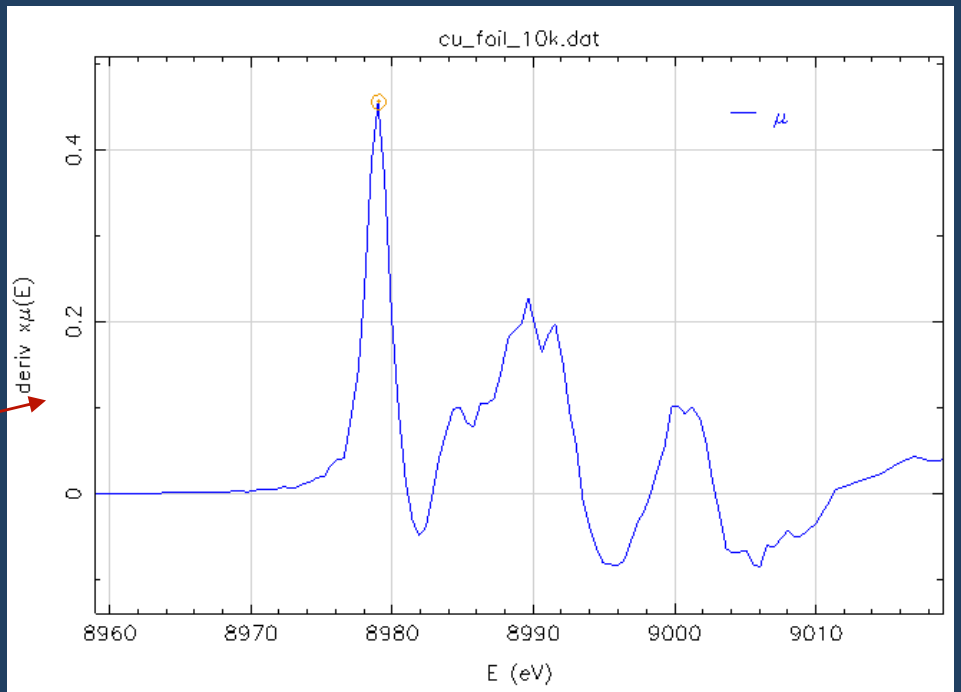


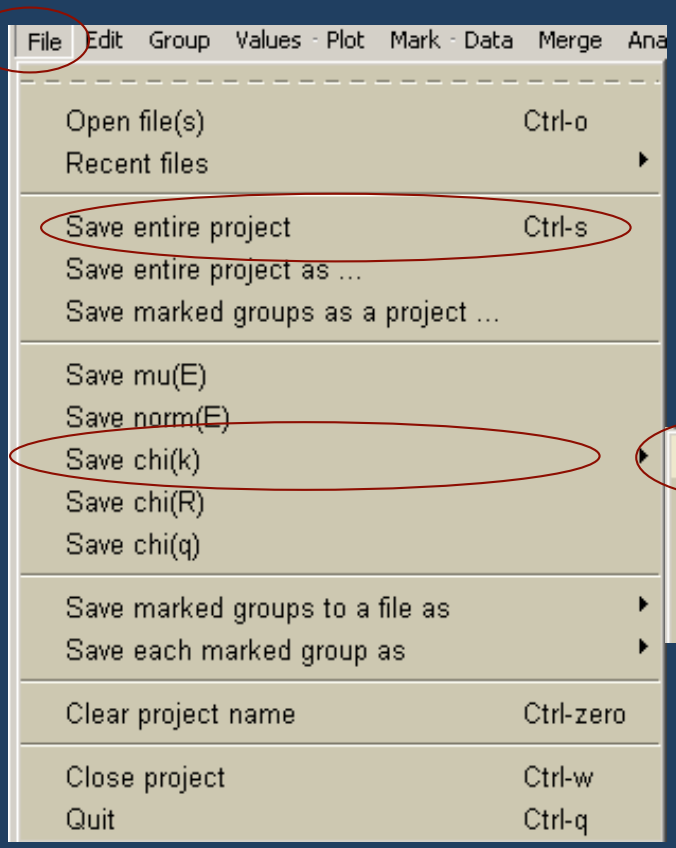
5: Data pre-treatment







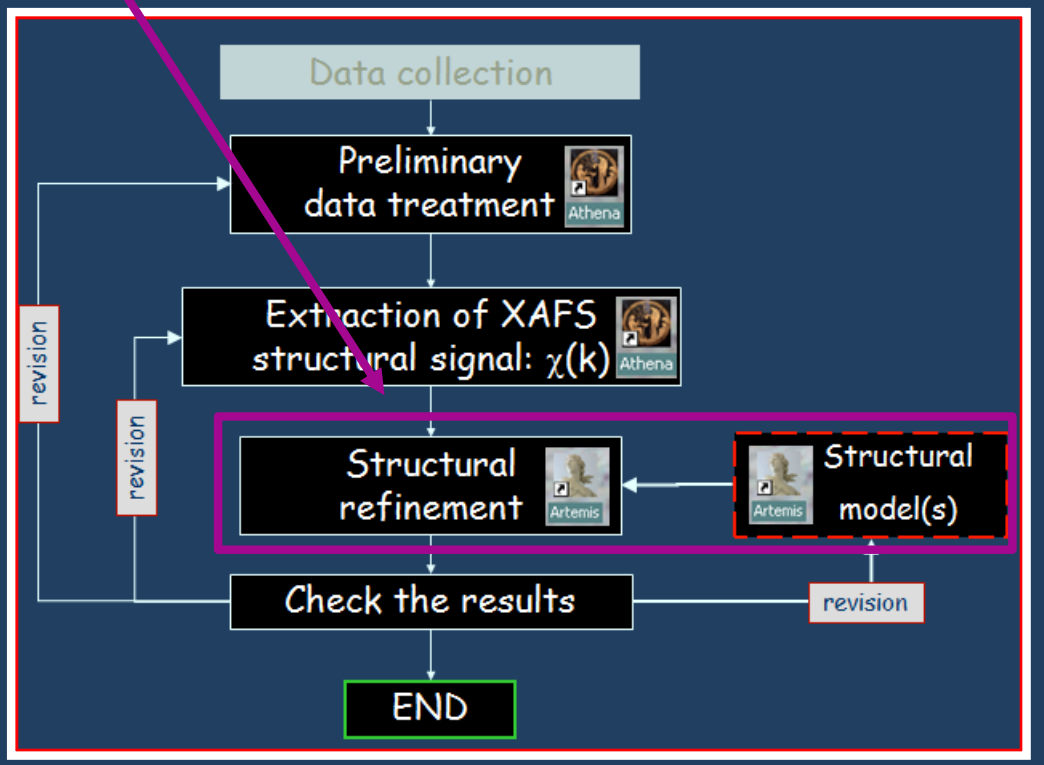




Save:

cu_foil_10k.dat.chi

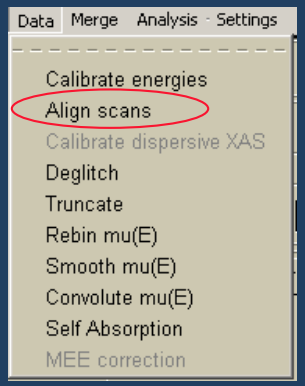
χ(k) is required for ARTEMIS

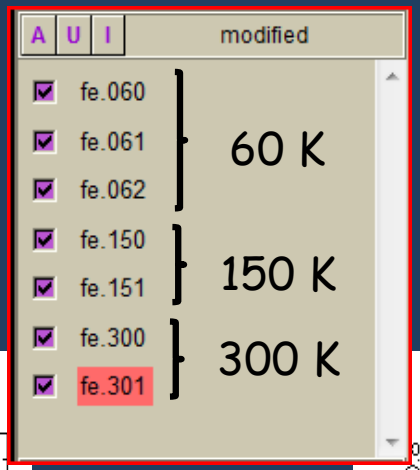


Working with several files

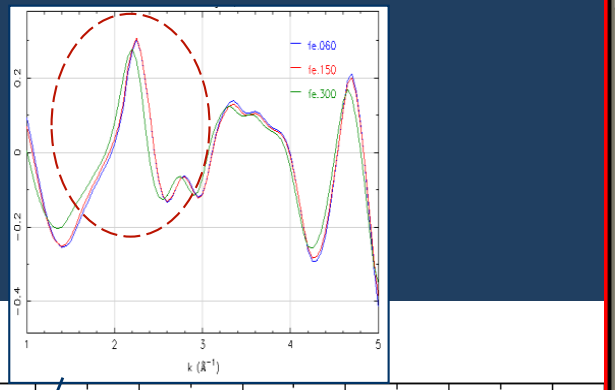
Go into the **Fe** directory

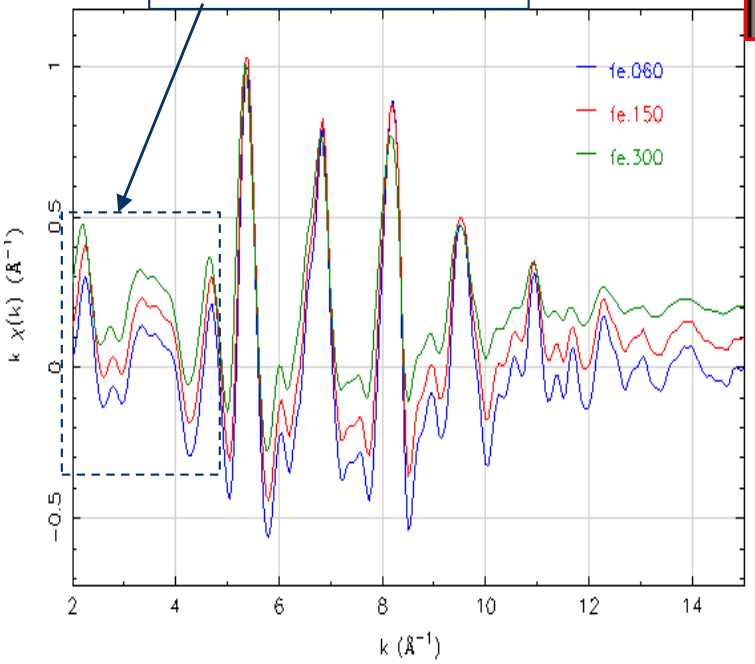
Open all the files (except README) into Athena

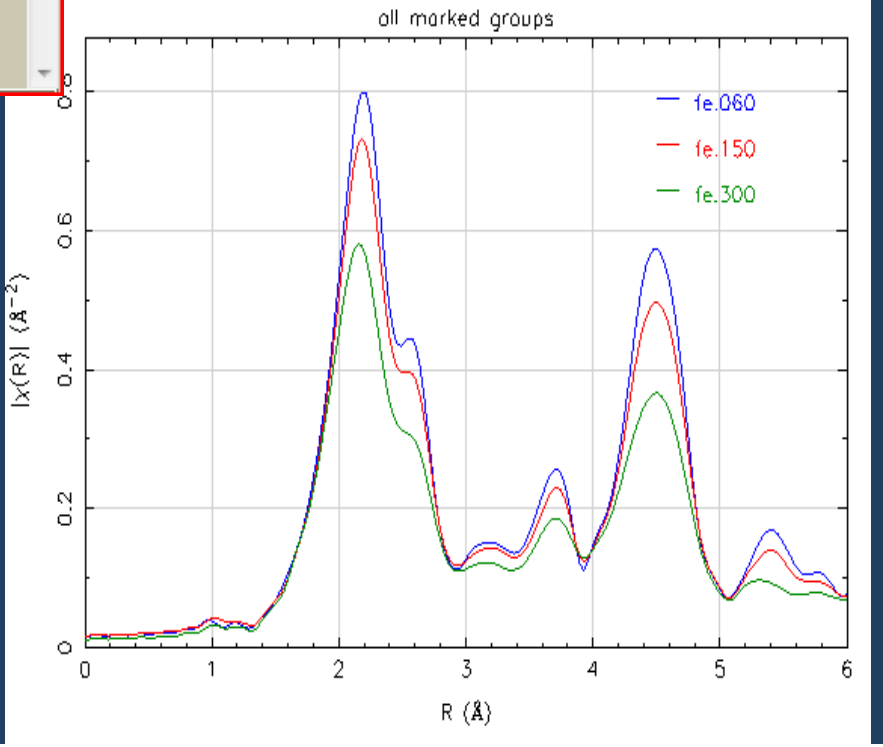




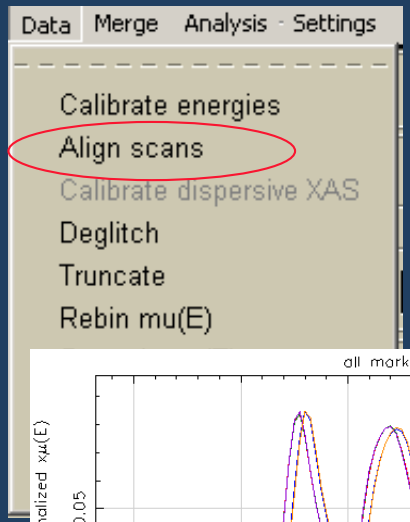
Themperature effect

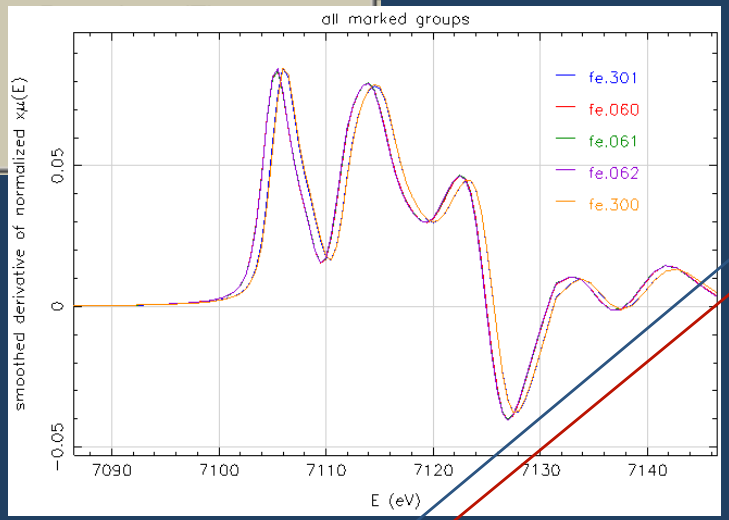


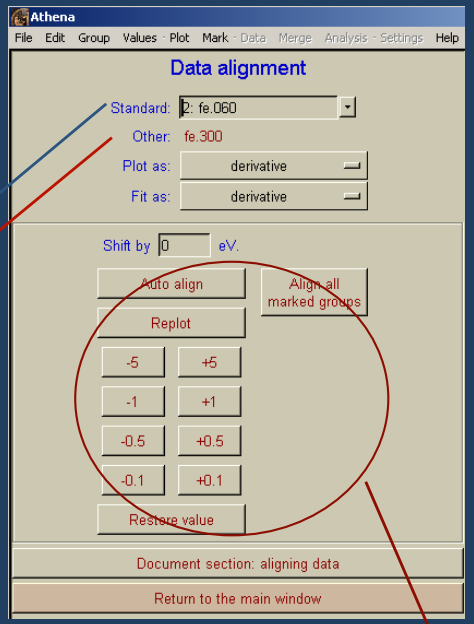




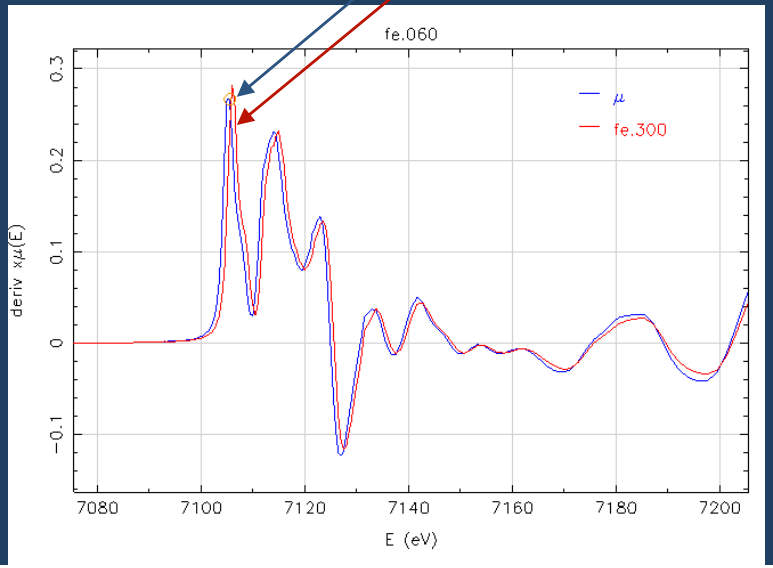
5: Data treatment: Align Eo

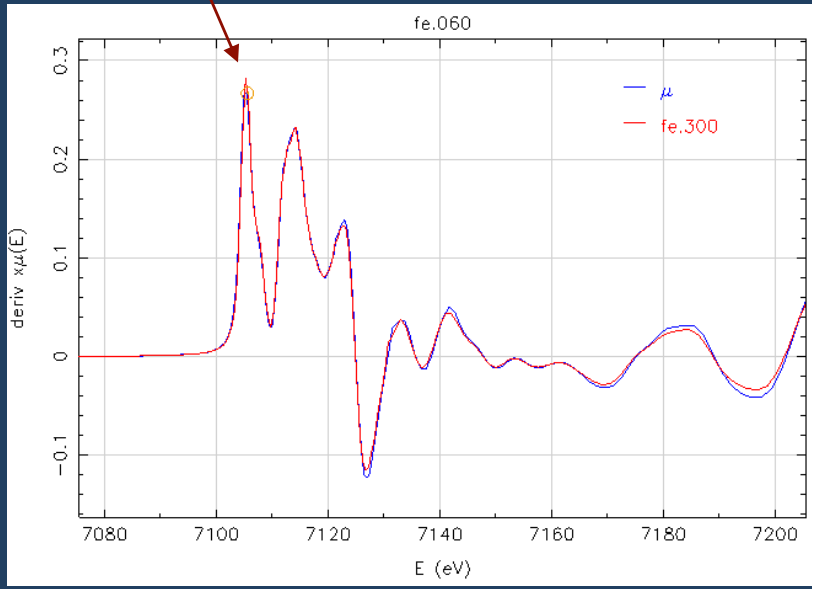




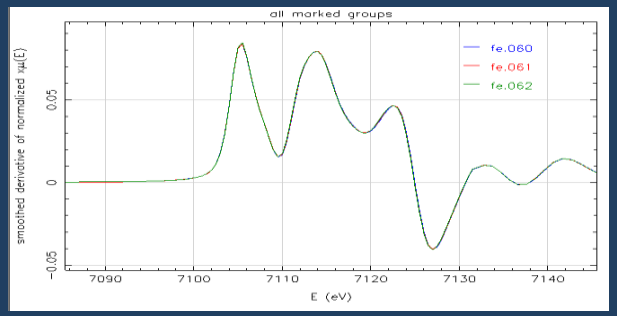


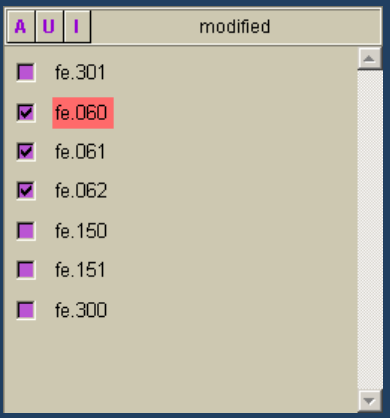
Eo appear shifted among the files

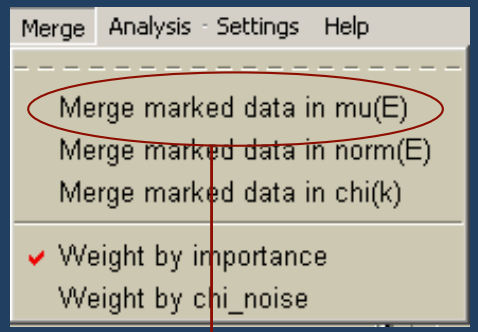


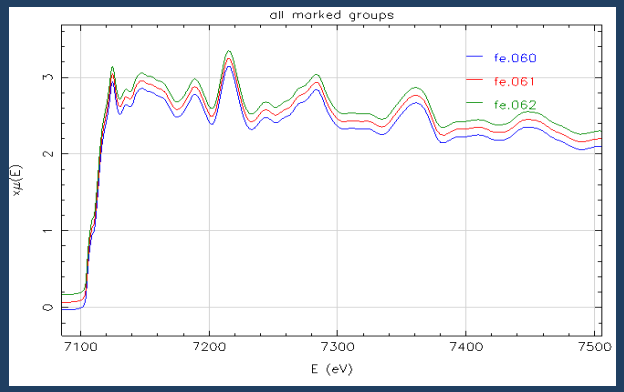


5: Data treatment: Merge several files

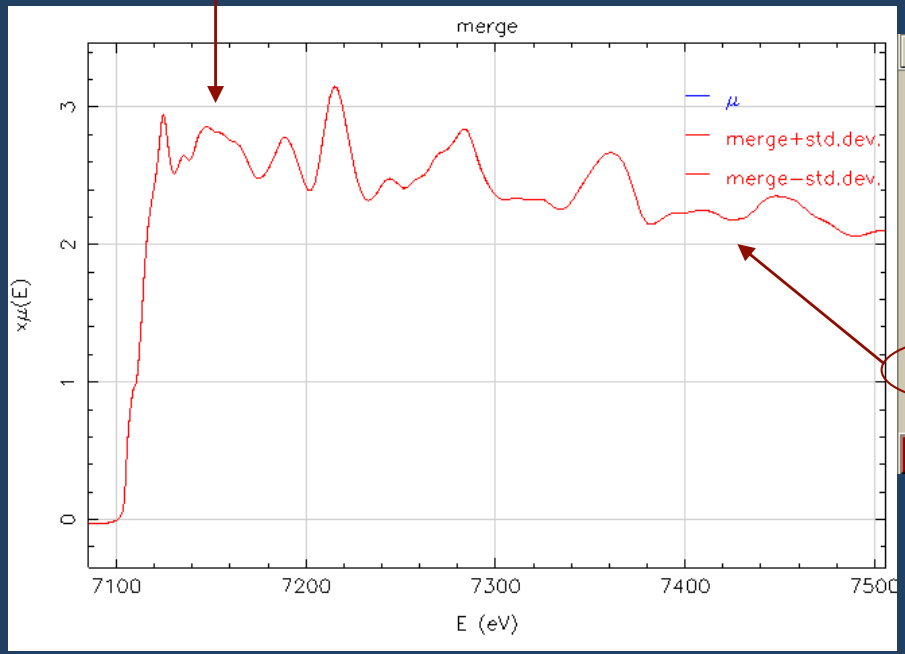


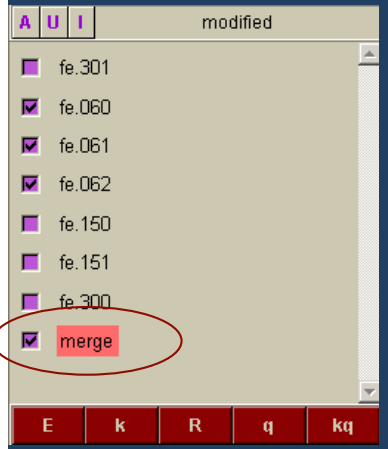


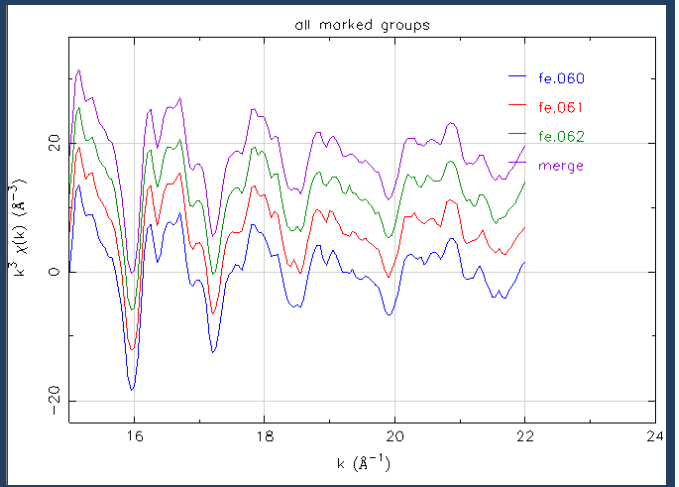




Fe 60 are aligned



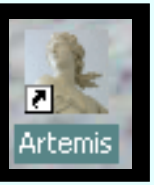




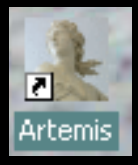
Exercise:

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

Structural refinement

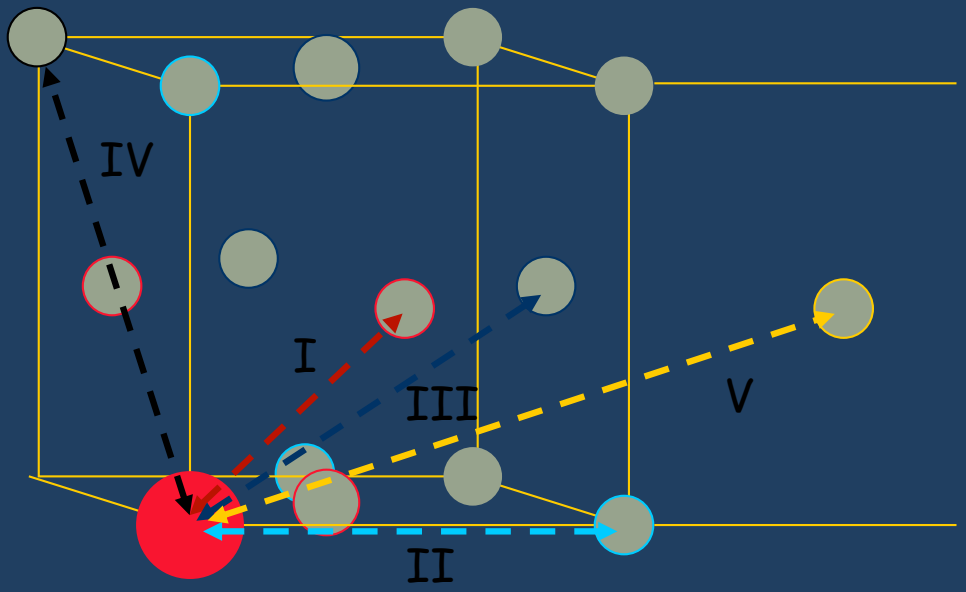


Structural model(s)



Cu-fcc

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

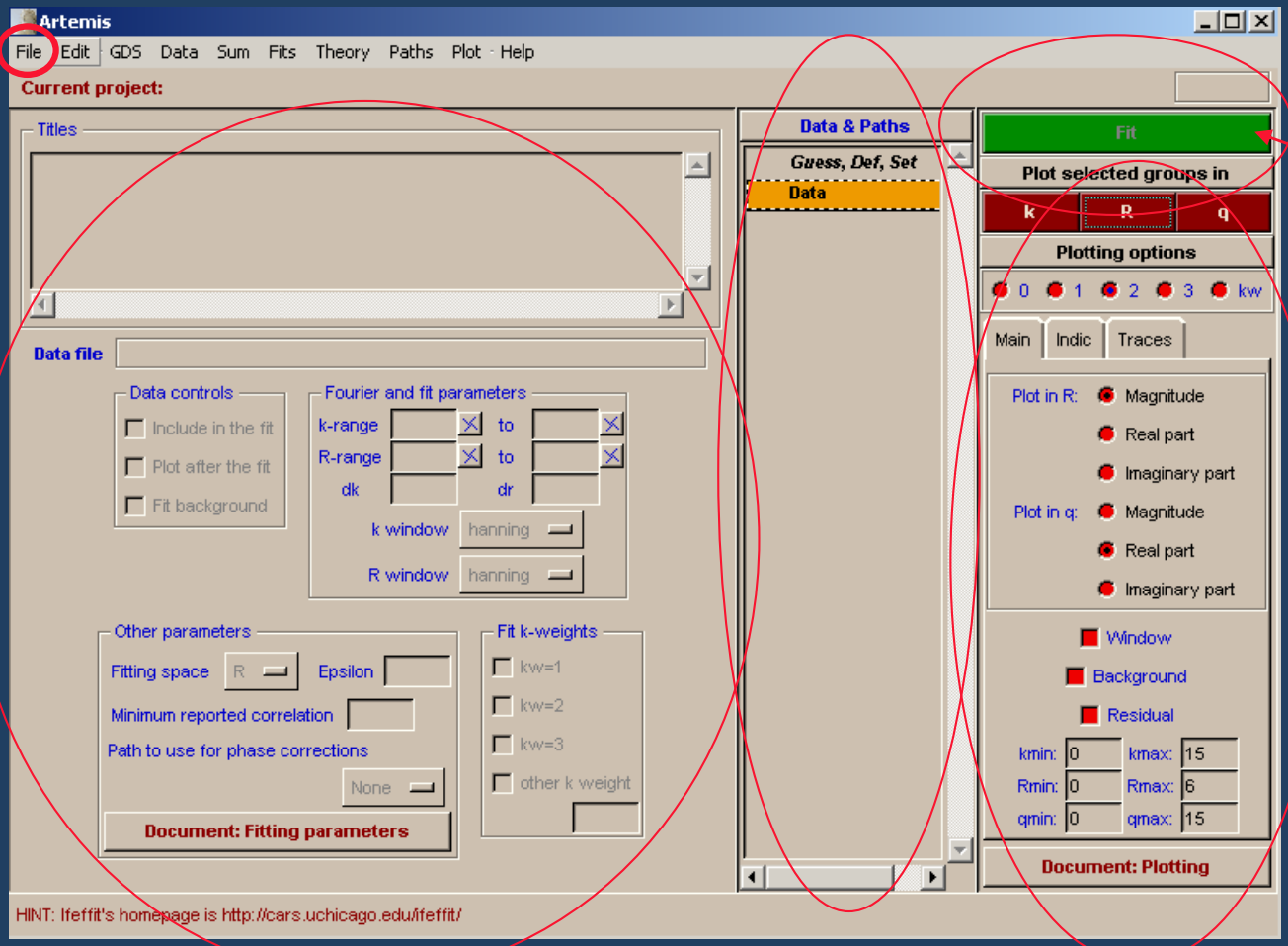


Sh	R	N	$R_{Cu}(A)$
I:	a/sqrt(2)	12	2.553
II:	a	6	3.610
III:	a·sqrt(1.5)	24	4.421
IV:	a·sqrt(2)	12	5.105
V:	a·sqrt(2.5)	24	5.708
....			

Structural model & Data refinement

Start ARTEMIS program

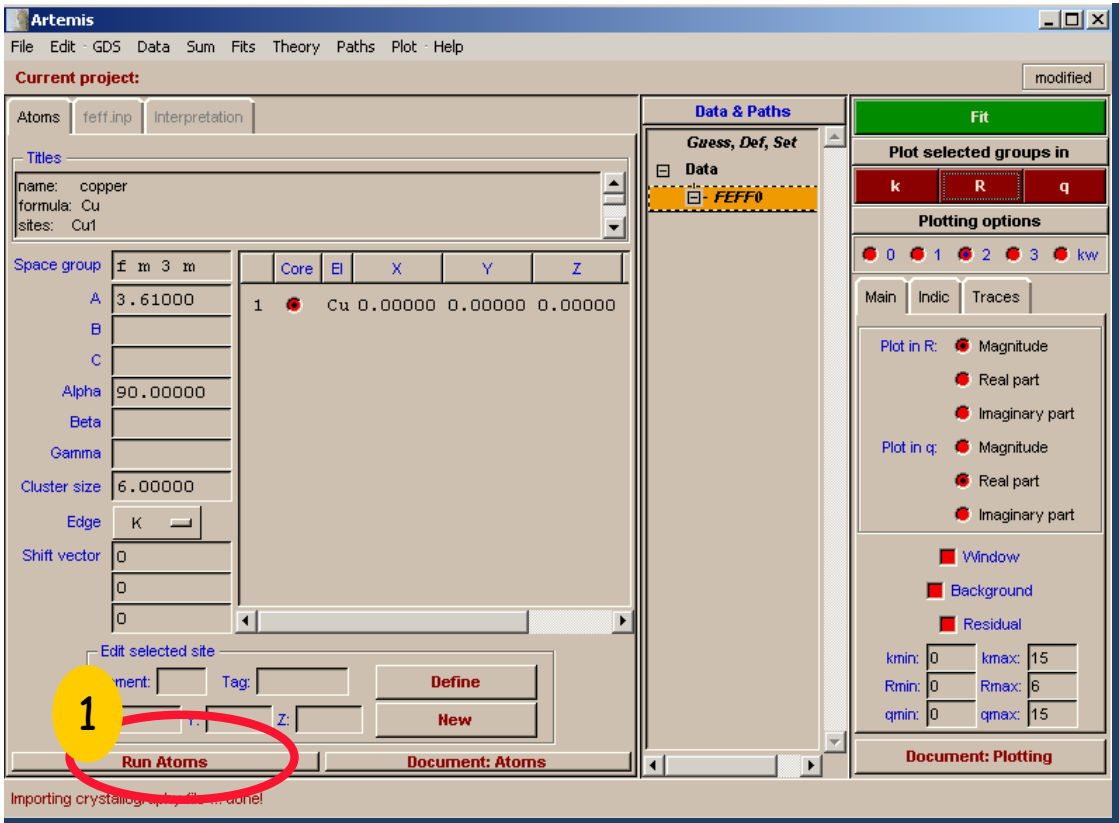
Open Cu.inp file from the Cu directory

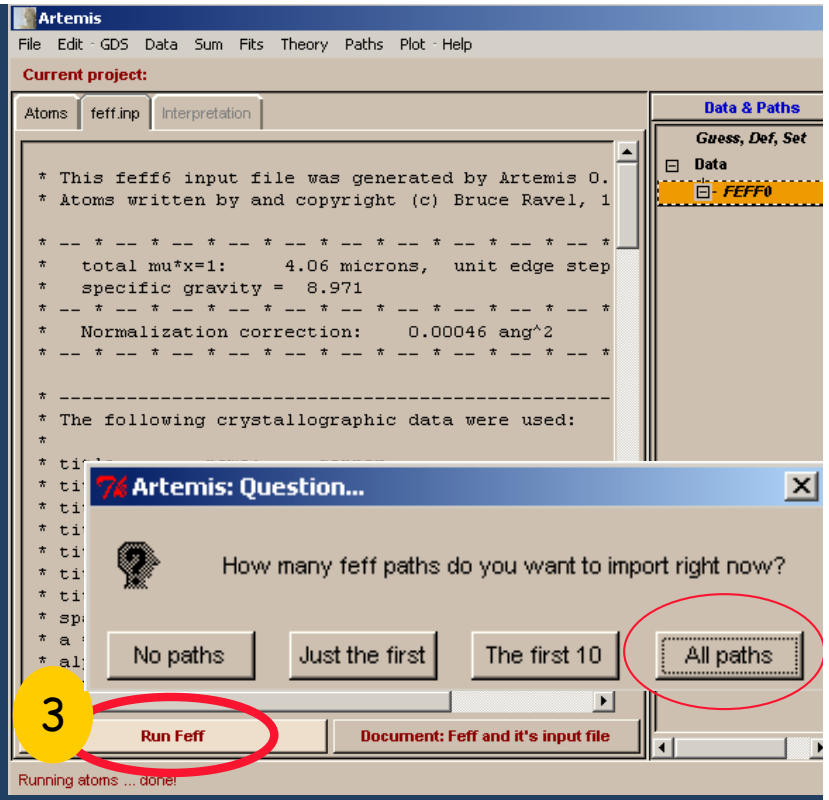


Start the refinement

Depends on what is highlighted in the Data & Paths panel

Controls for plotting

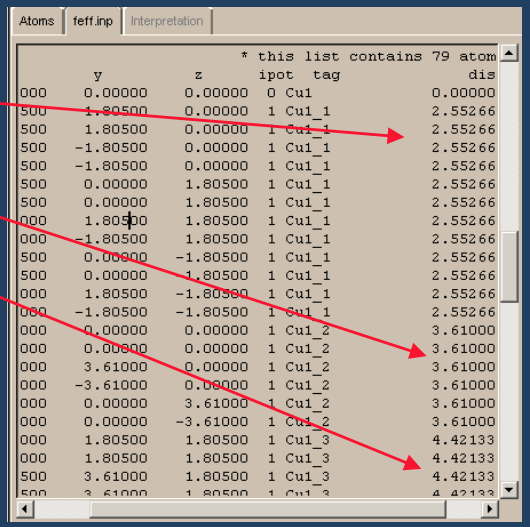




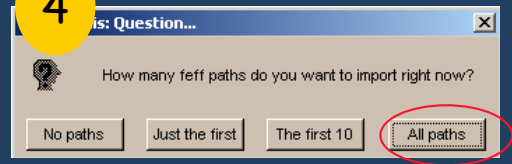
It builds the cluster

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

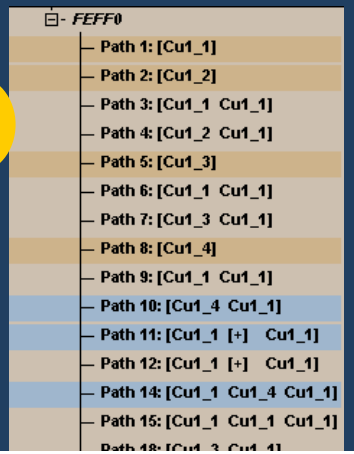
2

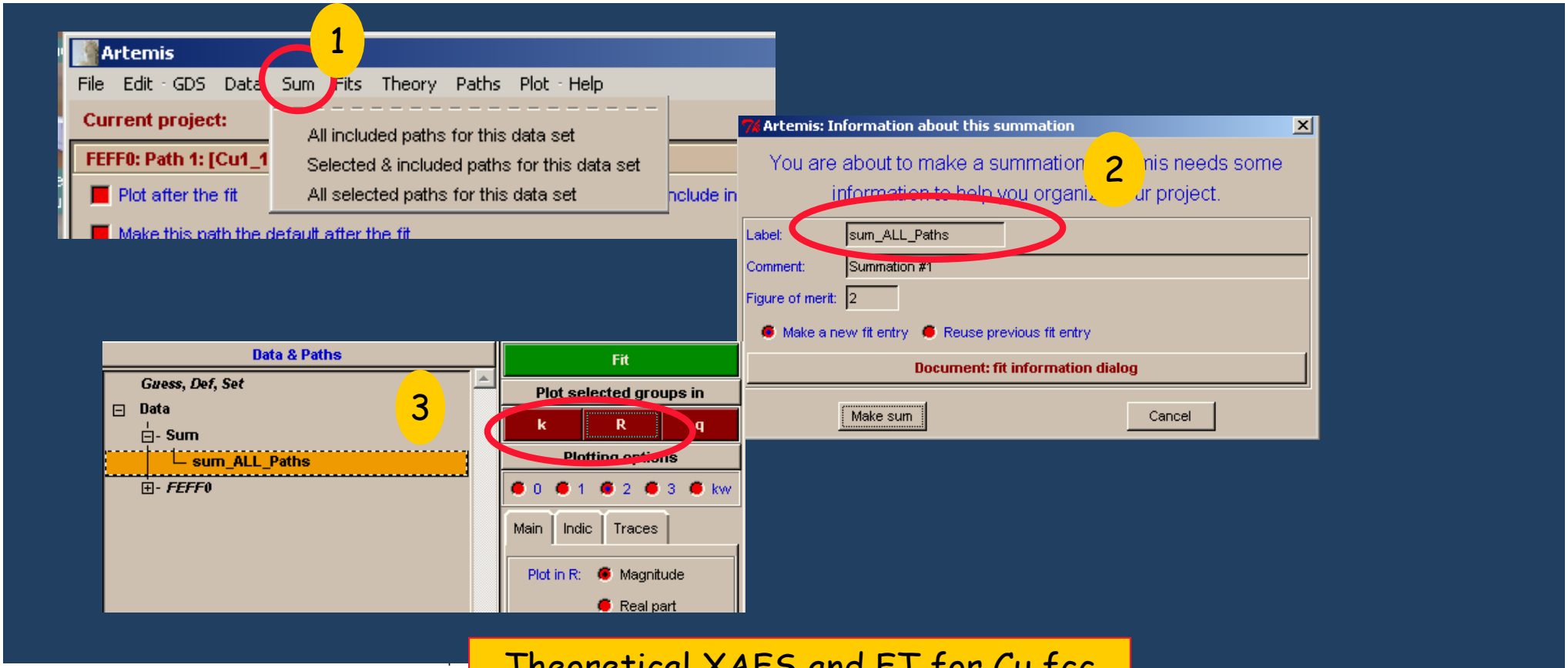


4

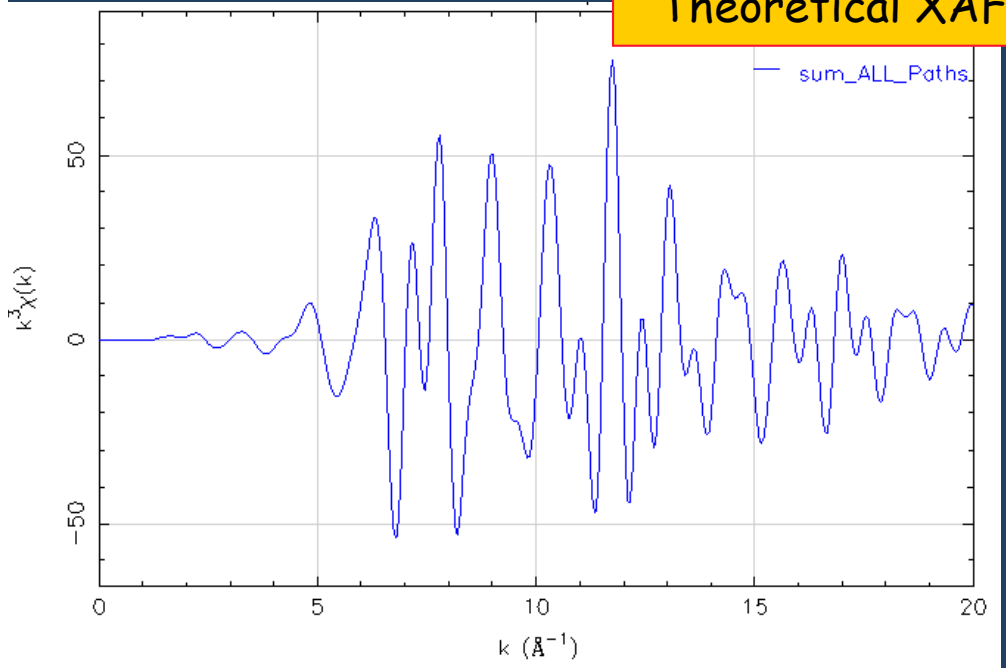


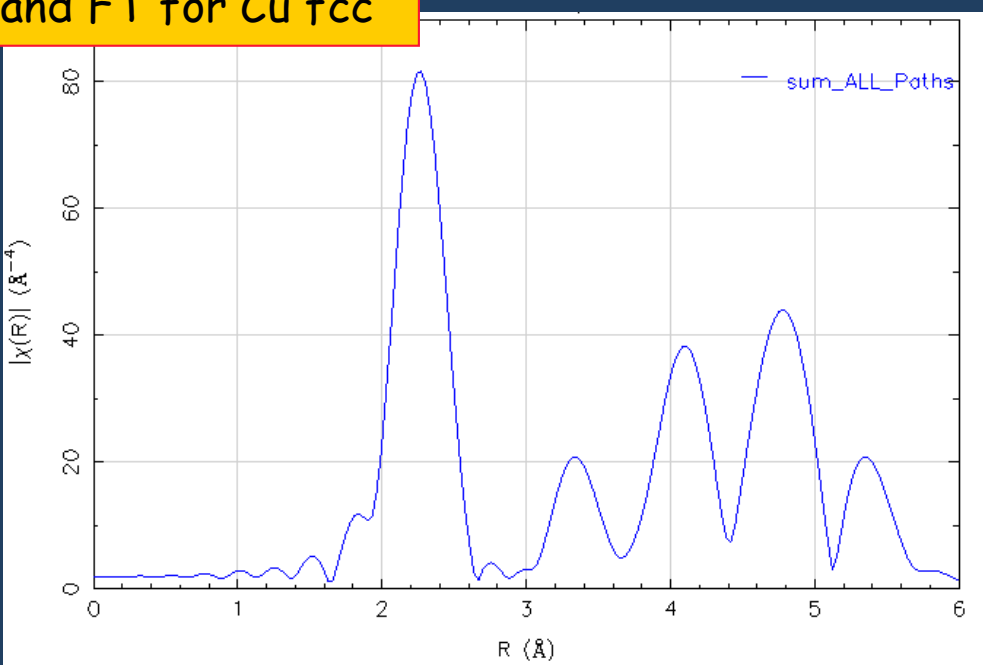
5





Theoretical XAFS and FT for Cu fcc

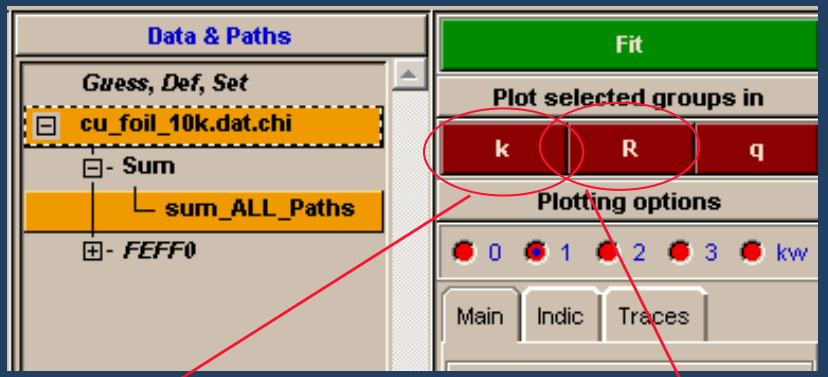


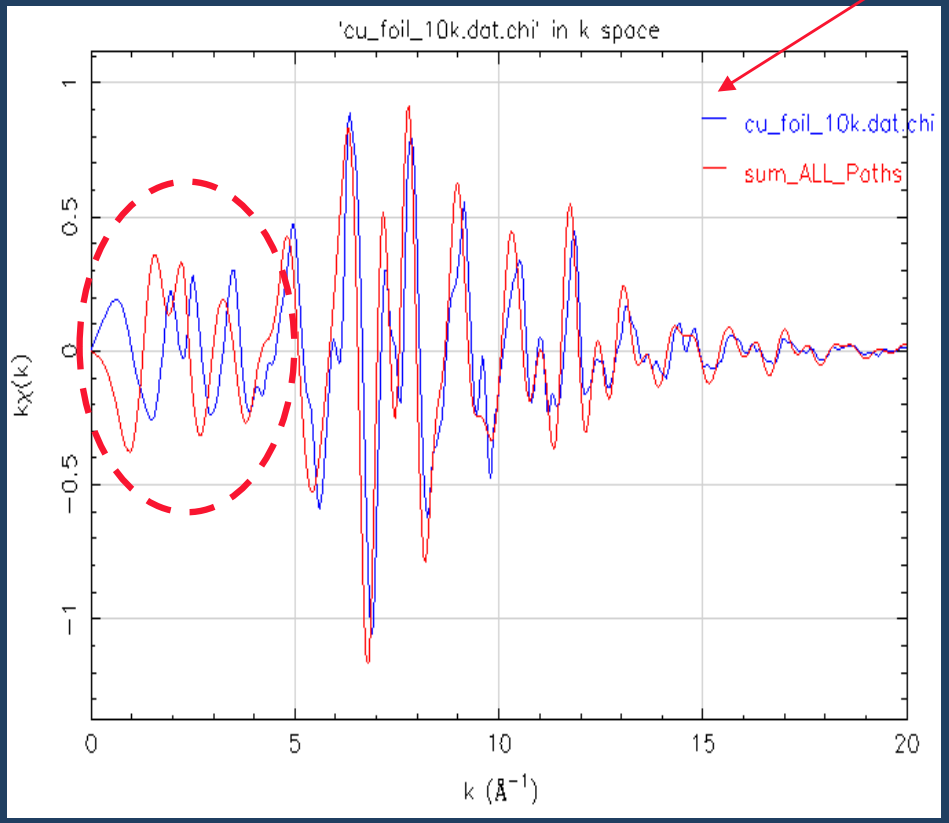


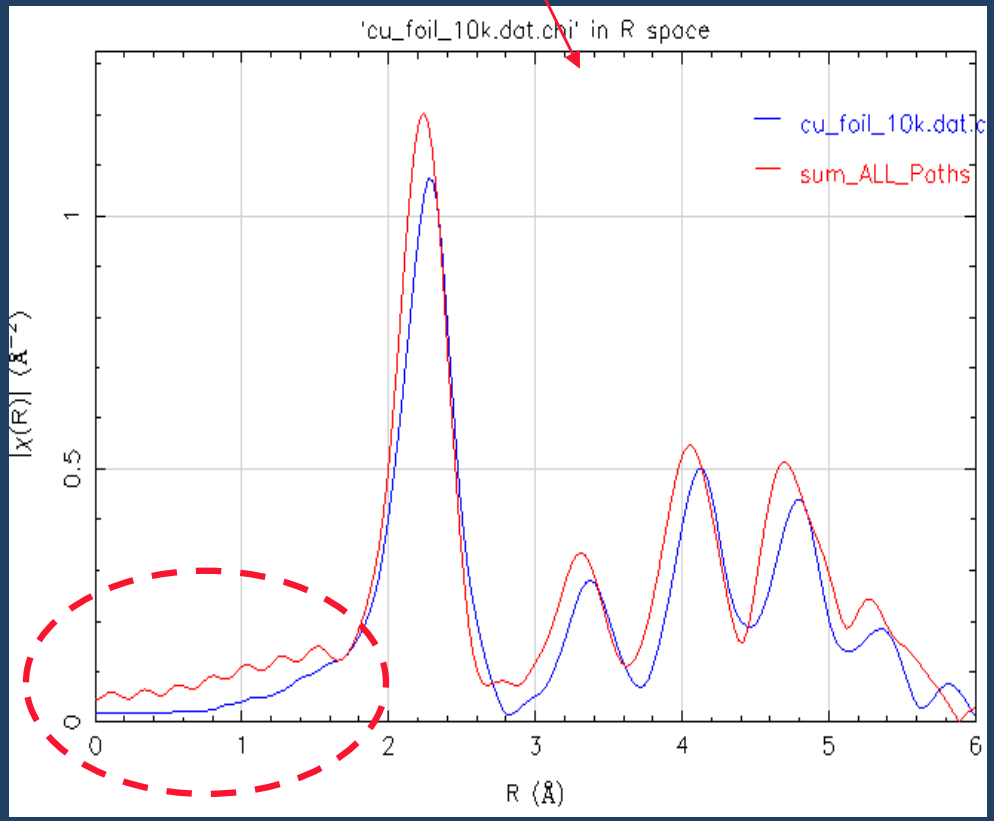
Compare model and experimental data

Open Cu010k.chi

Using CRTL key select groups for plot



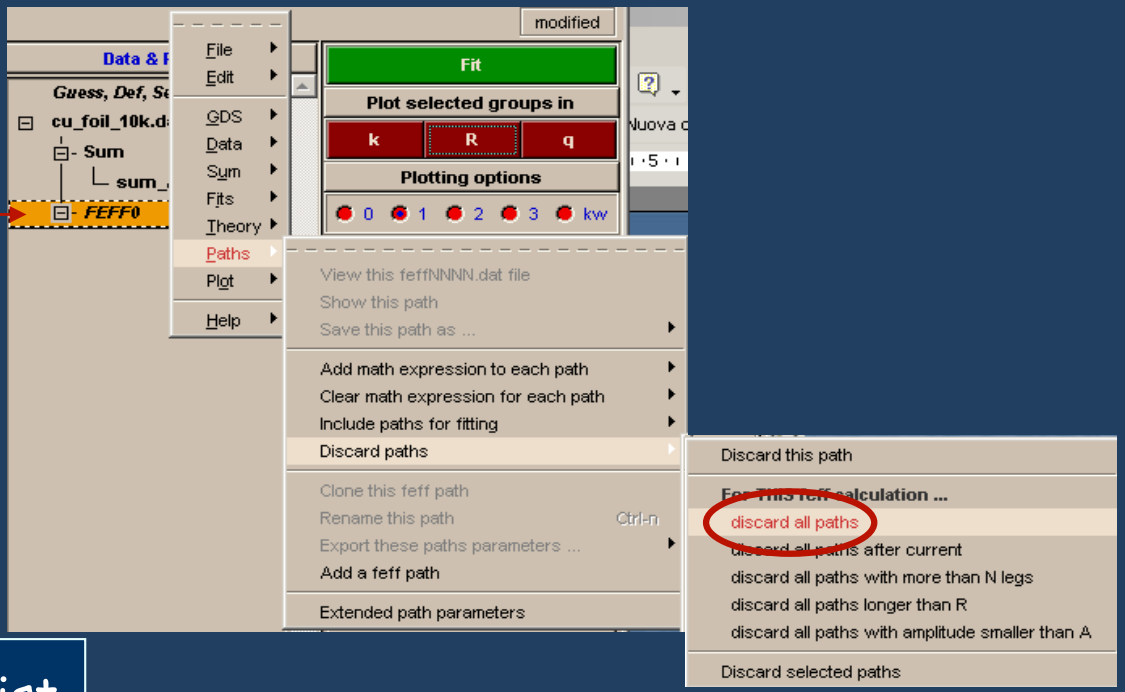




1st shell analysis

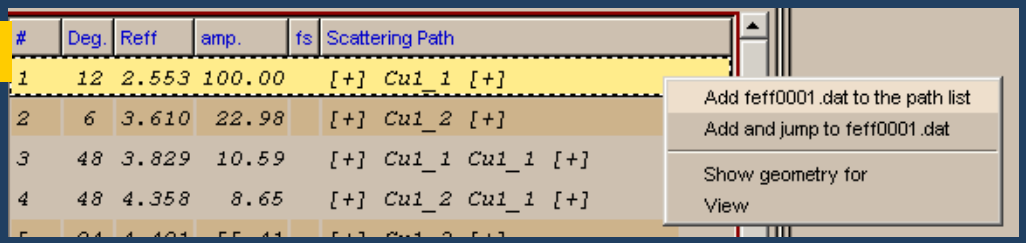
remove all paths or restart ARTEMIS

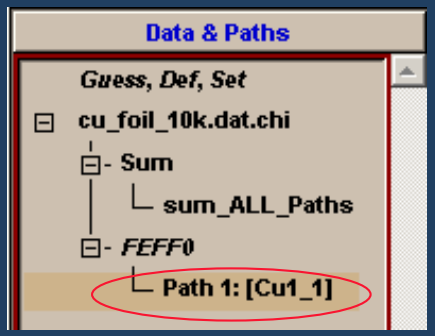
Right click

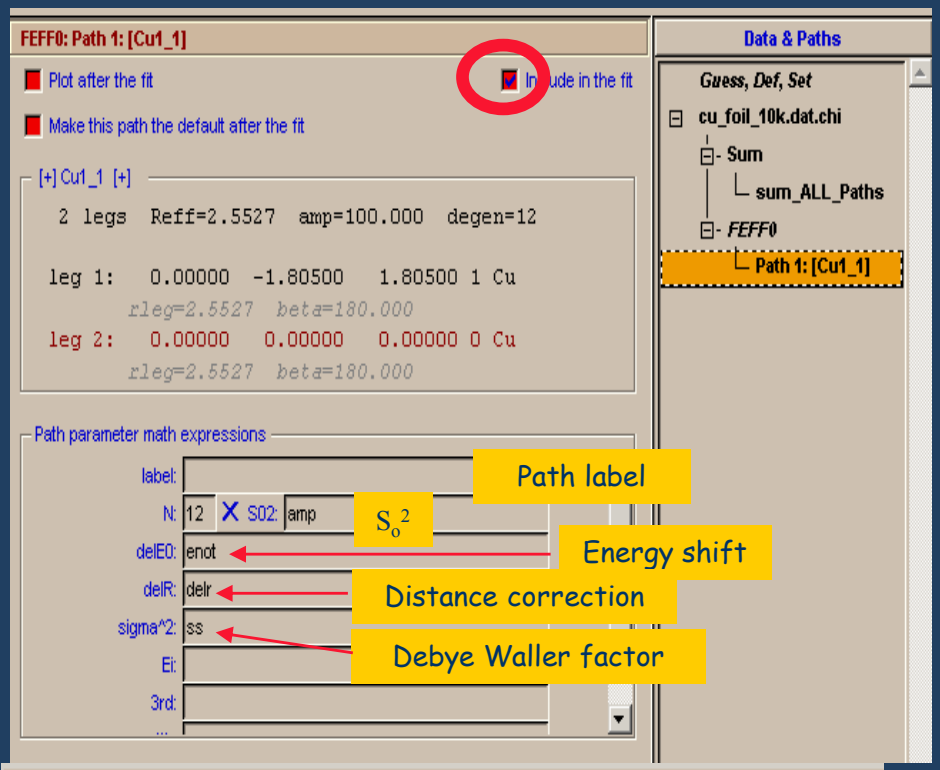


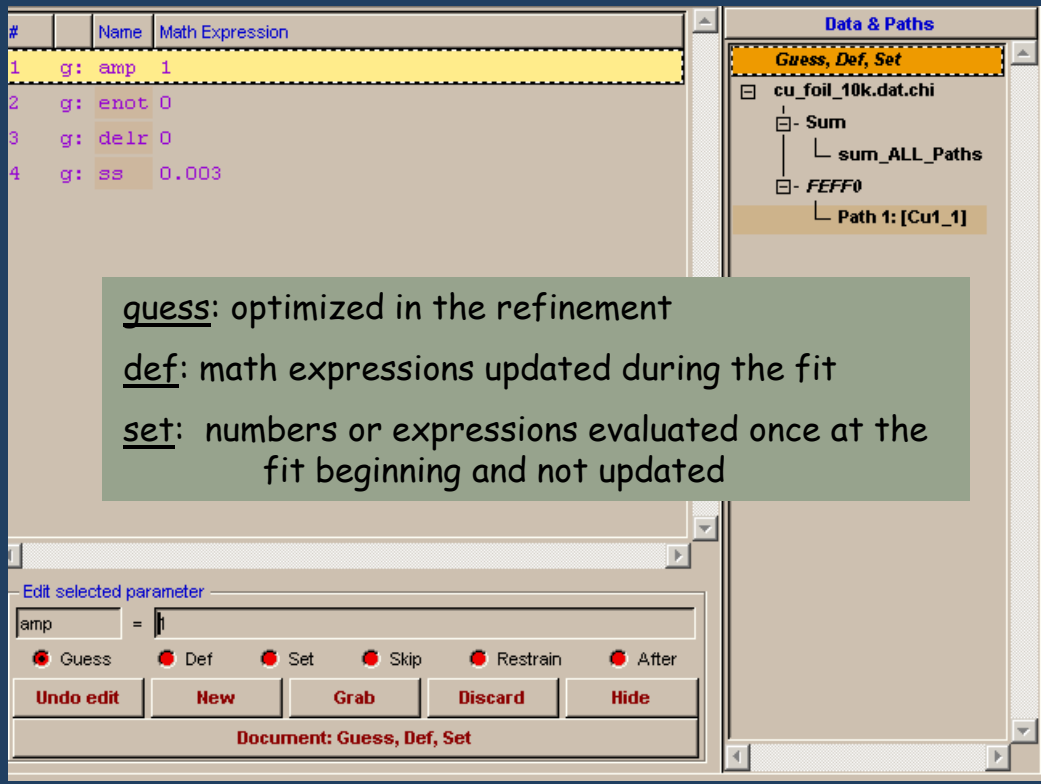
add 1st shell path to the list

select and Right click





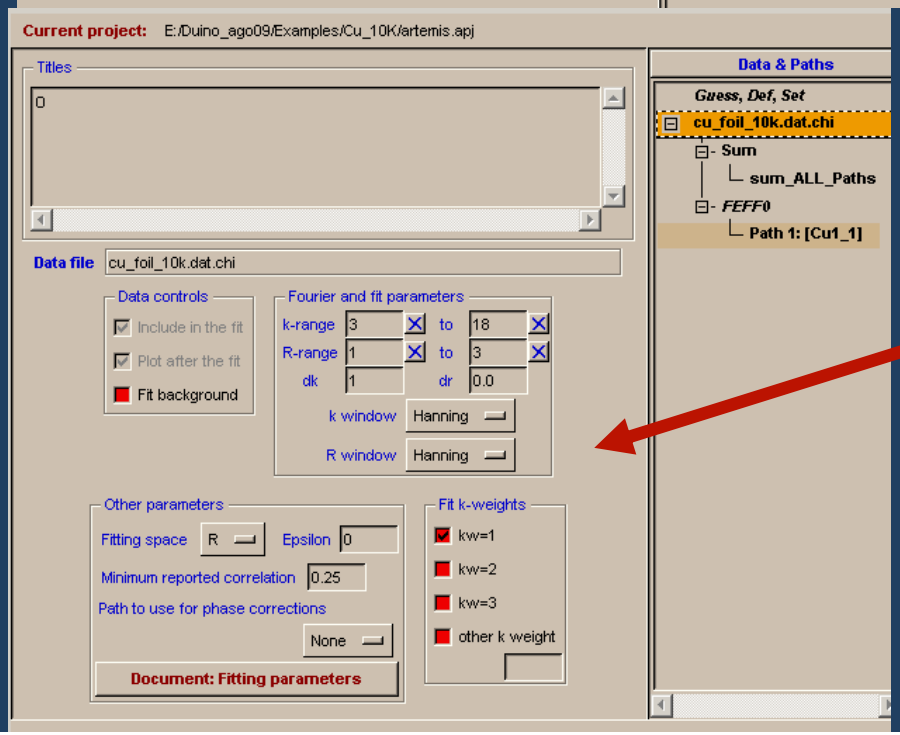




guess: optimized in the refinement

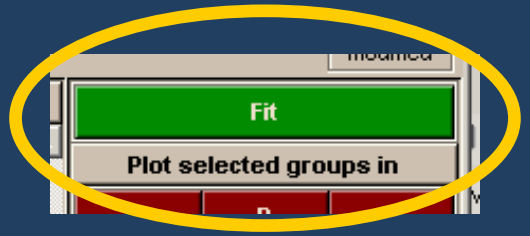
def: math expressions updated during the fit

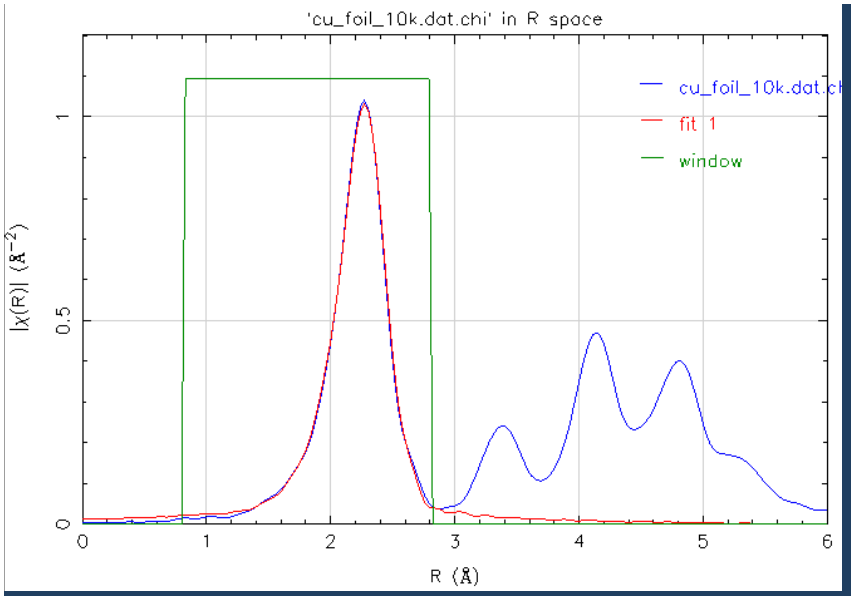
set: numbers or expressions evaluated once at the fit beginning and not updated

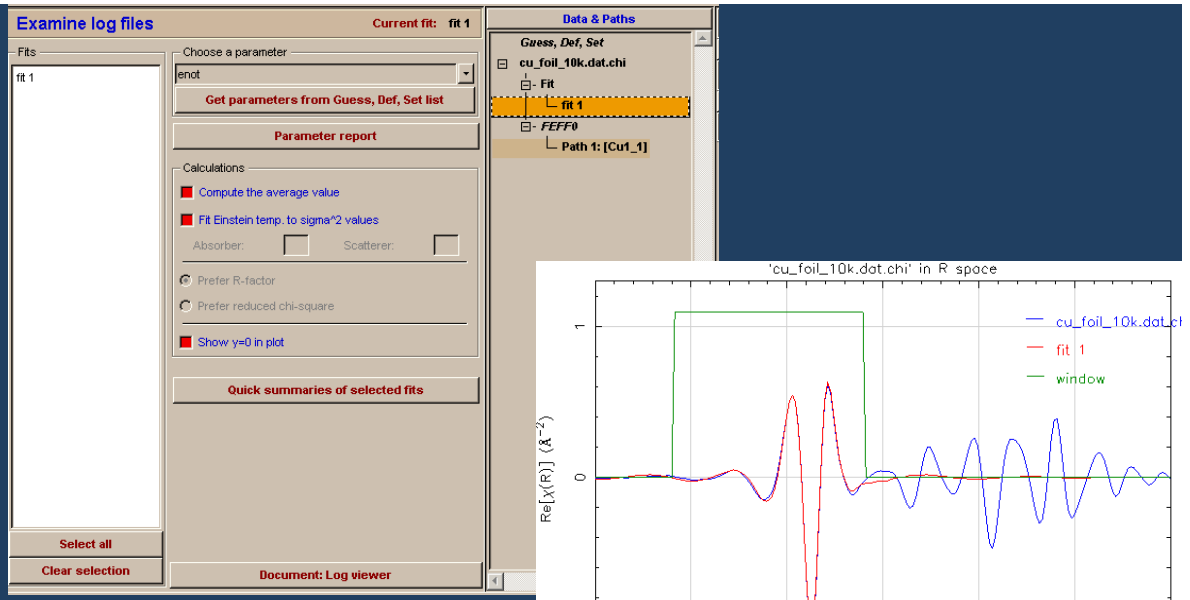


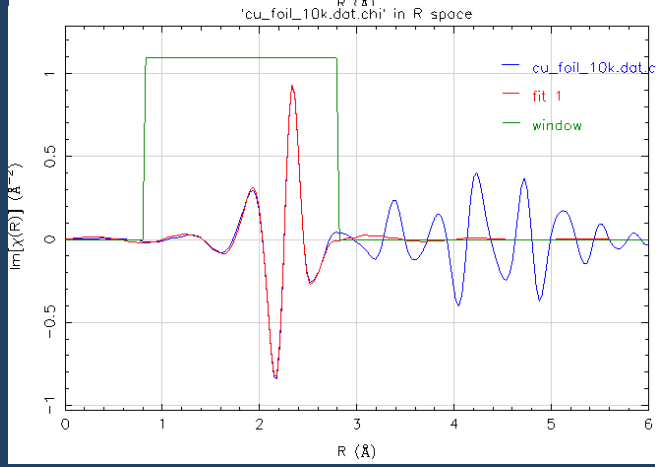
$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

The Data screen allow defining the fitting strategy and parameters









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

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

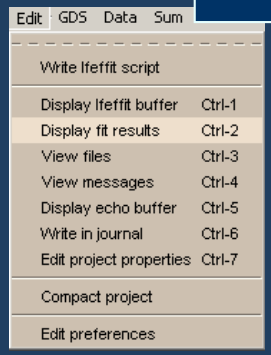
$\nu = N_{ind} - N_{var}$

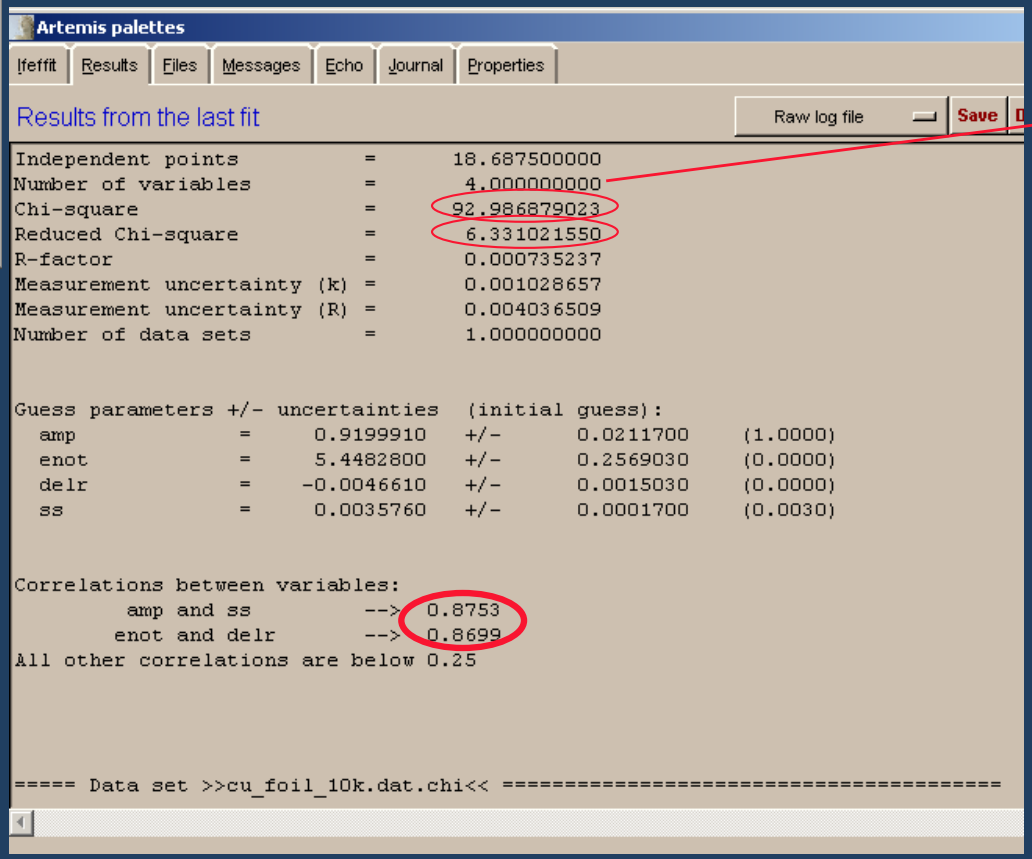
The refinement is performed on the Real and Imaginary parts of the FT

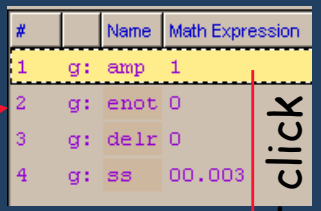
$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right]}{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i)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

Absolute misfit between experimental data and theory

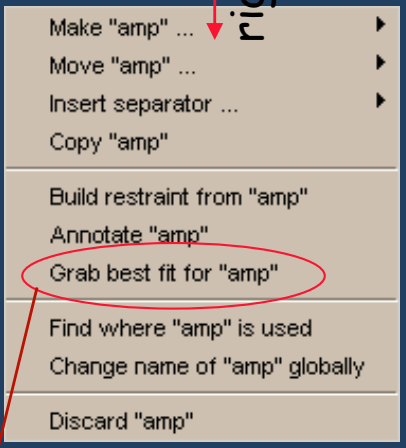
Structural results

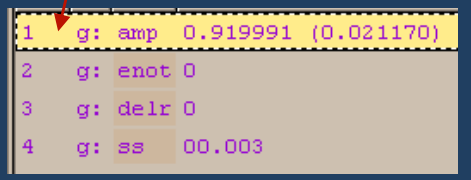






right click

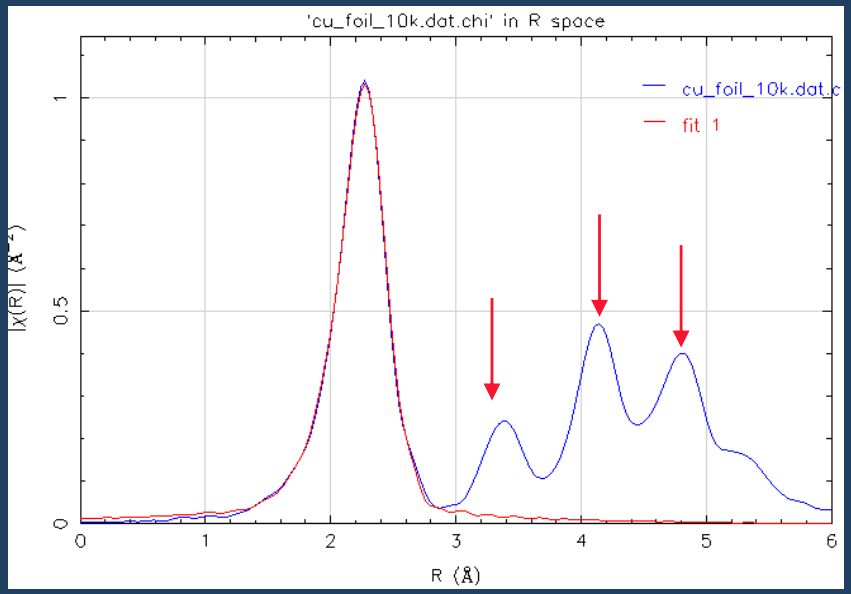


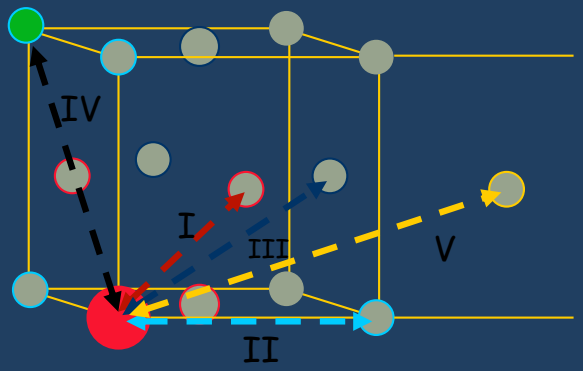


$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left(\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right)$$

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

Add new contributions





Atoms | feff.inp | Interpretation

Interpretation of the FEFF Calculation

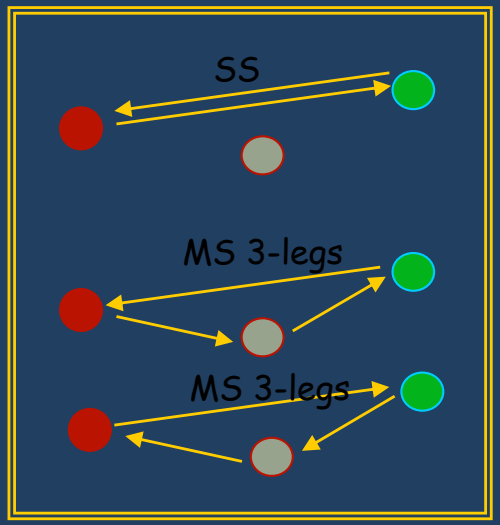
```
# TITLE name:    copper
# TITLE formula: Cu
# TITLE sites:   Cu1
# TITLE refer1:  Kittel, ISSP
# TITLE refer2:
```

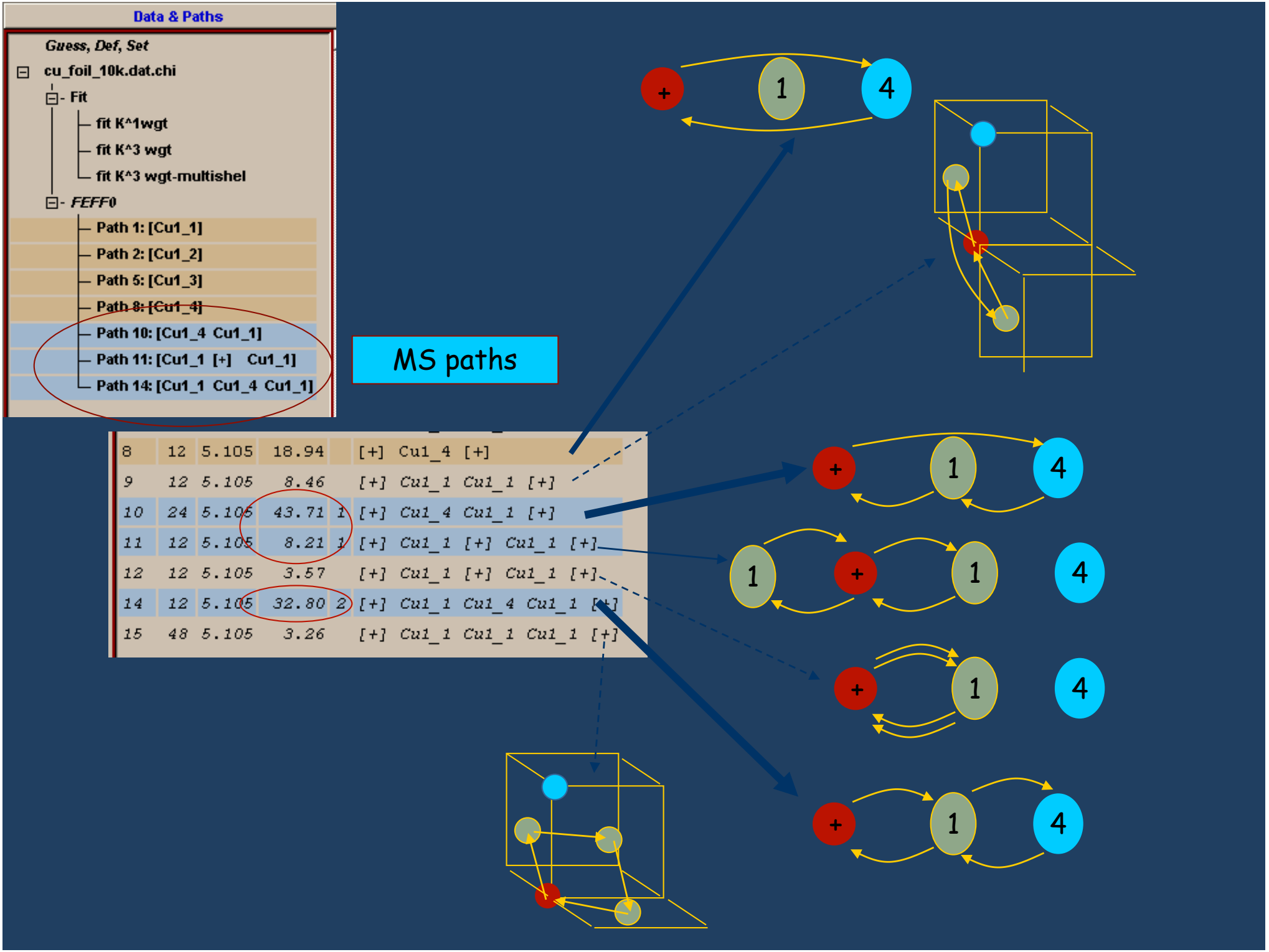
#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00		[+] Cu1_1 [+]
2	6	3.610	22.98		[+] Cu1_2 [+]
3	48	3.829	10.59		[+] Cu1_1 Cu1_1 [+]
4	48	4.358	8.65		[+] Cu1_2 Cu1_1 [+]
5	24	4.421	55.41		[+] Cu1_3 [+]
6	48	4.763	10.63		[+] Cu1_1 Cu1_1 [+]
7	96	4.763	21.81		[+] Cu1_3 Cu1_1 [+]
8	12	5.105	18.94	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

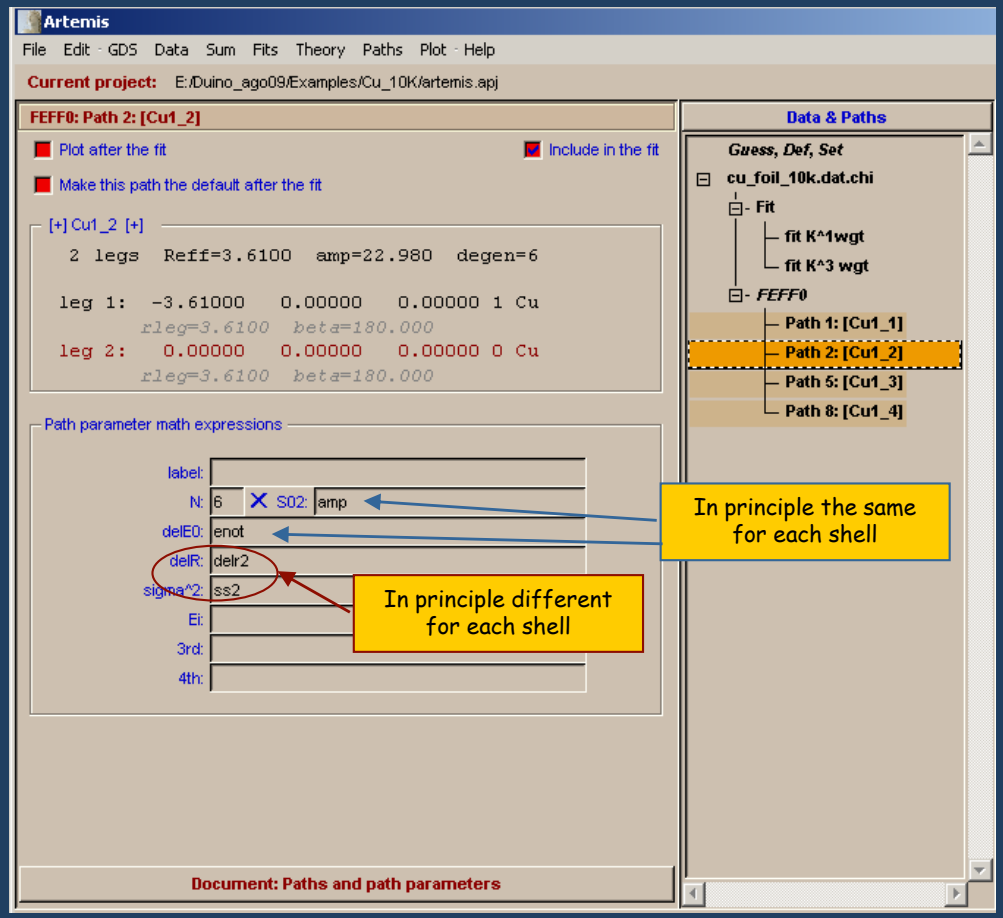
Document: Feff interpretation

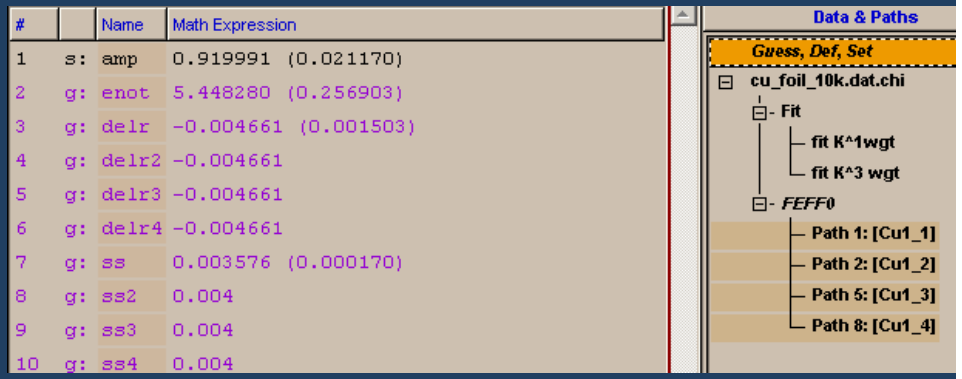
Single Scattering

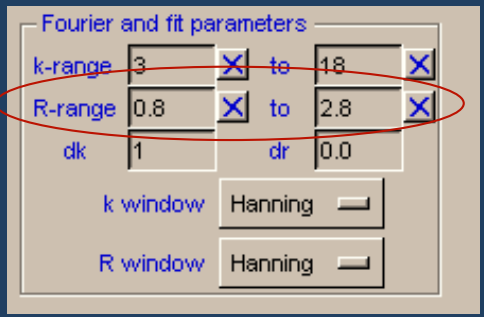
MS + Focusing




Data & Paths
Guess, Def, Set
cu_foil_10k.dat.chi
- Fit
fit K^1wgt
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 [+]
+
1
4





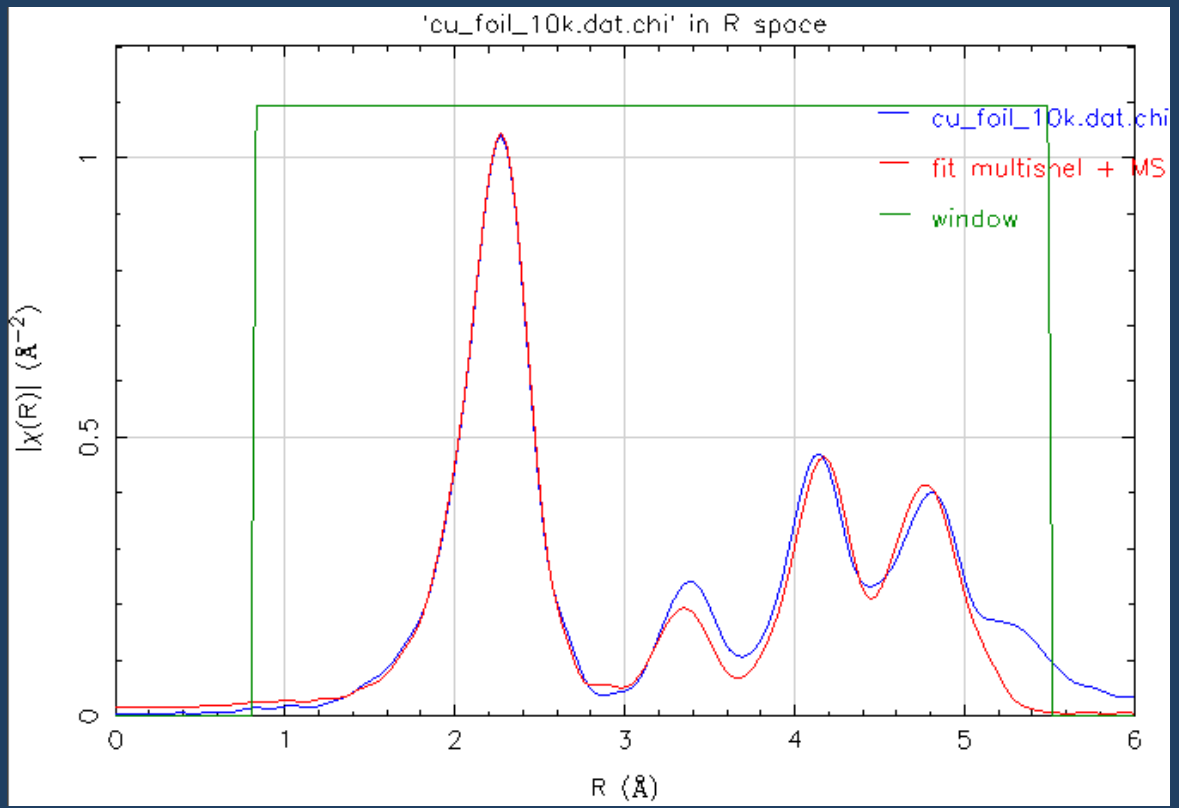


The used path must be inside the fit range

#		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
```

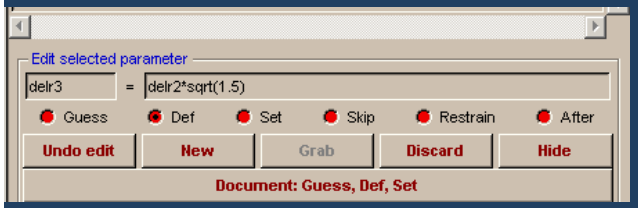
```
Correlations between variables:
          ss6 and ss7          -->  -0.8579
         enot and delr         -->   0.8206
         delr4 and ss5         -->  -0.6973
         enot and delr3        -->   0.6923
         delr and delr3        -->   0.5675
         enot and ss5          -->   0.4211
         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
```

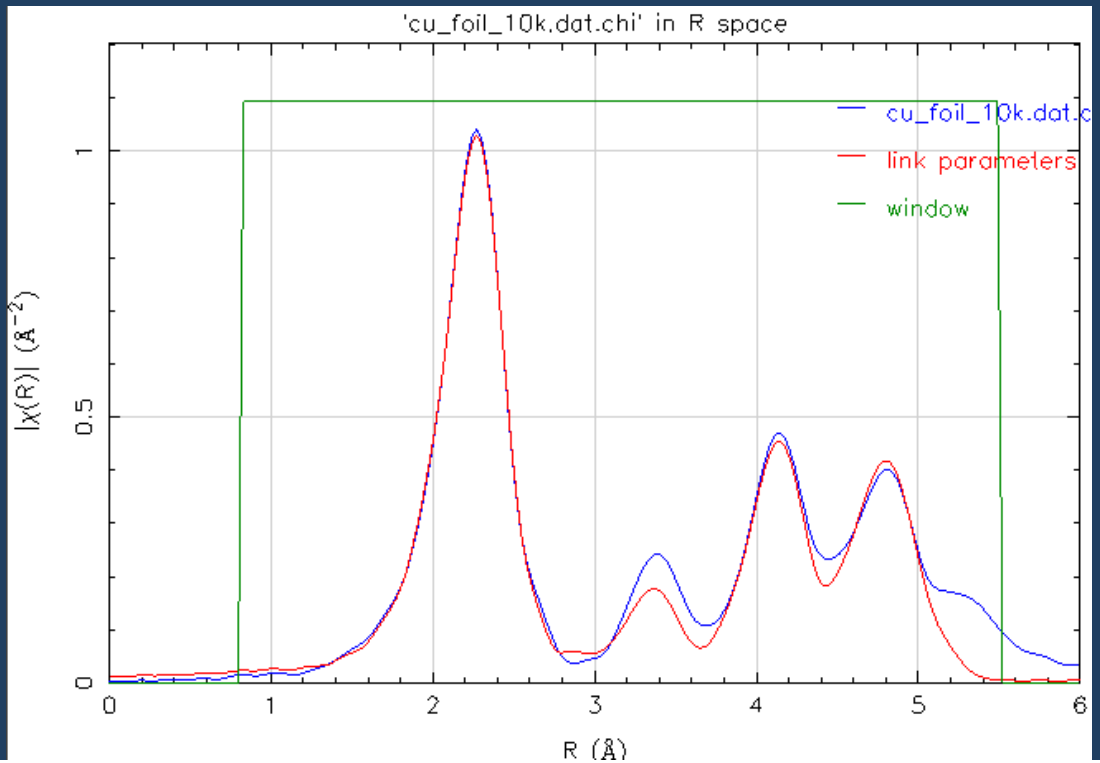


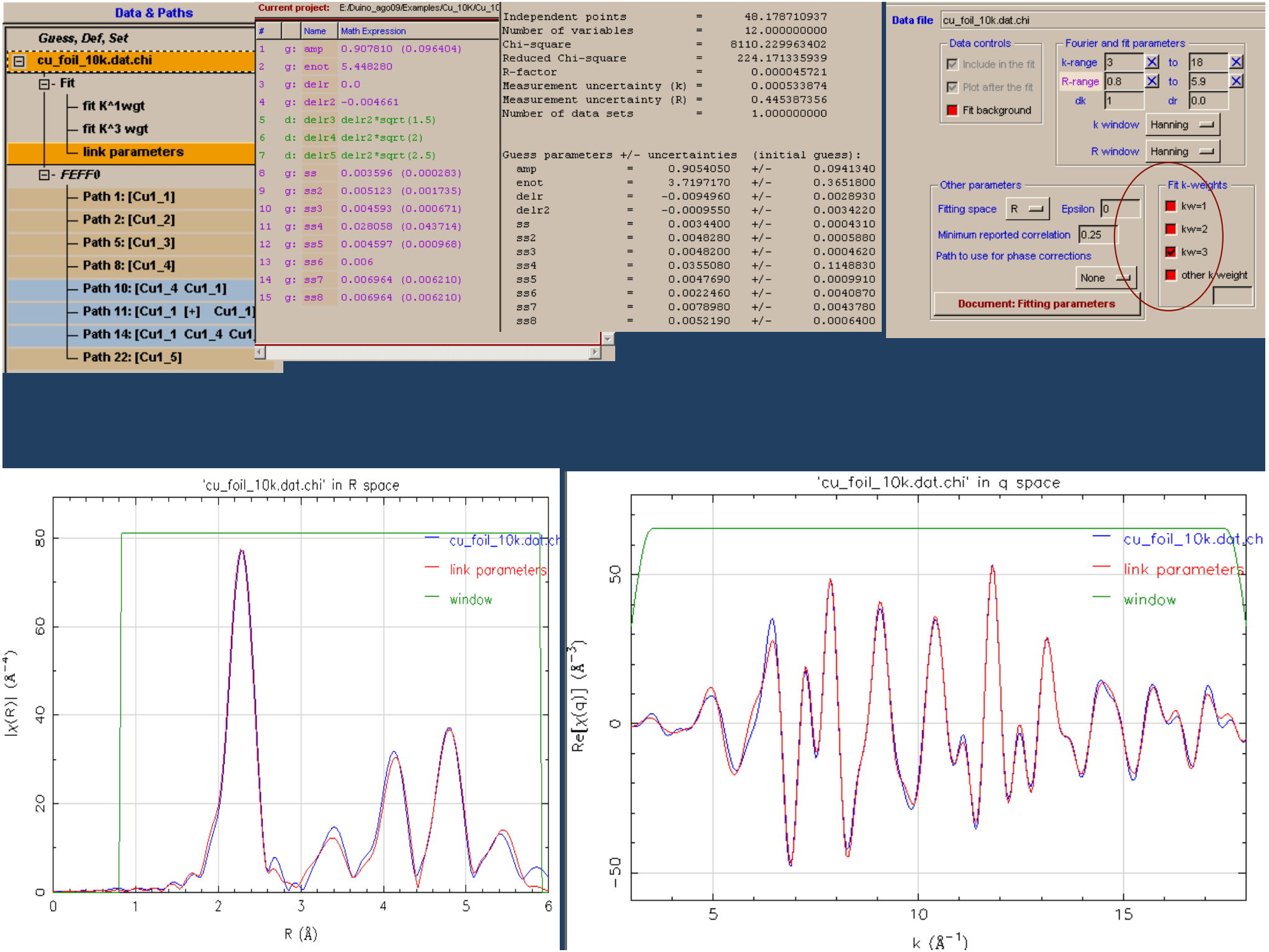
#		Name	Math Expression
1	s:	amp	0.919991
2	g:	enot	5.448280
3	d:	delr	delr2/sqrt(2)
4	g:	delr2	-0.004661
5	d:	delr3	delr2*sqrt(1.5)
6	d:	delr4	delr2*sqrt(2)
7	g:	ss	0.003596 (0.000283)
8	g:	ss2	0.005123 (0.001735)
9	g:	ss3	0.004593 (0.000671)
10	g:	ss4	0.028058 (0.043714)
11	g:	ss5	0.004597 (0.000968)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

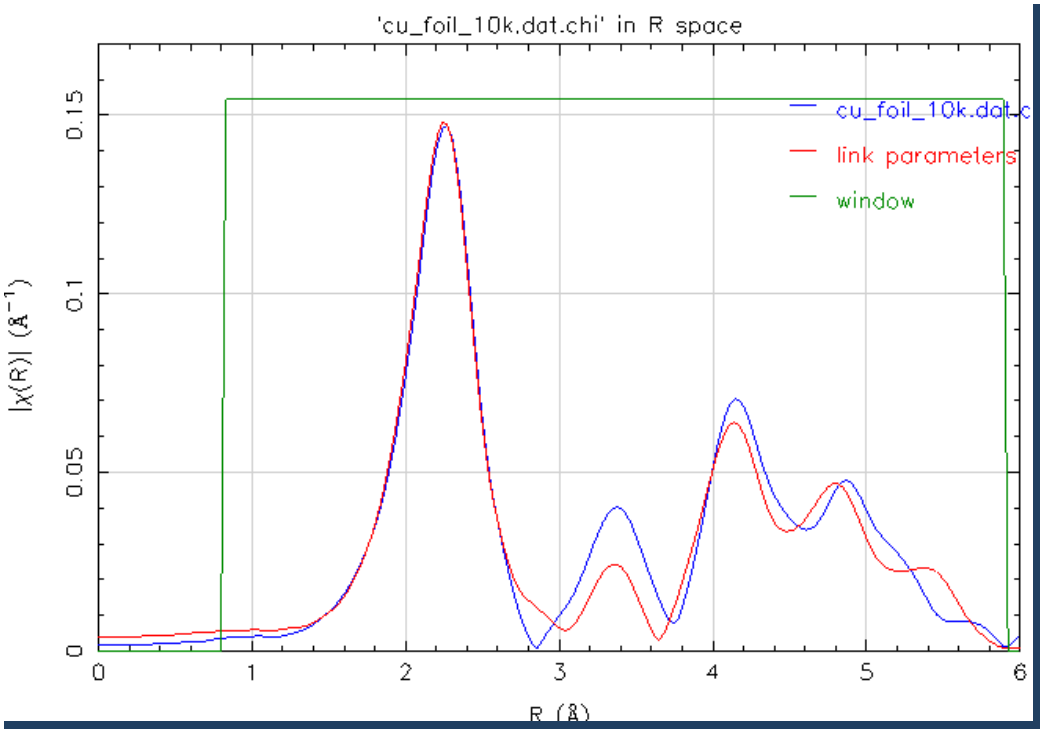
```
Independent points               =      44.382812500
Number of variables              =       9.000000000
Chi-square                       =    3499.926965502
Reduced Chi-square               =      98.916019339
R-factor                         =       0.022188660
Measurement uncertainty (k)    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


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
```

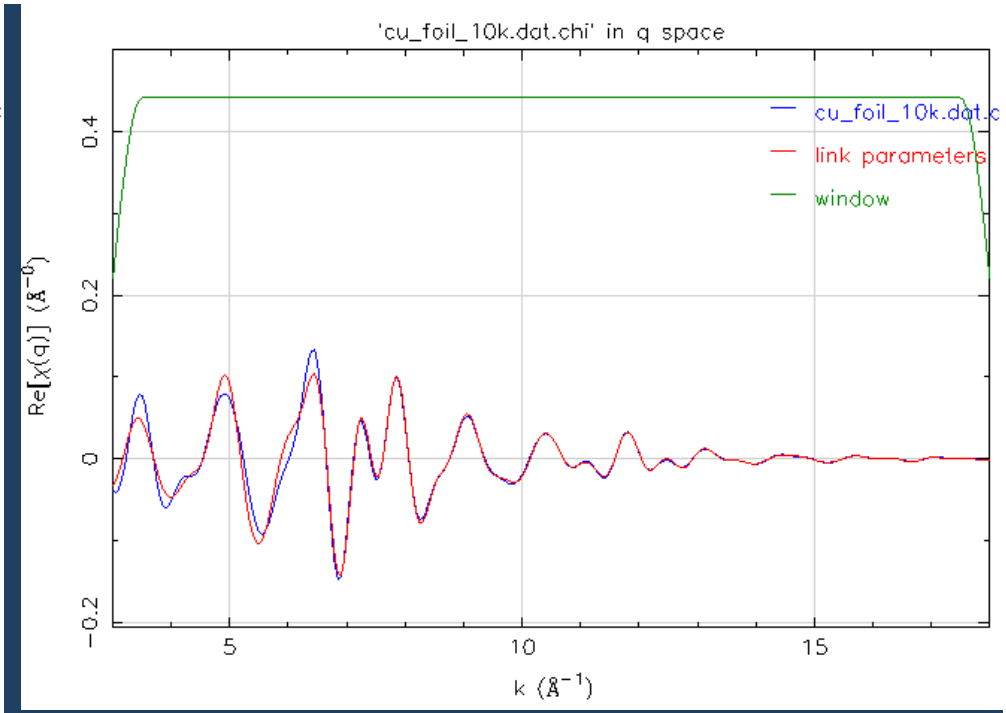
```
Correlations between variables:
          ss6 and ss7          -->  -0.9544
         enot and delr2        -->   0.8598
          ss4 and ss5          -->   0.6684
          ss5 and ss7          -->   0.6517
          ss4 and ss7          -->   0.6019
          ss5 and ss6          -->  -0.5675
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

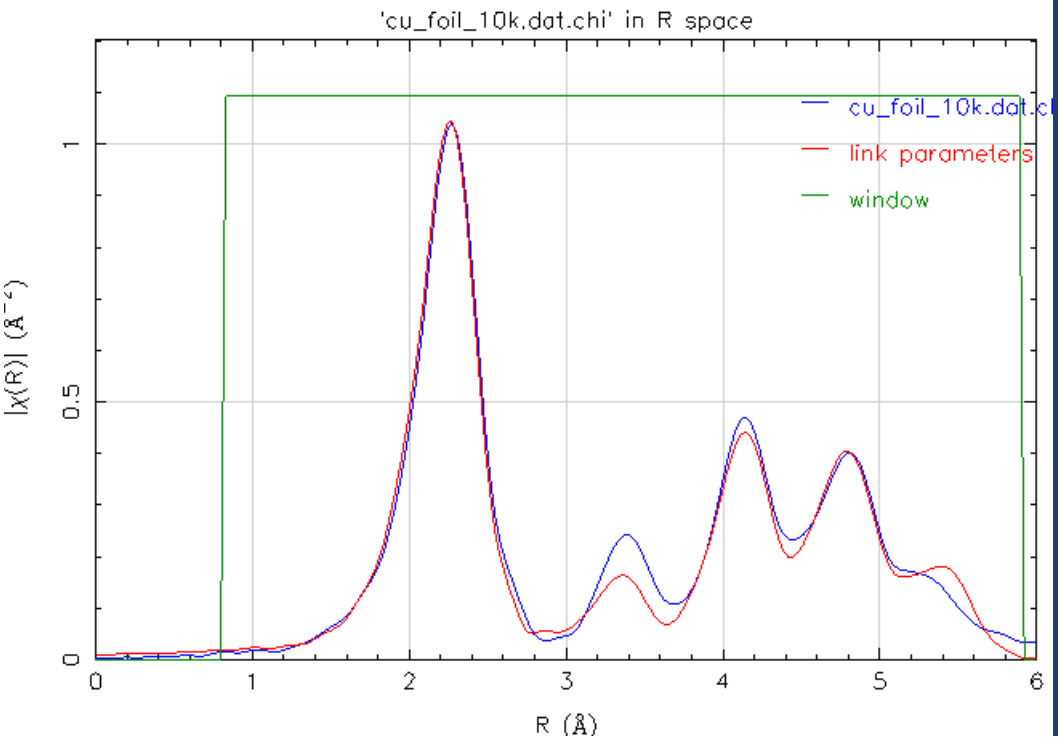


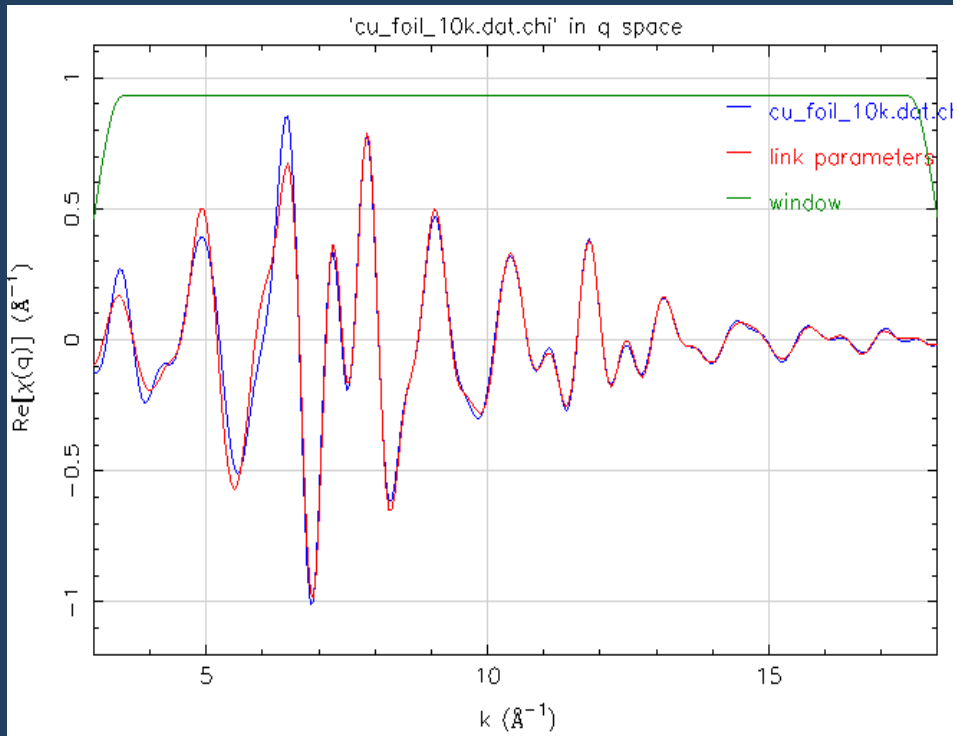



Data & Paths
Guess, Def, Set
cu_foil_10k.dat.chi
- Fit
fit K^1wgt
fit K^3 wgt
link parameters
- FEFF0
Path 1: [Cu1_1]
Path 2: [Cu1_2]
Path 5: [Cu1_3]
Path 8: [Cu1_4]
Path 10: [Cu1_4 Cu1_1]
Path 11: [Cu1_1 [+] Cu1_1]
Path 14: [Cu1_1 Cu1_4 Cu1
Path 22: [Cu1_5]
Current project: E:/Duino_ago09/Examples/Cu_10K/Cu_10
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
Document: Fitting parameters
Fit k-weights
kw=1
kw=2
kw=3
other k-weight
'cu_foil_10k.dat.chi' in R space
cu_foil_10k.dat.ch
link parameters
window
|χ(R)| (Å⁻⁴)
R (Å)
'cu_foil_10k.dat.chi' in q space
cu_foil_10k.dat.ch
link parameters
window
Re[χ(q)] (Å⁻³)
k (Å⁻¹)


'cu_foil_10k.dat.chi' in R space
cu_foil_10k.dat.c
link parameters
window
|χ(R)| (Å⁻¹)
R (Å)


'cu_foil_10k.dat.chi' in q space
cu_foil_10k.dat.c
link parameters
window
Re[χ(q)] (Å⁻⁰)
k (Å⁻¹)


'cu_foil_10k.dat.chi' in R space
cu_foil_10k.dat.c
link parameters
window
|χ(R)| (Å⁻²)
R (Å)


'cu_foil_10k.dat.chi' in q space
cu_foil_10k.dat.c
link parameters
window
Re[χ(q)] (Å⁻¹)
k (Å⁻¹)

it's your work now!

a. amorphous Ge

b. GeO

c. Pt