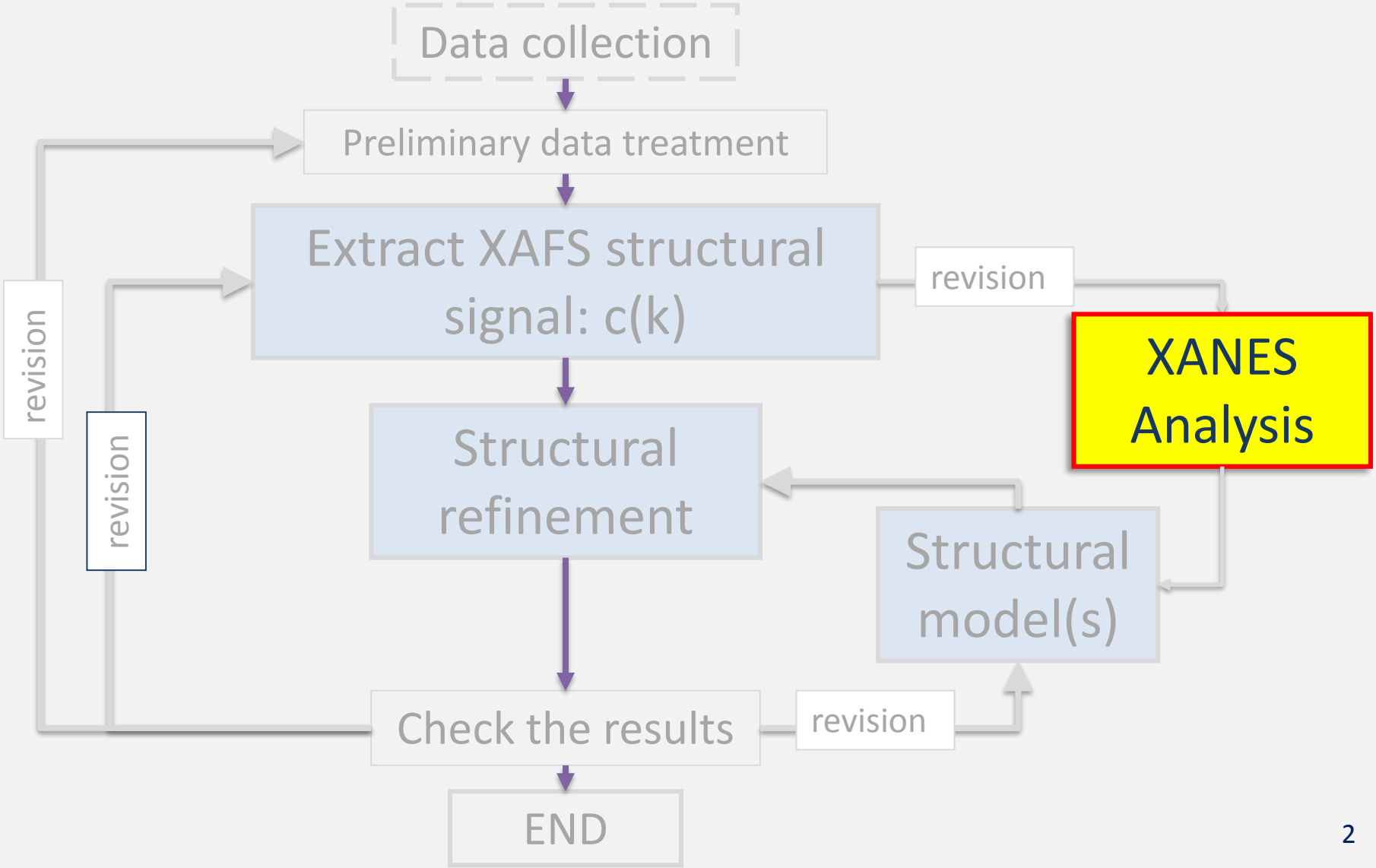
Data analysis of XAFS data

1. XAFS data analysis and related software
2. From XAS to XAFS: data treatment procedures
3. Training: EXAFS data refinement
4. **Training: XANES data analysis**
    1. **Linear combination Analysis**
    2. **pre-edge analysis**

https://tinyurl.com/SRSelettra2021

Contacts:
Prof. Carlo Meneghini
Dip. Di Scienze, Università Roma Tre, Roma
carlo.meneghini@uniroma3.it

XAFS data ANALYSIS: from the experimental data to structural details

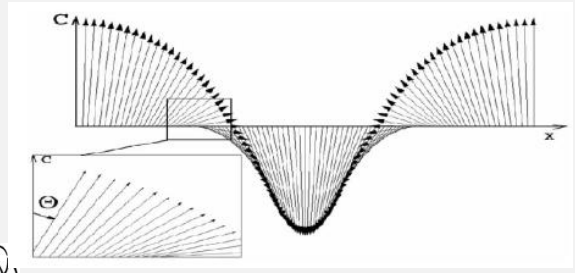


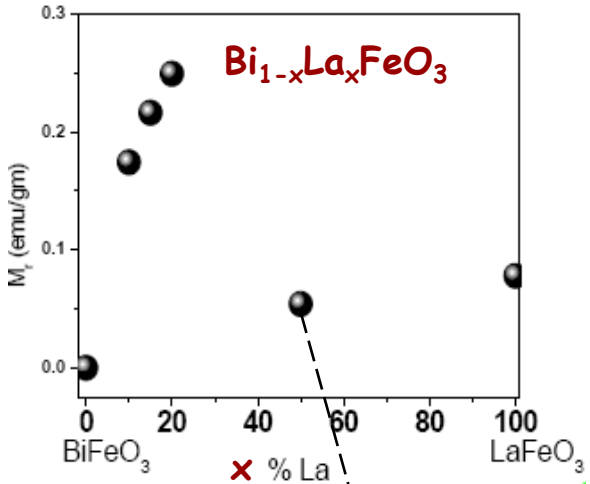
Analysis of mixtures: Linear Combination Analysis

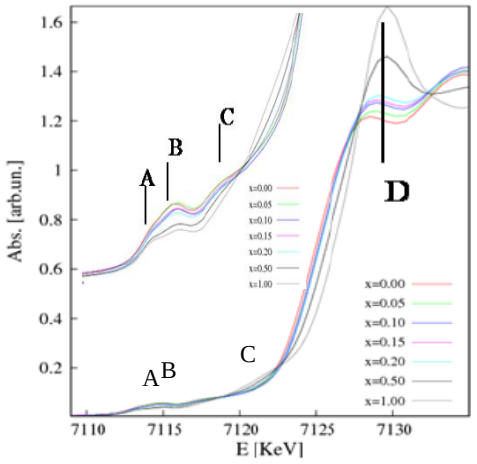
Magnetic properties of La doped $Bi_{1-x}La_xFeO_3$ improves doping with La till x~0.2 then M suddenly drops down.

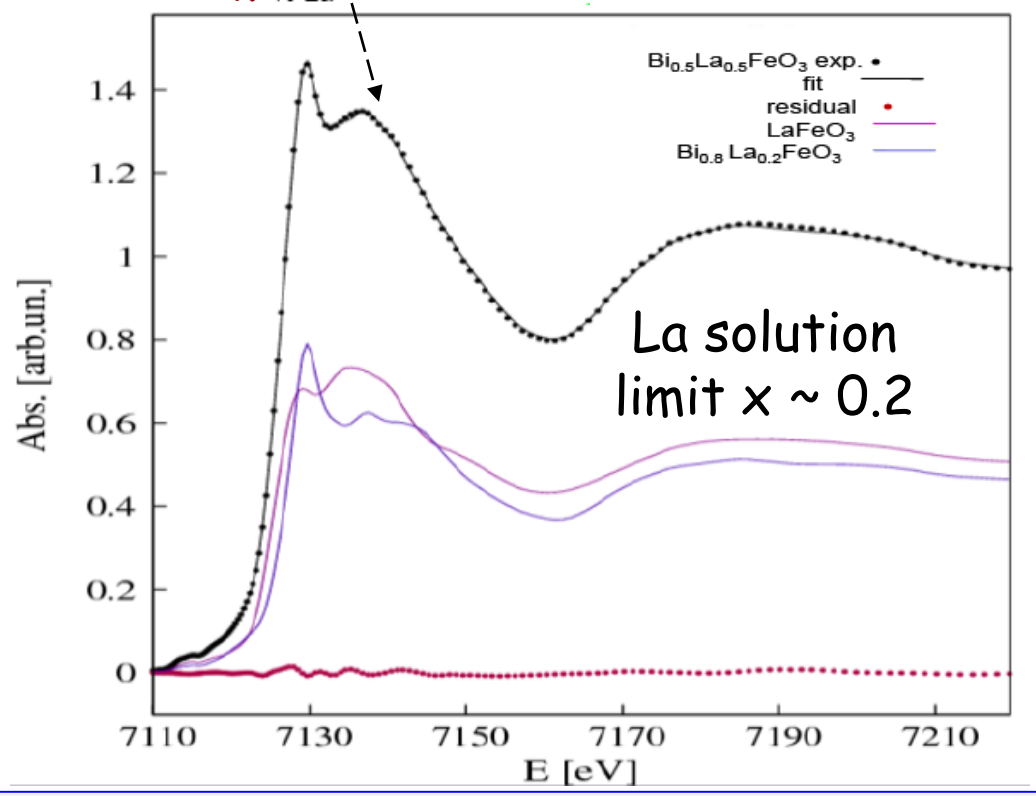
Why?

Above x~0.2 $LaFeO_3$ phase separate out (solution limit) worsening the overall property of the system



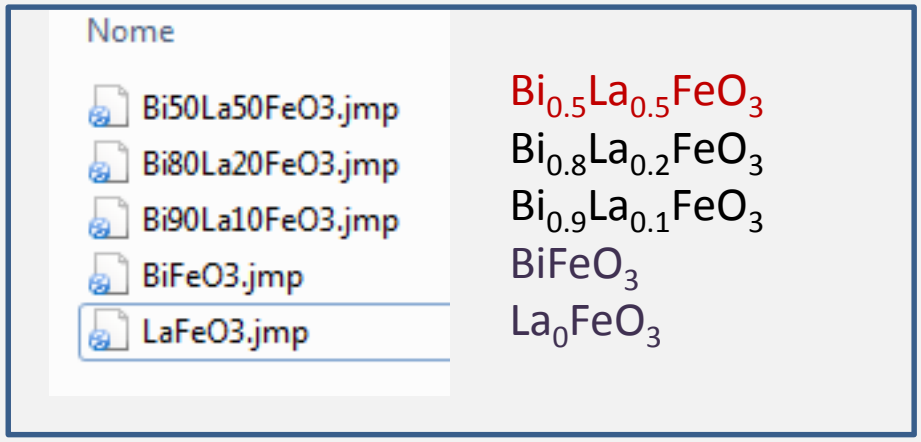


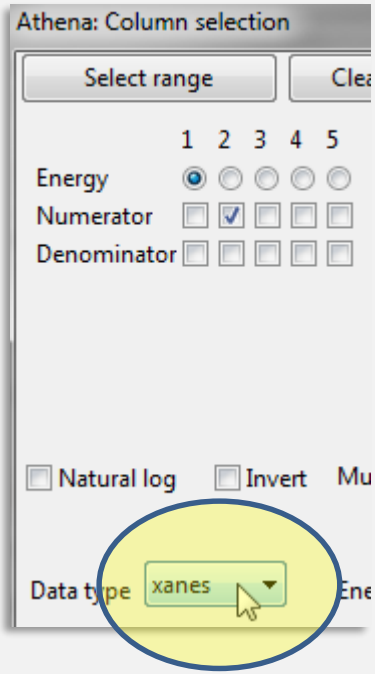




Pap. No. : L-173
Title : **Structural and magnetic study of La doped multiferroic BiFeO3**
Authors : Deepti KOTHARI, Sanjay Upadhya, Carlo Meneghini, Raghavendra Reddy, Giuliana Aquilanti, Ajay Gupta

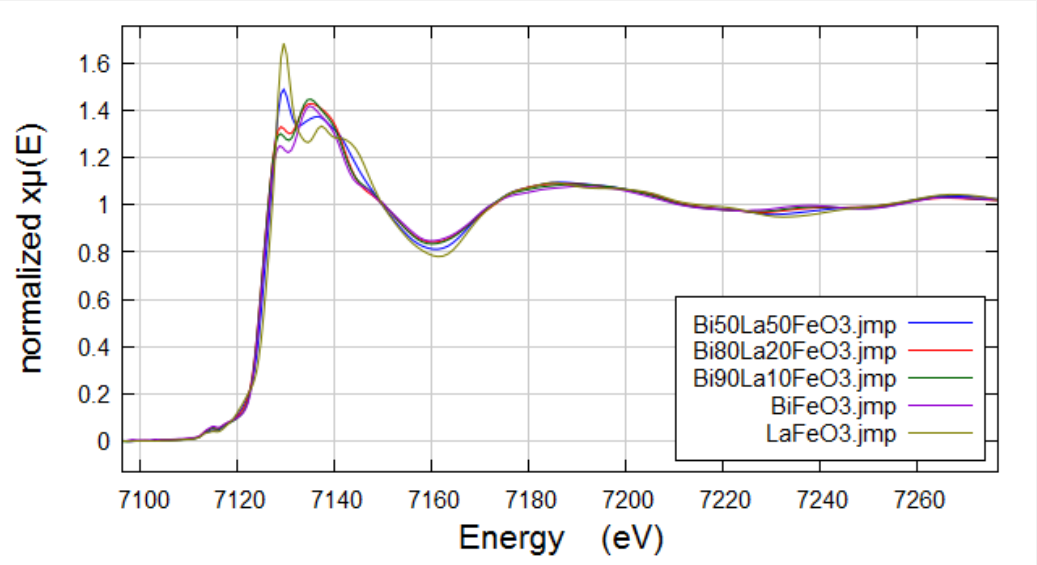
Data on: LCA-BiLaFeO

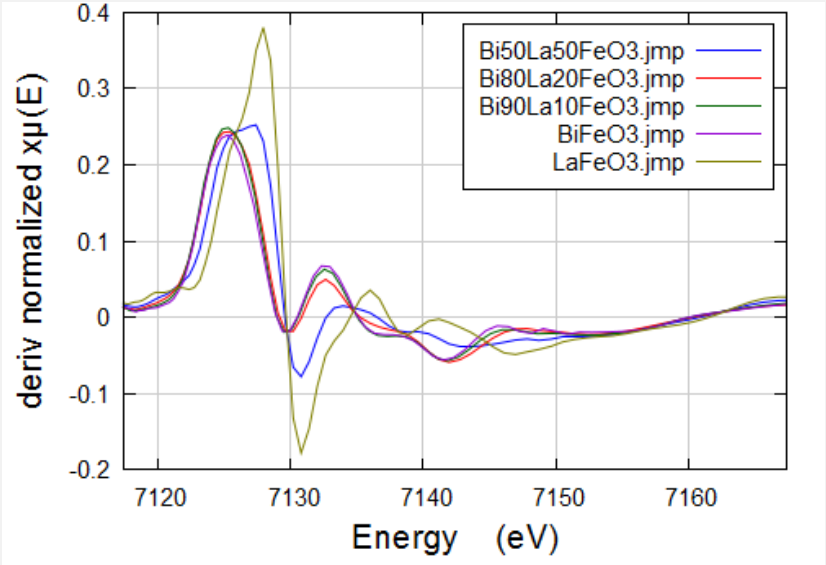


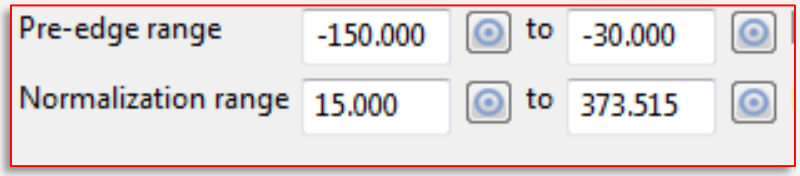


- Start Athena
- load all the files (columns 1,2)
- Import as XANES (simplified background extraction)

1. Check data & normalization



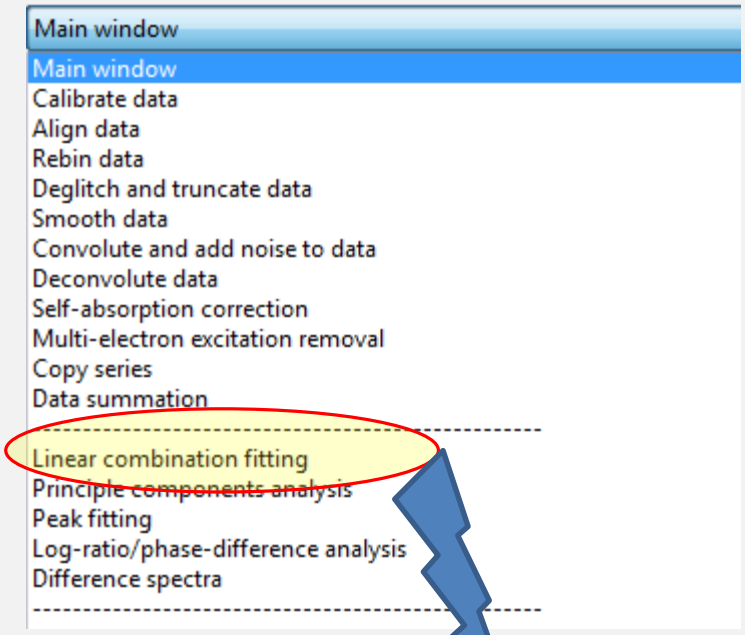




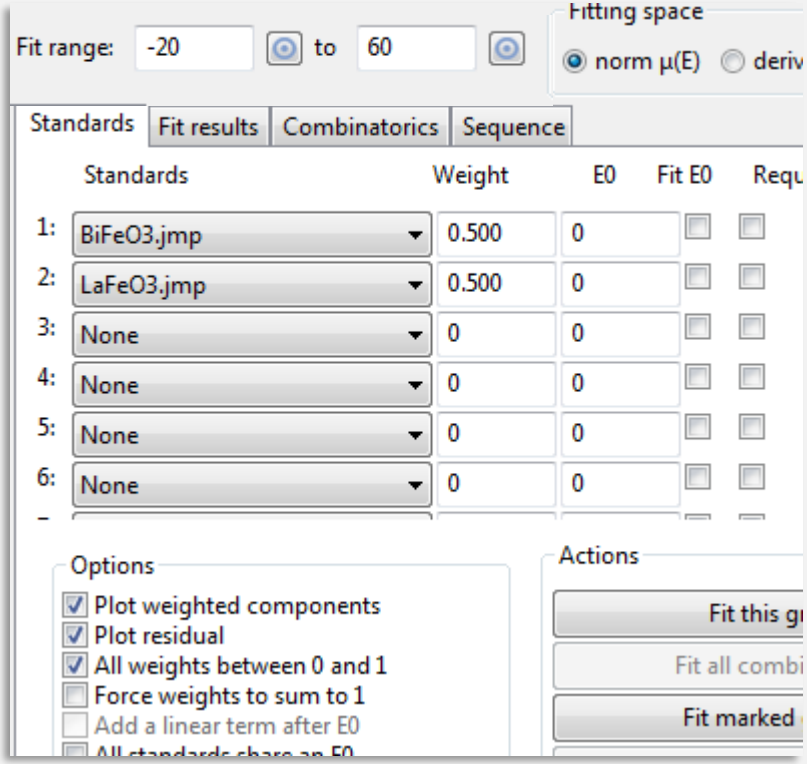
Check derivatives for energy scale alignement

Use the same normalization parameters for all the spectra to avoid artefacts

2. Linear combination fit

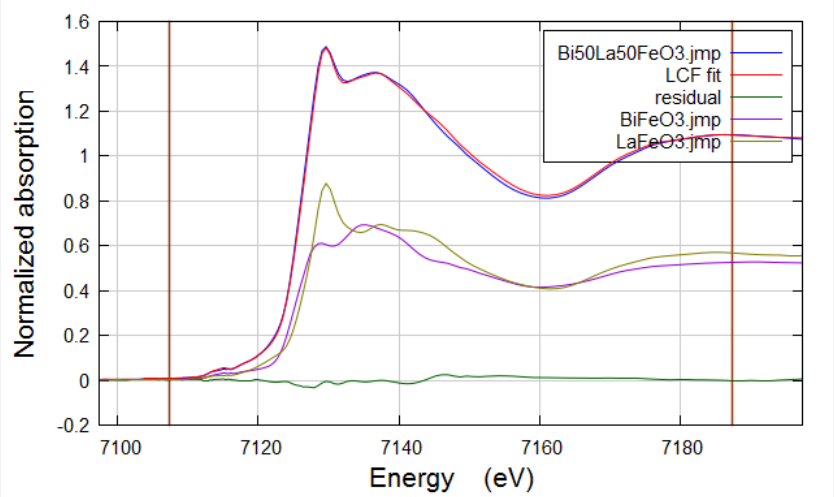


usually crashes!
Save the project and restart before doing LCA



Check the results

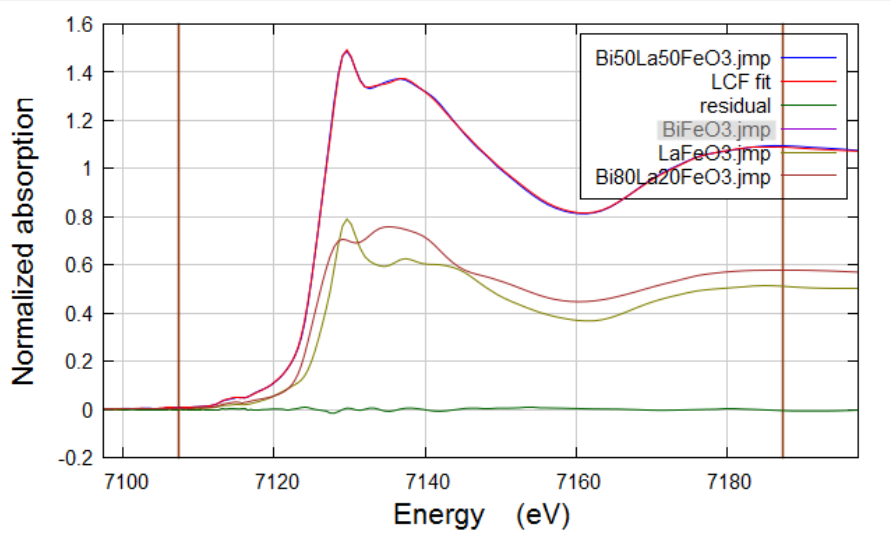
1:	BiFeO3.jmp	0.000	0.000
2:	LaFeO3.jmp	0.470	0.000
3:	Bi80La20FeO3.jmp	0.531	0.000




```
Fit included 143 data points and 2 variables, and approximately
60.045 measurements
Weights sum to 1: no
Weights forced between 0 and 1: yes
Overall e0 shift used: no
Noise added to data: 0
R-factor = 0.0003747
Chi-square = 0.01542
Reduced chi-square = 0.0001086

.    standard              weight           e0
=========================================================
.   BiFeO3.jmp             0.490 (0.010)    0.000 (0.000)
.   LaFeO3.jmp             0.522 (0.010)    0.000 (0.000)

.         sum ........... 1.011
```

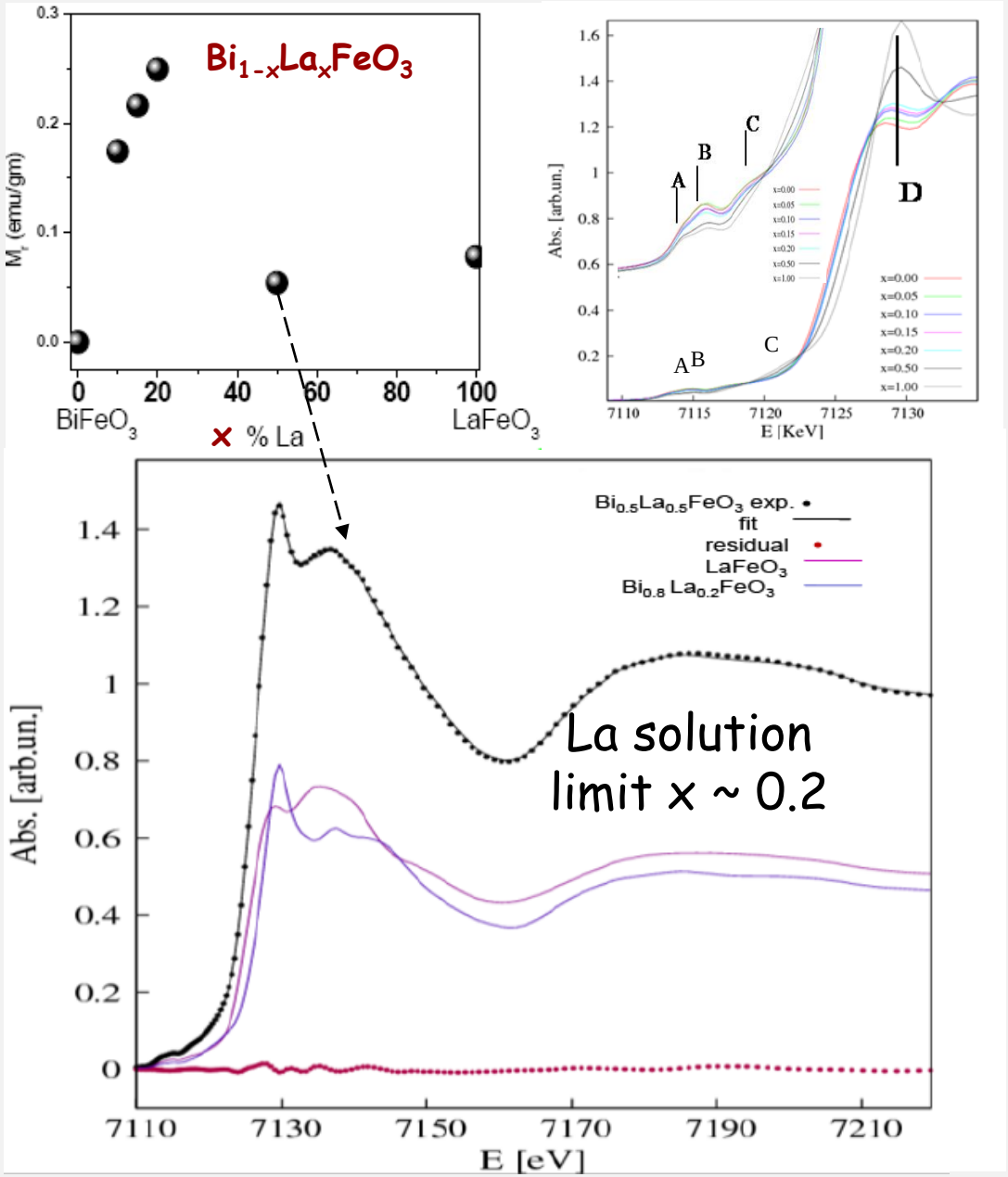



```
Weights sum to 1: no
Weights forced between 0 and 1: yes
Overall e0 shift used: no
Noise added to data: 0
R-factor = 0.0000494
Chi-square = 0.00206
Reduced chi-square = 0.0000146

.    standard              weight           e0
=========================================================
.   BiFeO3.jmp             0.000 (0.018)    0.000 (0.000)
.   Bi80La20FeO3.jmp       0.531 (0.020)    0.000 (0.000)
.   LaFeO3.jmp             0.470 (0.004)    0.000 (0.000)

.         sum ........... 1.001
```

Analysis of mixtures: Linear Combination Analysis

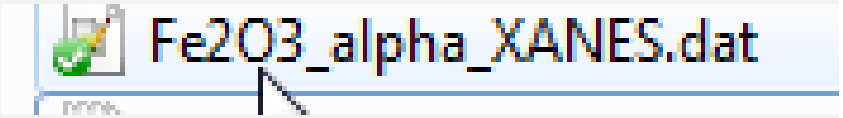


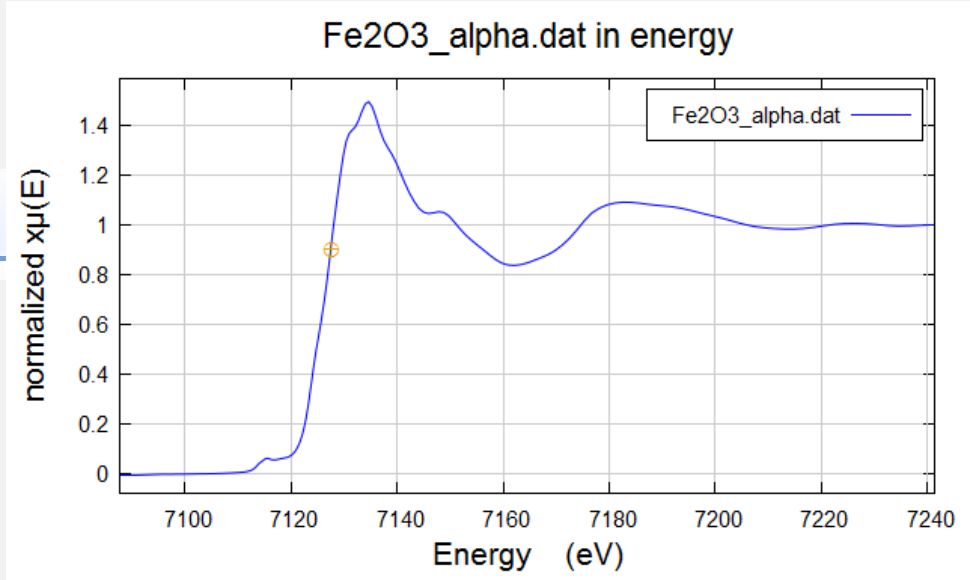
Above x =0.2 a phase separation occurs with local

$LaFeO_3 + Bi_{0.8}La_{0.2}FeO_3$

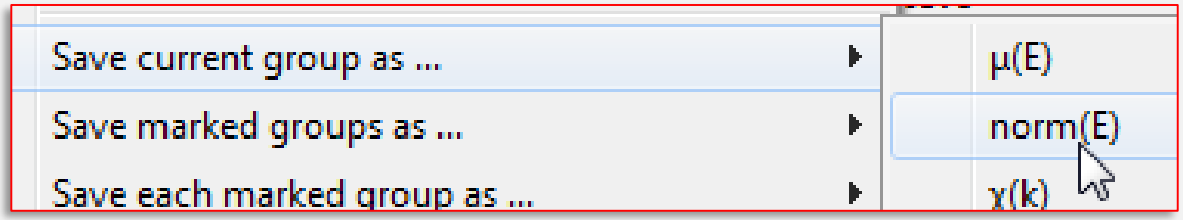
2. Analysis of pre-edge

1. Normalize Fe_2O_3 XANES data with Athena





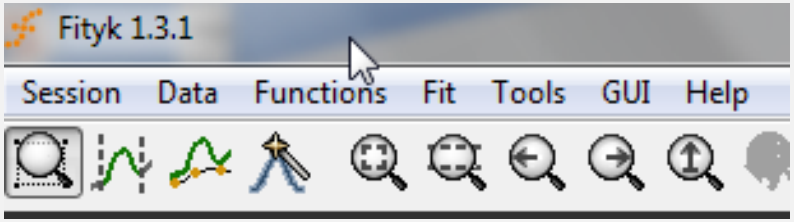
2. Save Fe_2O_3 Normalized XANES spectrum



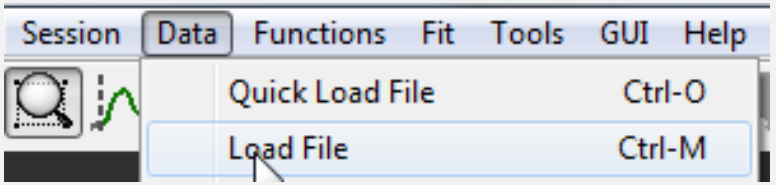
Fe2O3_alpha_XANES.nor

2. Analysis of pre-edge

3. Start Fityk

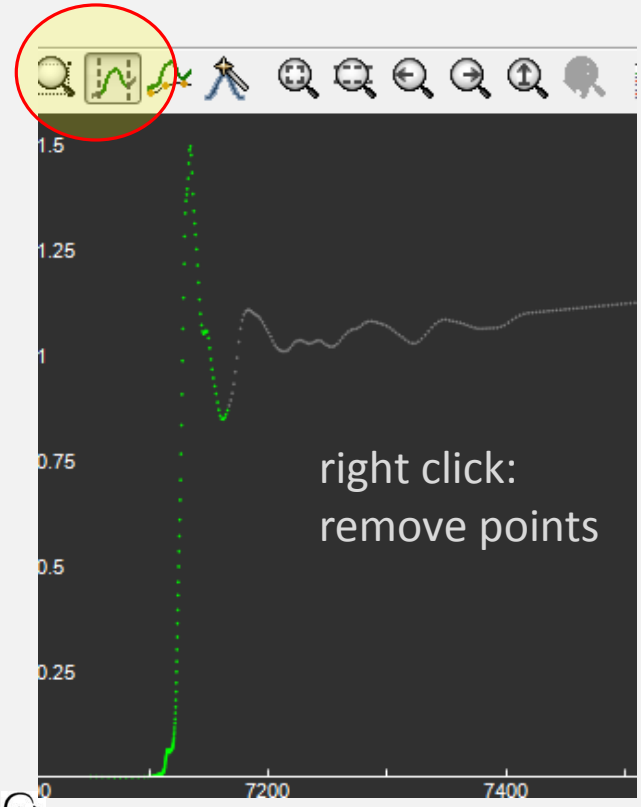


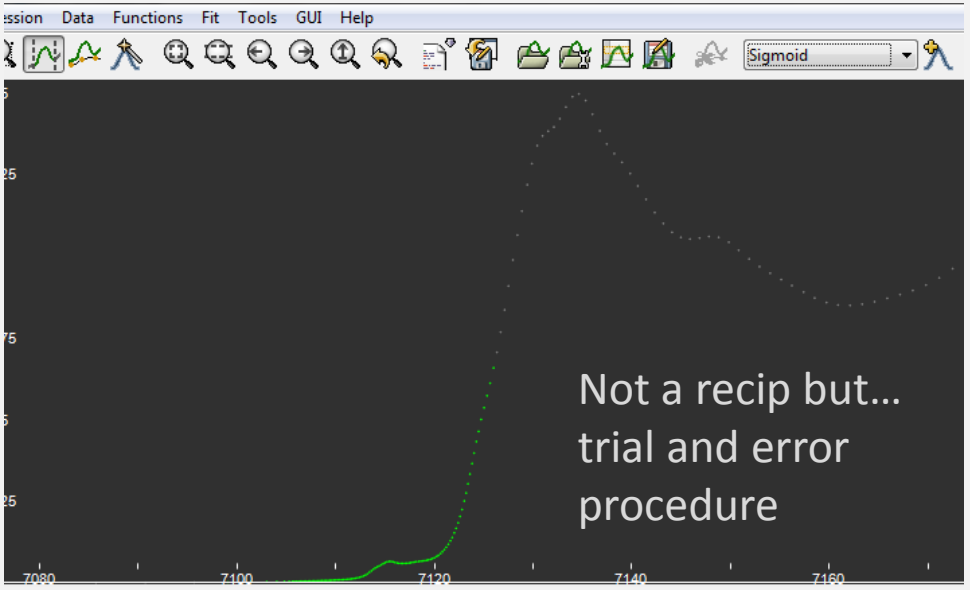
4. Load normalized spectrum



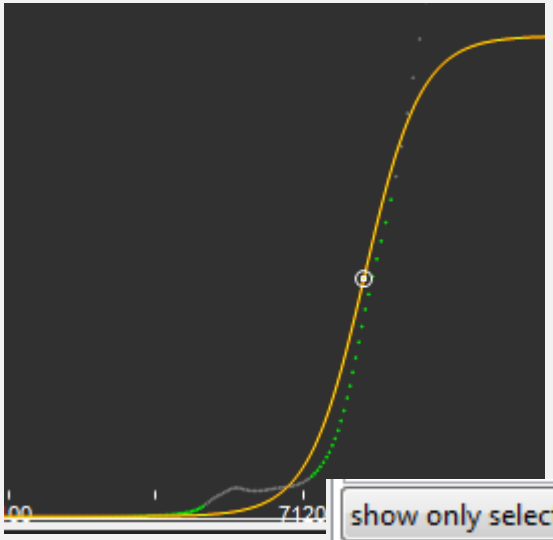
Fe2O3_alpha_XANES.nor

5. select the pre-edge region

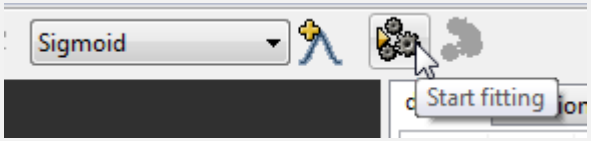


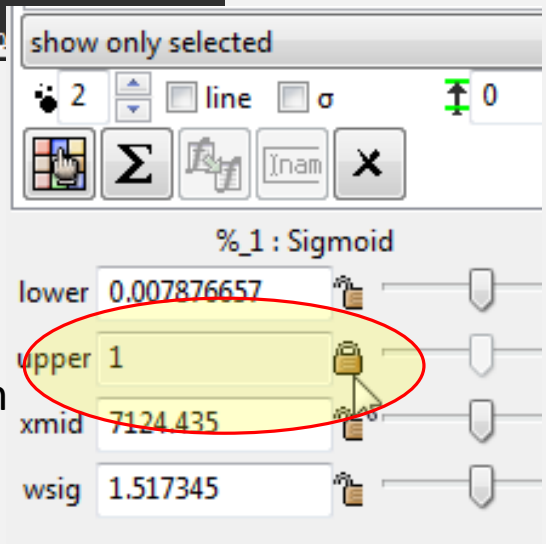


2. Analysis of pre-edge

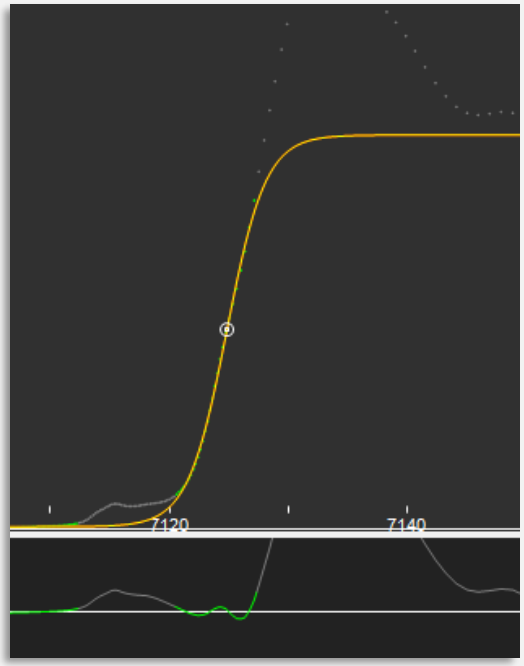


6. add the step functin (sigmoid)





fix the maximum



2. Analysis of pre-edge