XAFS
Experimental &data Analysis

1. XAFS data analysis software
2. From XAS to XAFS: how to deal with the data
3. Training: EXAFS data refinement
4. **Training: Linear combination analysis of XANES**

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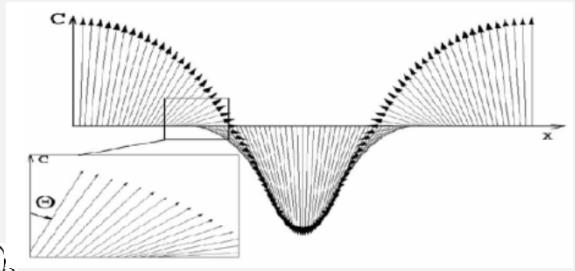
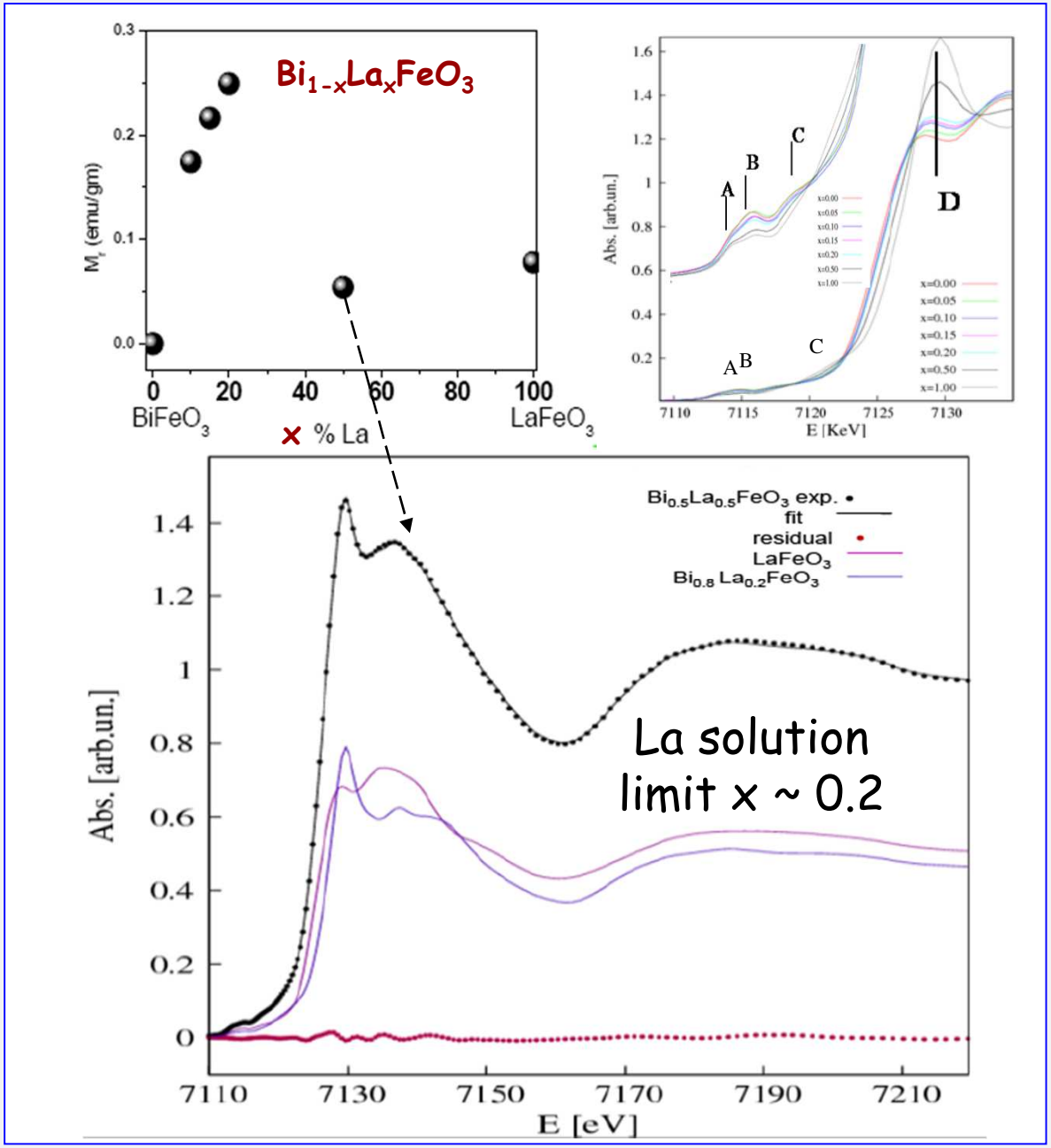
Analysis of mixtures: Linear Combination Analysis

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

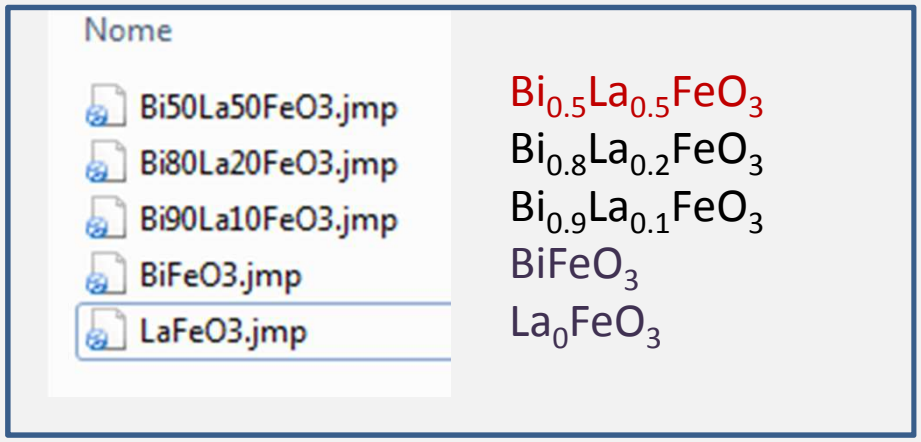
Why?

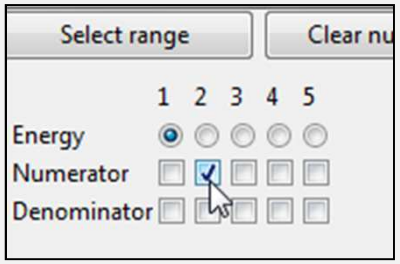
Above x~0.2 $LaFeO_3$ phase separate out (solution limit) worsening the overall property of the system





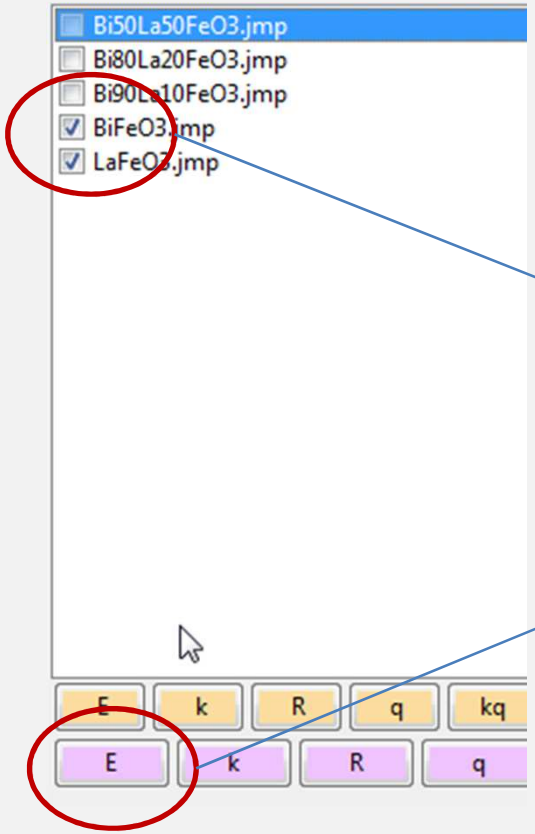
Data on: LCA-BiLaFeO

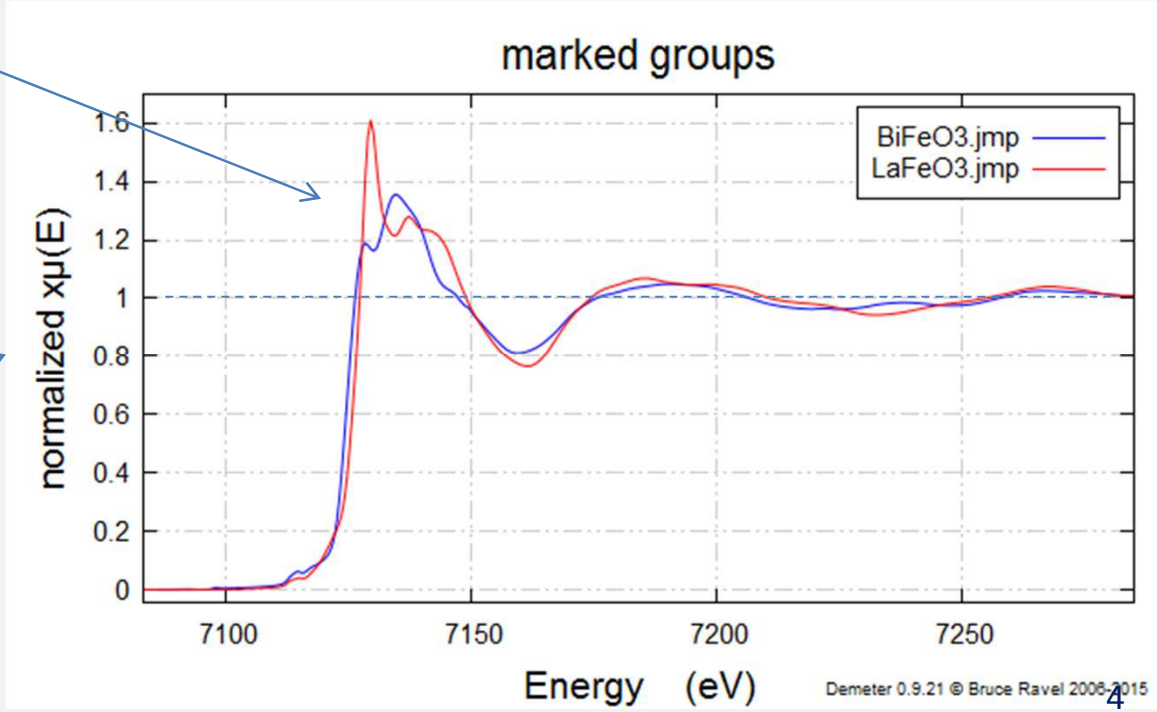




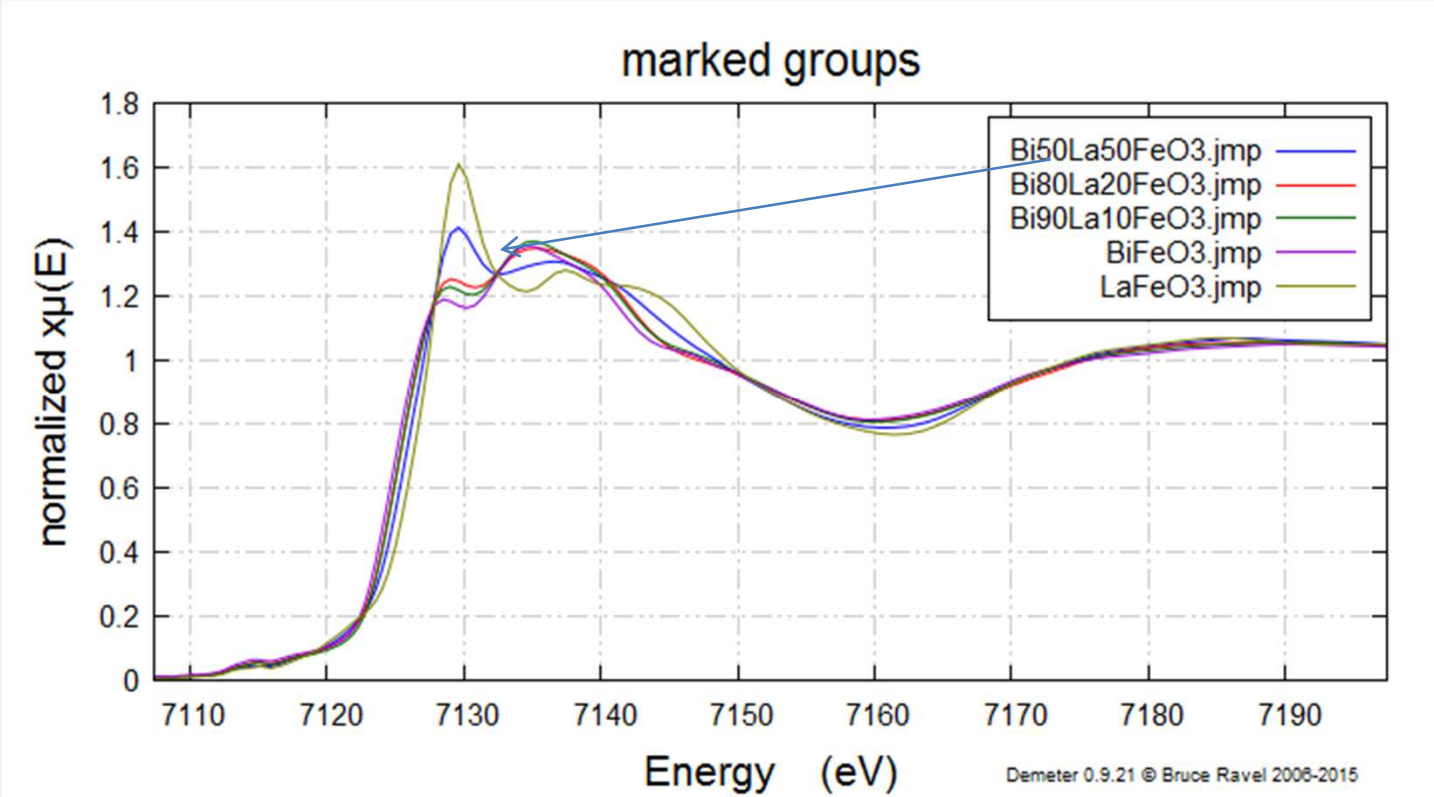
- Start Athena
- load all the files (columns 1,2)

Compare end member Normalized spectra

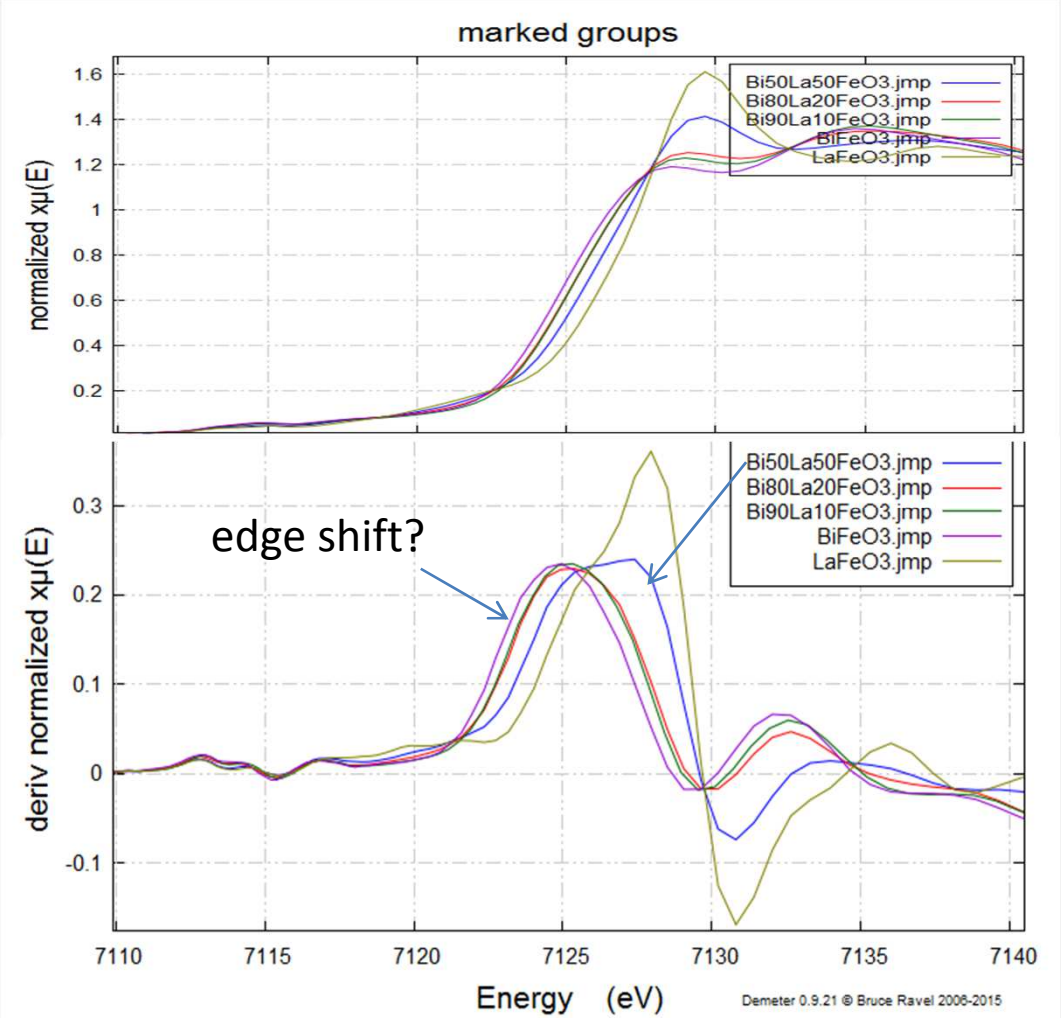




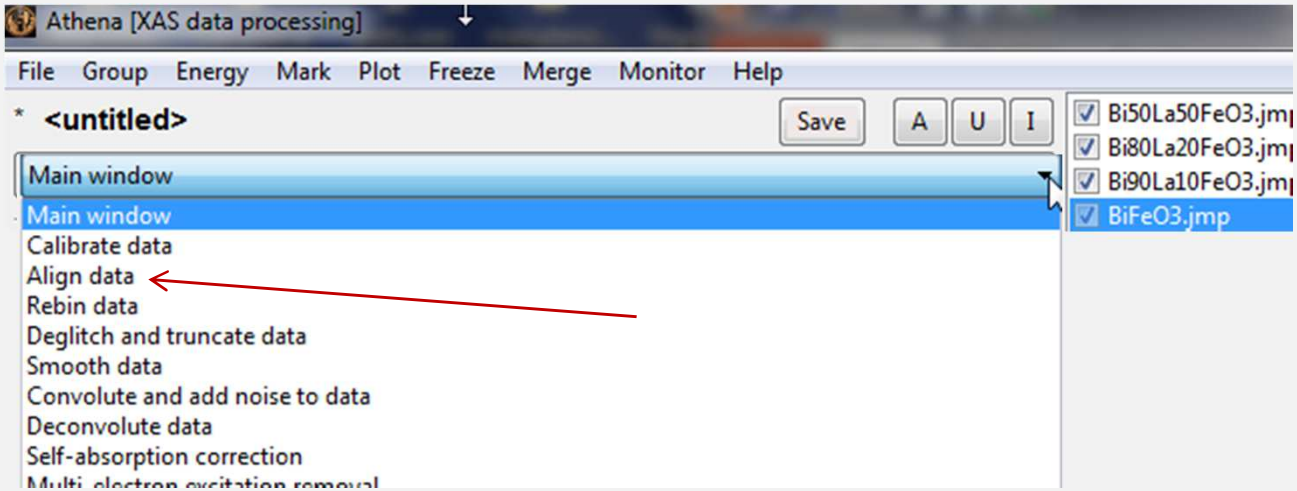
Compare spectra with the end compounds

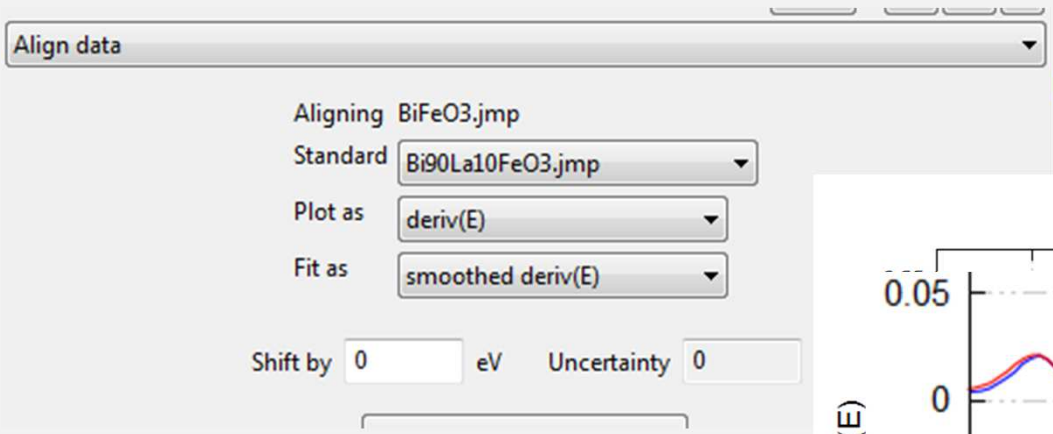


Compare derivatives

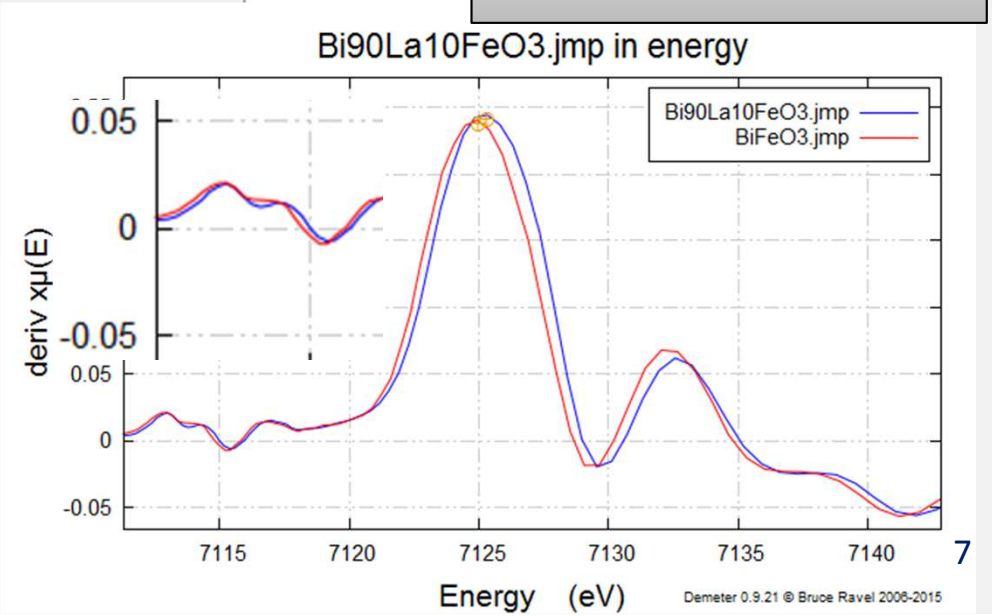


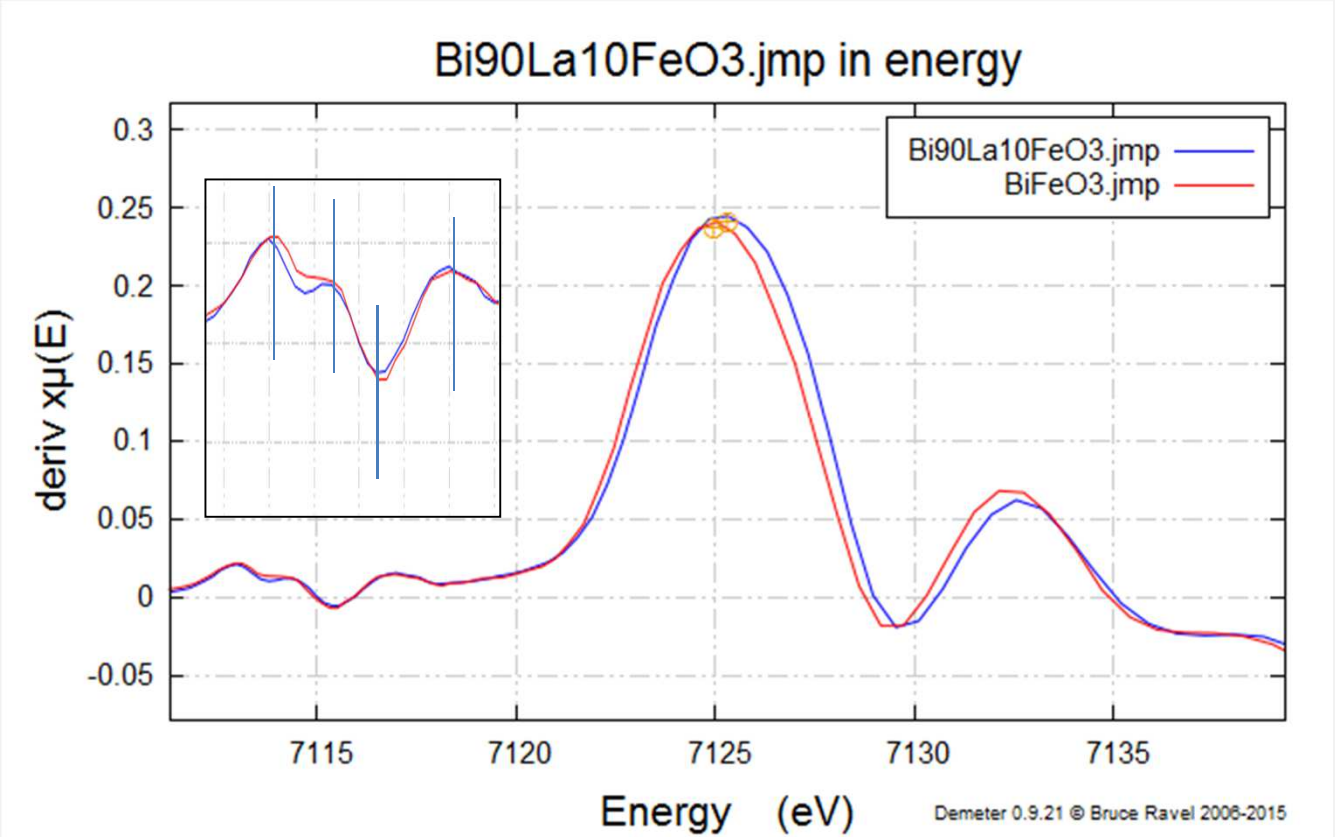
Align the data (If you need)



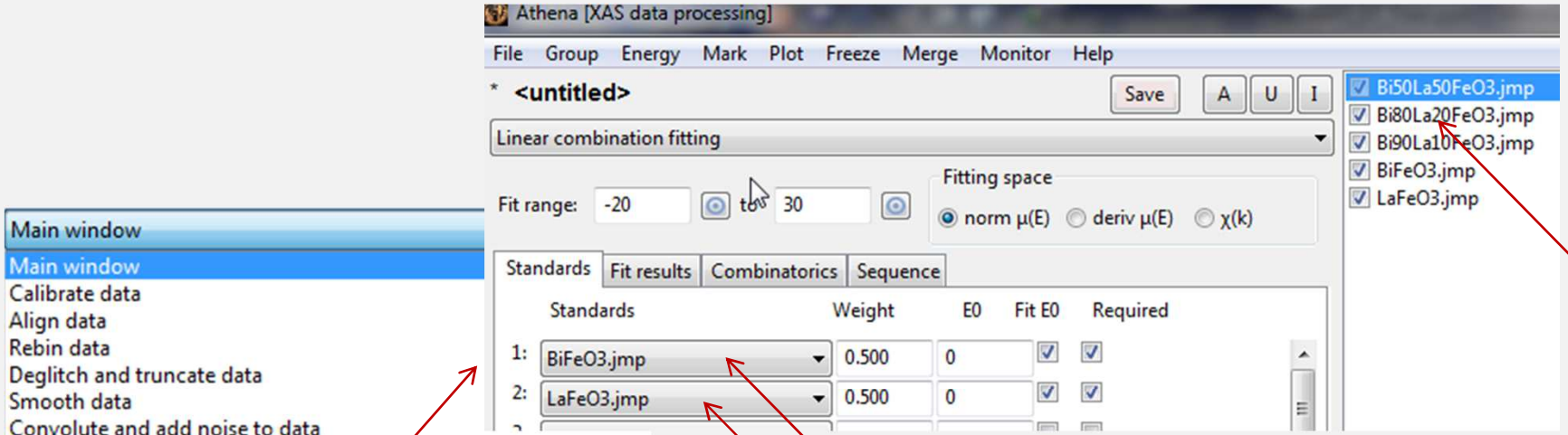


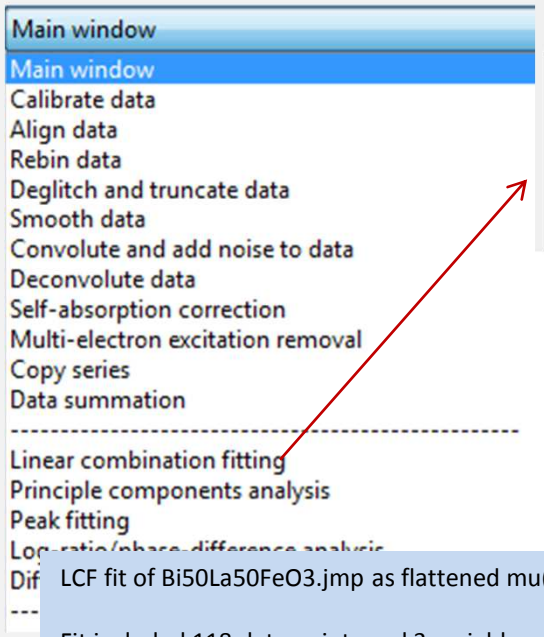
It is likely a rigid shift between BiFeO3 and Bi09La01FeO3 data





Generally pre-edge region derivative is more stable (transition to localized states)



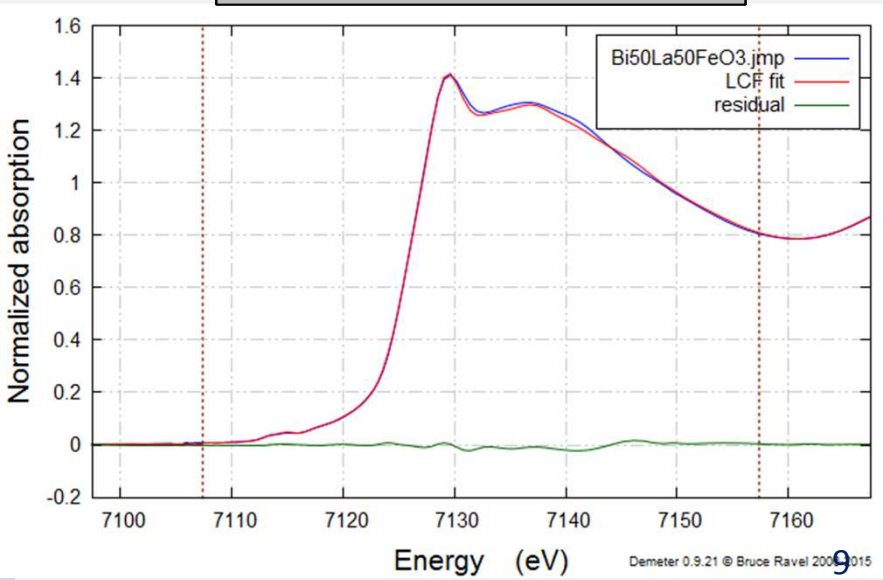


$Bi_{0.5}La_{0.5}FeO_3$ =
0.44 $BiFeO_3$
+ 0.56 La_0FeO_3

LCF fit of Bi50La50FeO3.jmp as flattened mu(E) from 7107.411 to 7157.411

Fit included 118 data points and 3 variables, and approximately 37.528 measurements
Weights sum to 1: yes
Weights forced between 0 and 1: yes
Overall e0 shift used: no
Noise added to data: 0
R-factor = 0.0001869
Chi-square = 0.00614
Reduced chi-square = 0.0000534

.	standard	weight	e0
.	BiFeO3.jmp	0.443 (0.008)	-0.008 (0.034)
.	LaFeO3.jmp	0.557 (0.008)	-0.119 (0.019)



R-factor = 0.0001869
Chi-square = 0.00614
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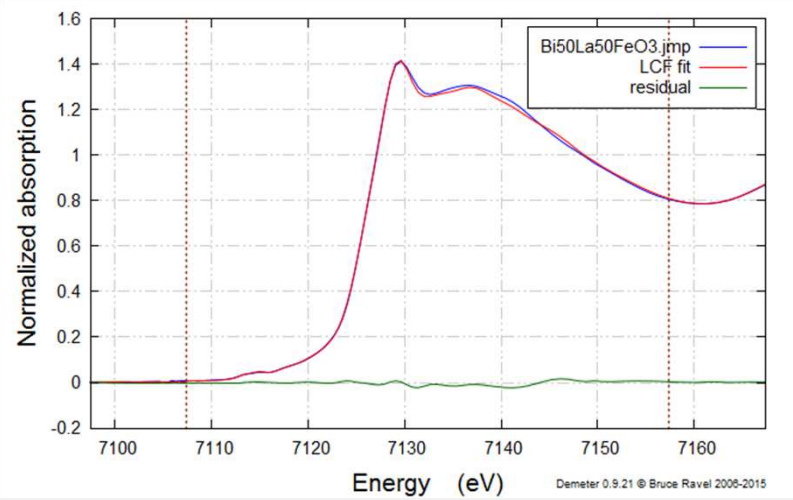

LCF fit of Bi50La50FeO3.jmp as flattened mu(E) from 7107.411 to 7157.411

Fit included 118 data points and 3 variables, and approximately 37.528 measurements
Weights sum to 1: yes
Weights forced between 0 and 1: yes
Overall e0 shift used: no
Noise added to data: 0
R-factor = 0.0000378
Chi-square = 0.00124
Reduced chi-square = 0.0000108

.	standard	weight	e0
.	Bi80La20FeO3.jmp	0.532 (0.004)	0.047 (0.014)
.	LaFeO3.jmp	0.468 (0.004)	-0.087 (0.012)

$Bi_{0.5}La_{0.5}FeO_3$=
0.53 $Bi_{0.8}La_{0.2}FeO_3$+
0.47 La_0FeO_3