

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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**XIV School on Synchrotron Radiation:
Fundamentals, Methods and Applications**
Muggia, Italy / 18-29 September 2017

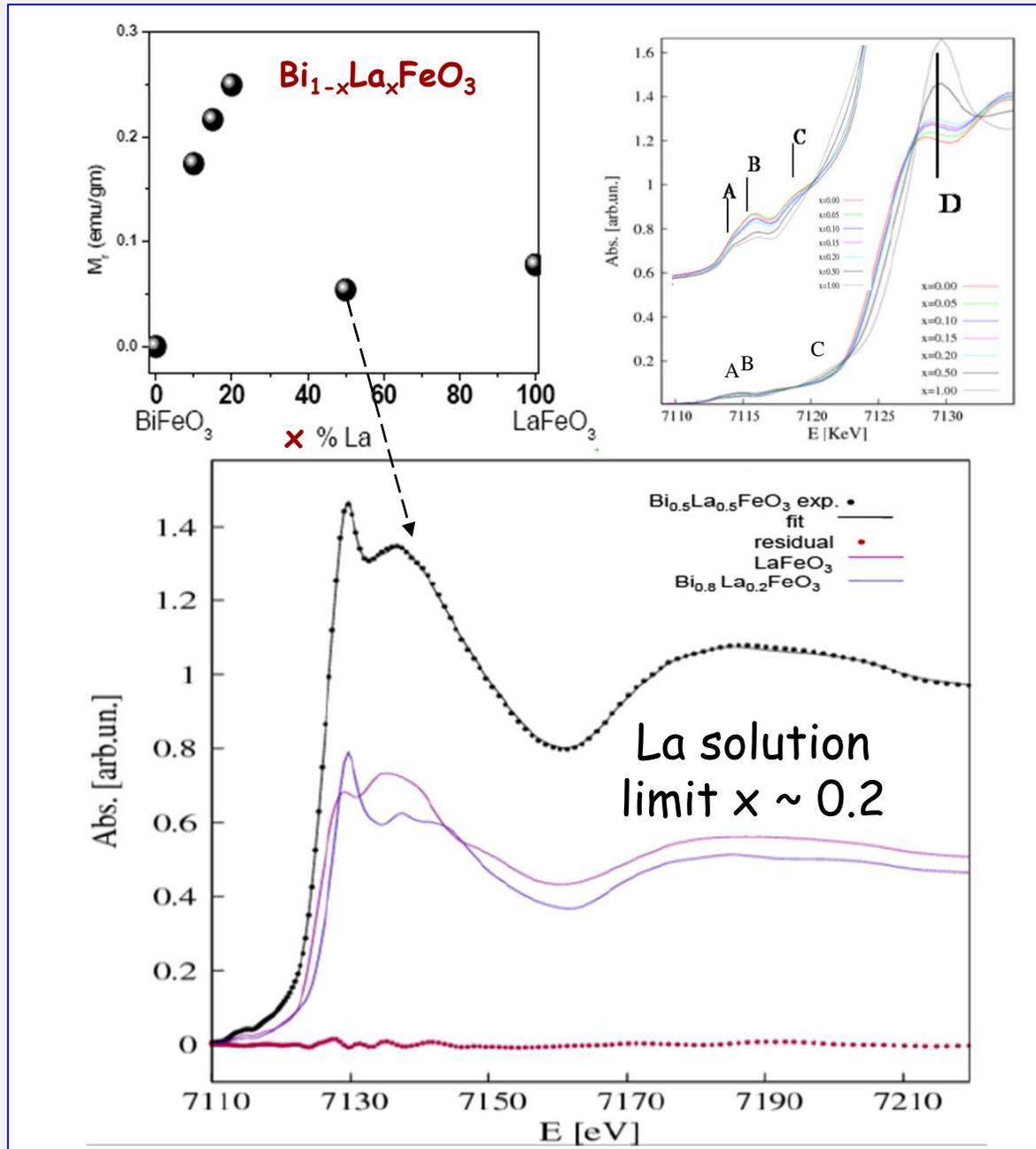
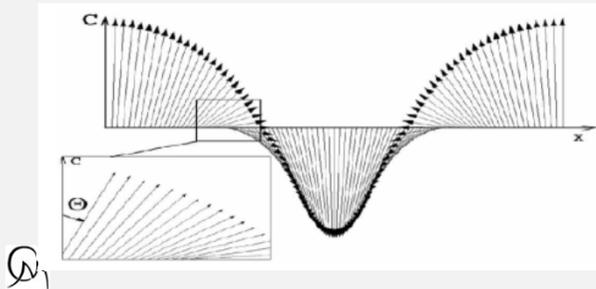


Analysis of mixtures: Linear Combination Analysis

Magnetic properties of La doped $\text{Bi}_{1-x}\text{La}_x\text{FeO}_3$ improves doping with La till $x \sim 0.2$ then M suddenly drops down.

Why?

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



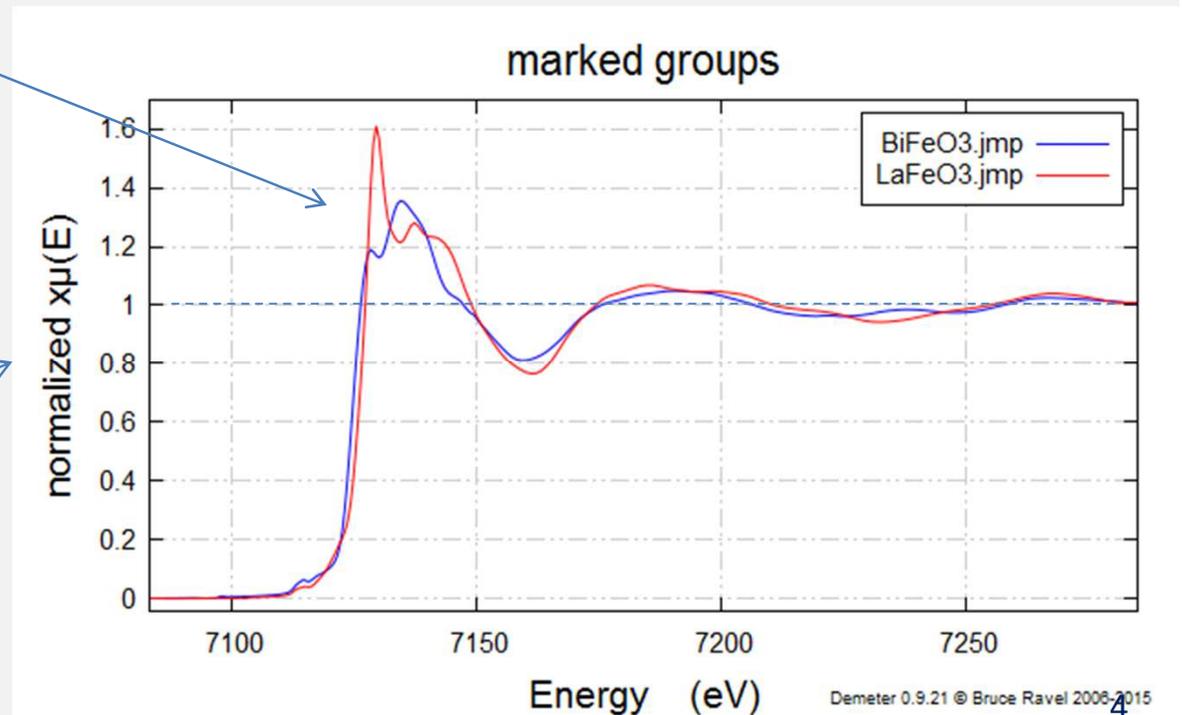
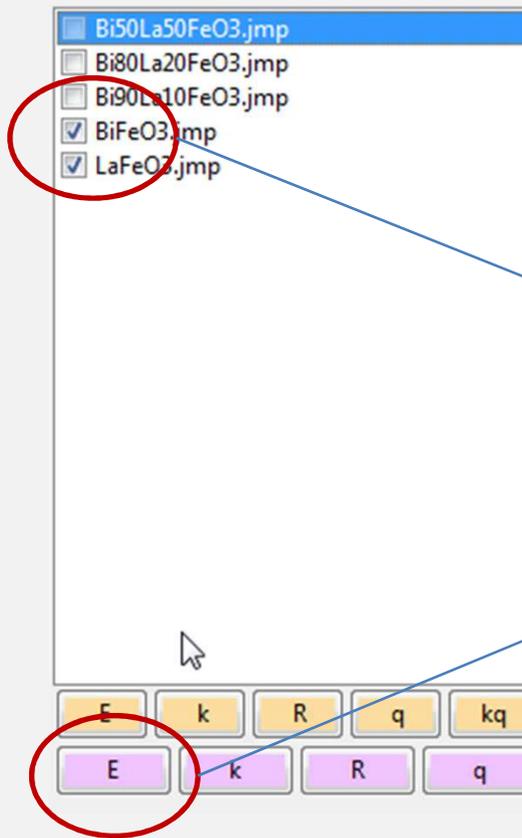
Data on: LCA-BiLaFeO

Nome	
Bi50La50FeO3.jmp	$\text{Bi}_{0.5}\text{La}_{0.5}\text{FeO}_3$
Bi80La20FeO3.jmp	$\text{Bi}_{0.8}\text{La}_{0.2}\text{FeO}_3$
Bi90La10FeO3.jmp	$\text{Bi}_{0.9}\text{La}_{0.1}\text{FeO}_3$
BiFeO3.jmp	BiFeO_3
LaFeO3.jmp	La_0FeO_3

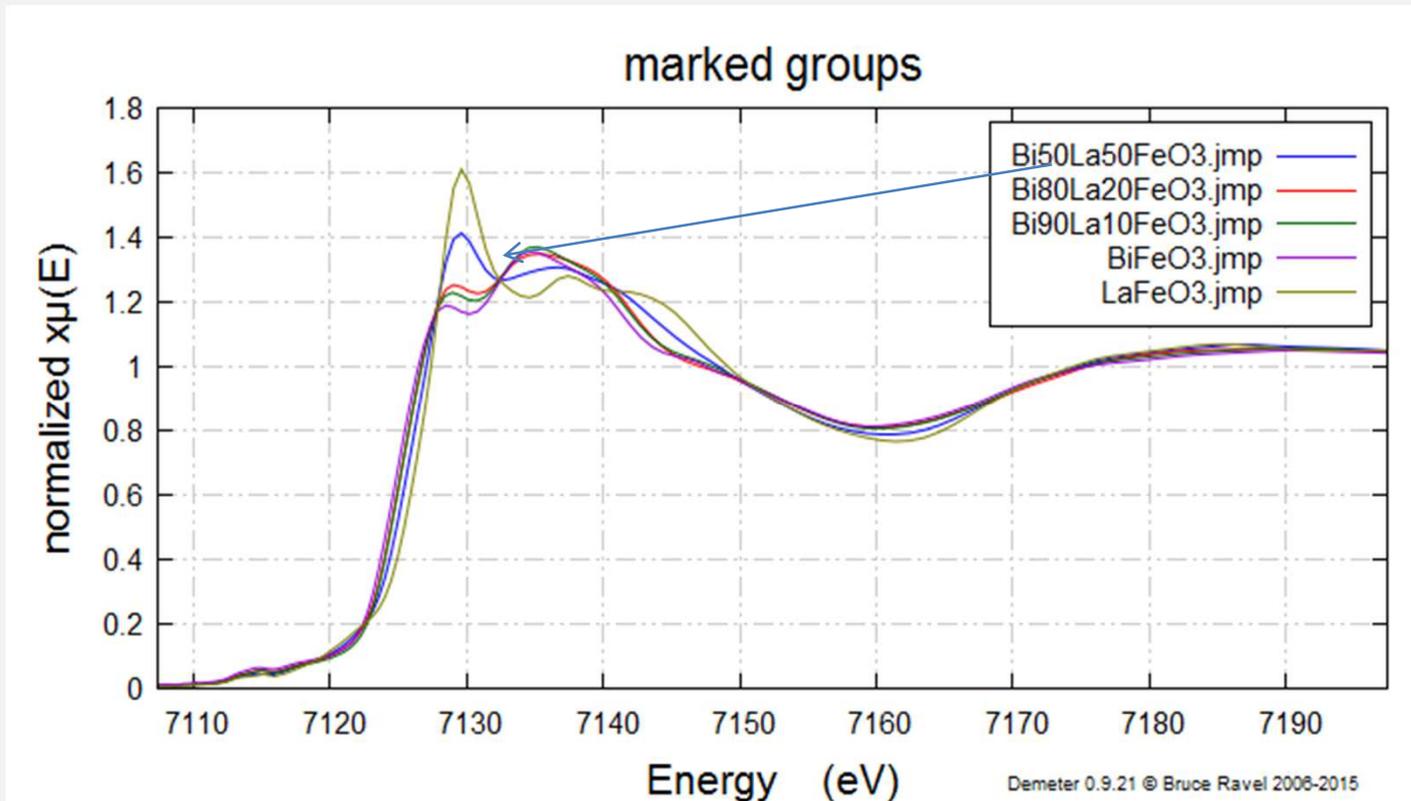
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Numerator	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Denominator	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

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

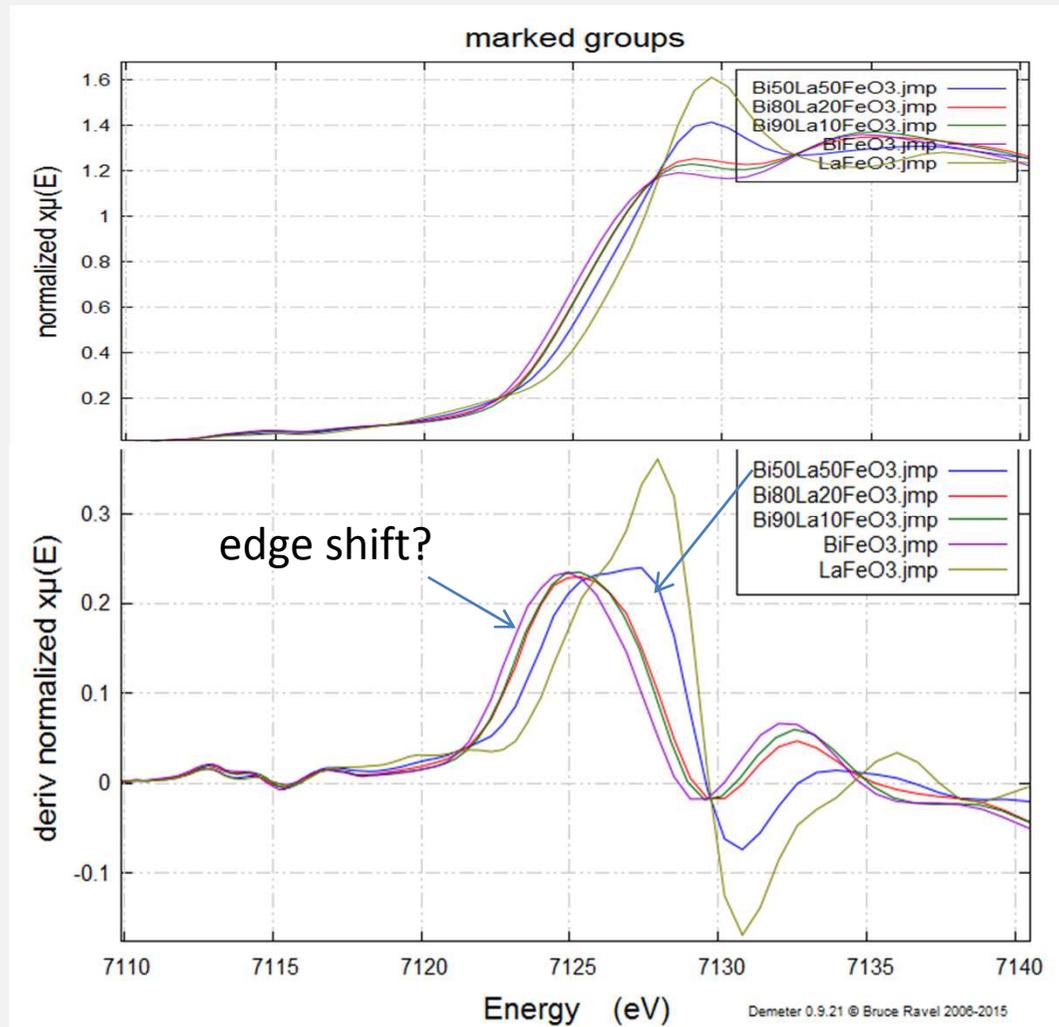
Compare end member Normalized spectra



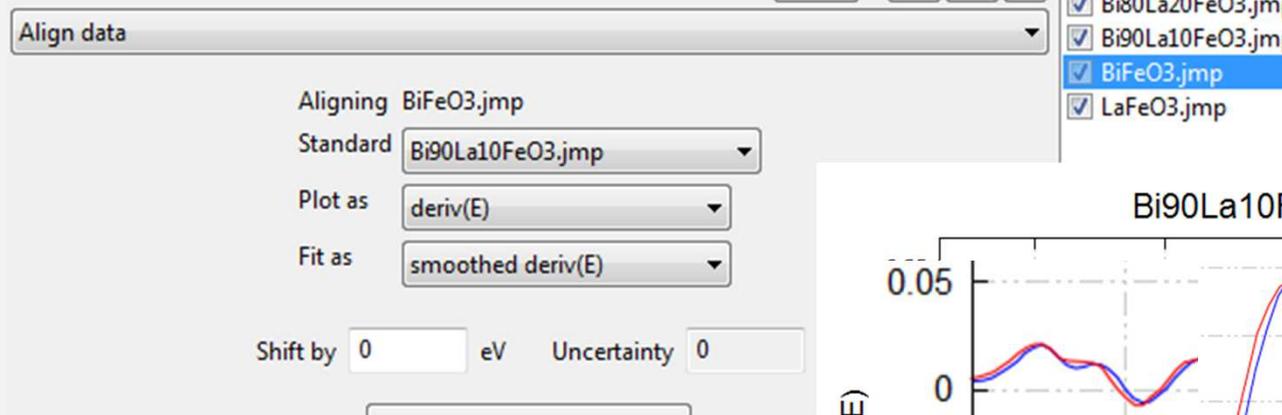
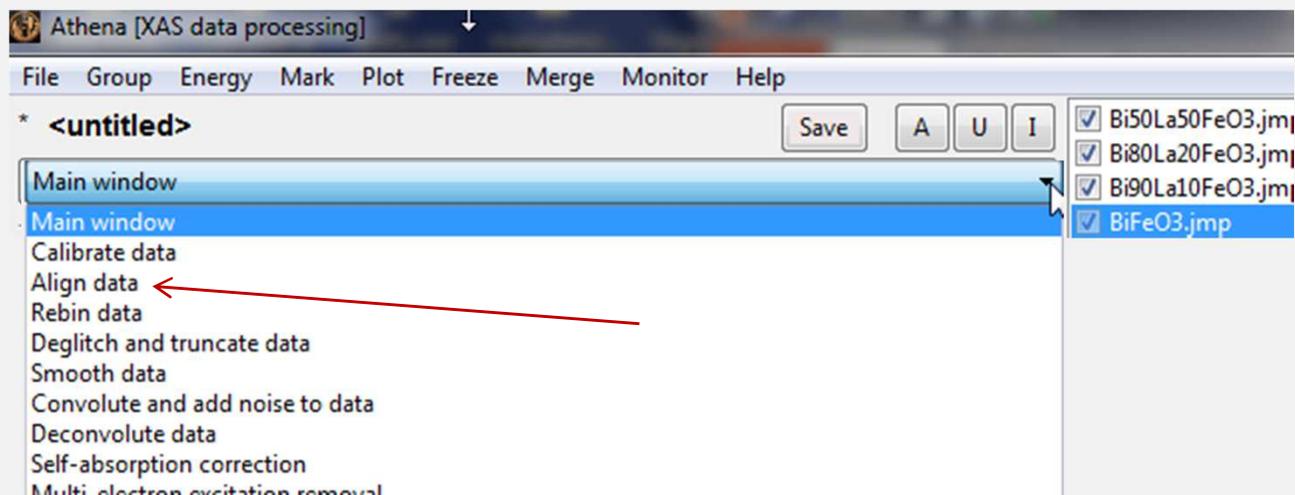
Compare spectra with the end compounds



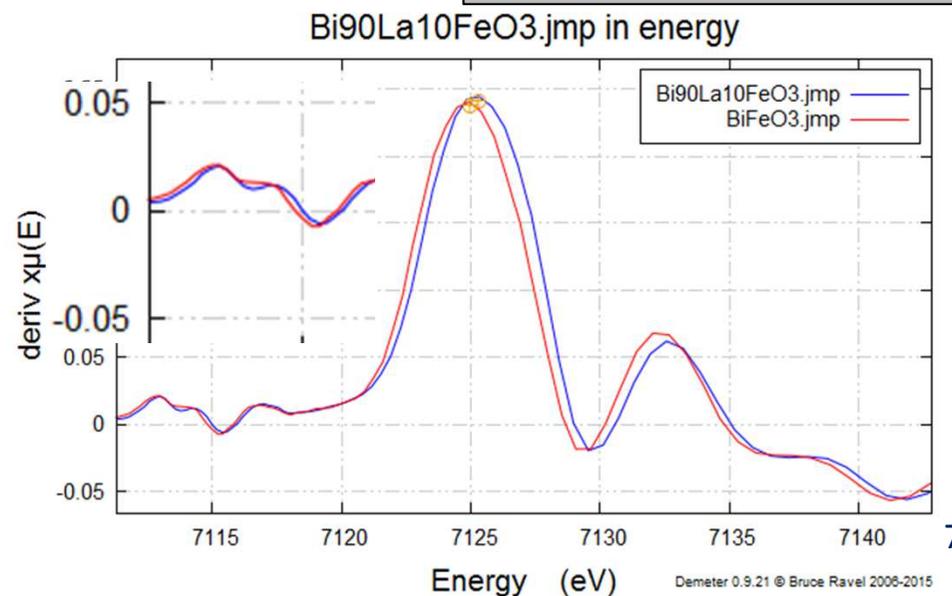
Compare derivatives



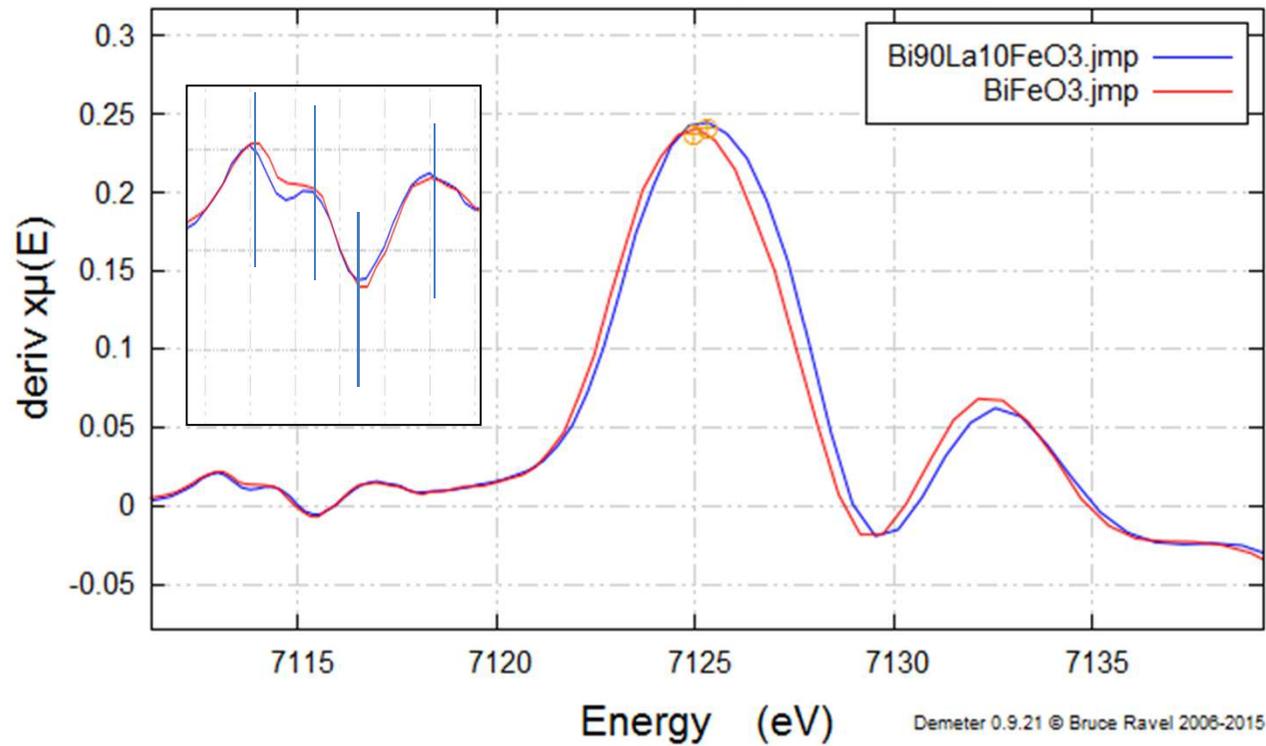
Align the data (If you need)



It is likely a rigid shift between BiFeO3 and Bi09La01FeO3 data



Bi90La10FeO3.jmp in energy



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

Athena [XAS data processing]

File Group Energy Mark Plot Freeze Merge Monitor Help

* <untitled> Save A U I

Linear combination fitting

Fit range: -20 to 30 Fitting space: norm $\mu(E)$ deriv $\mu(E)$ $\chi(k)$

Standards Fit results Combinatorics Sequence

Standards	Weight	E0	Fit E0	Required
1: BiFeO3.jmp	0.500	0	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
2: LaFeO3.jmp	0.500	0	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Bi50La50FeO3.jmp
 Bi80La20FeO3.jmp
 Bi90La10FeO3.jmp
 BiFeO3.jmp
 LaFeO3.jmp

- Main window
- Calibrate data
 - Align data
 - Rebin data
 - Deglitch and truncate data
 - Smooth data
 - Convolute and add noise to data
 - Deconvolute data
 - Self-absorption correction
 - Multi-electron excitation removal
 - Copy series
 - Data summation

- Linear combination fitting
- Principle components analysis
- Peak fitting
- Log-ratio/phase difference analysis
- Dif 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

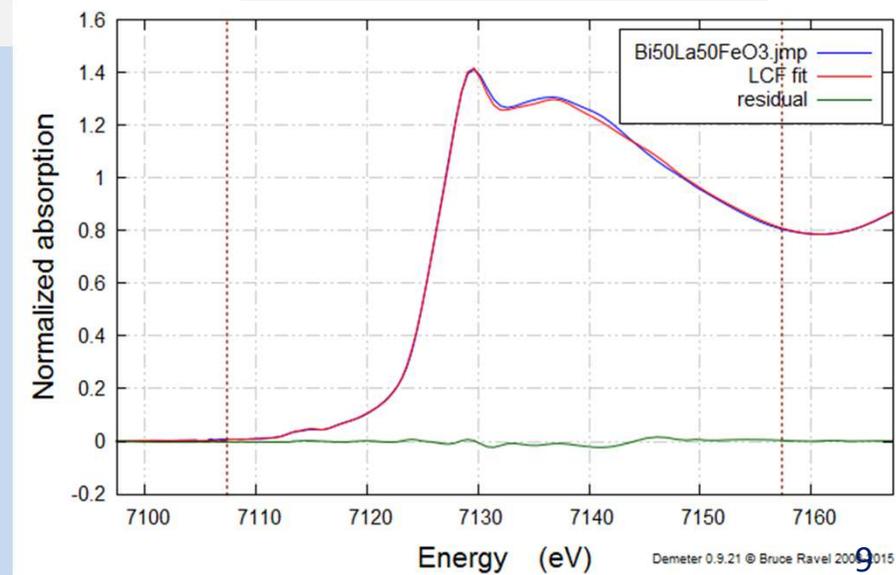
Noise added to data: 0

R-factor = 0.0001869

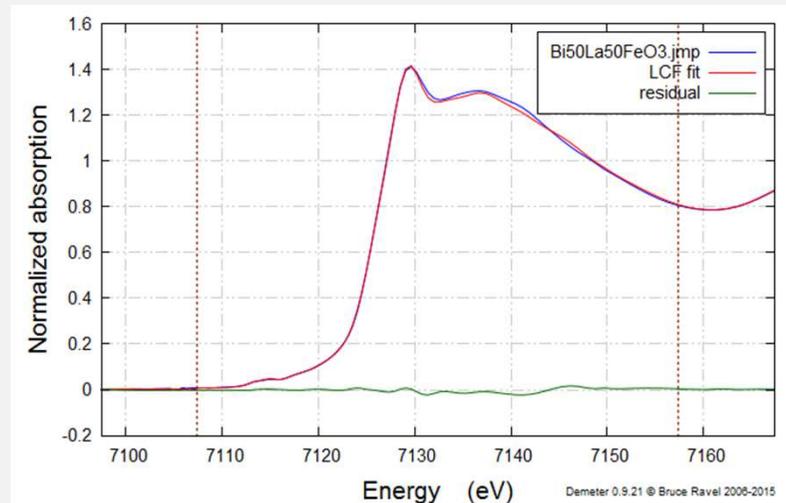
Chi-square = 0.00614

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
 Reduced chi-square = 0.0000534



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

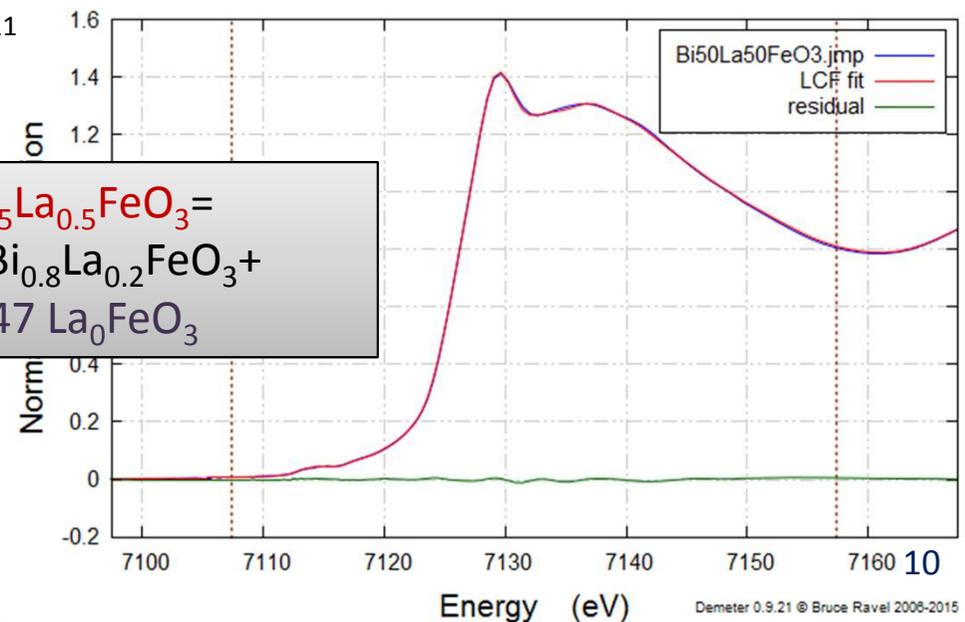
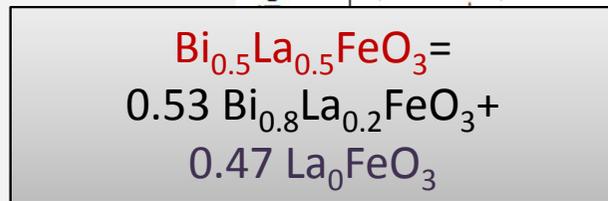
Overall e0 shift used: no

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)

