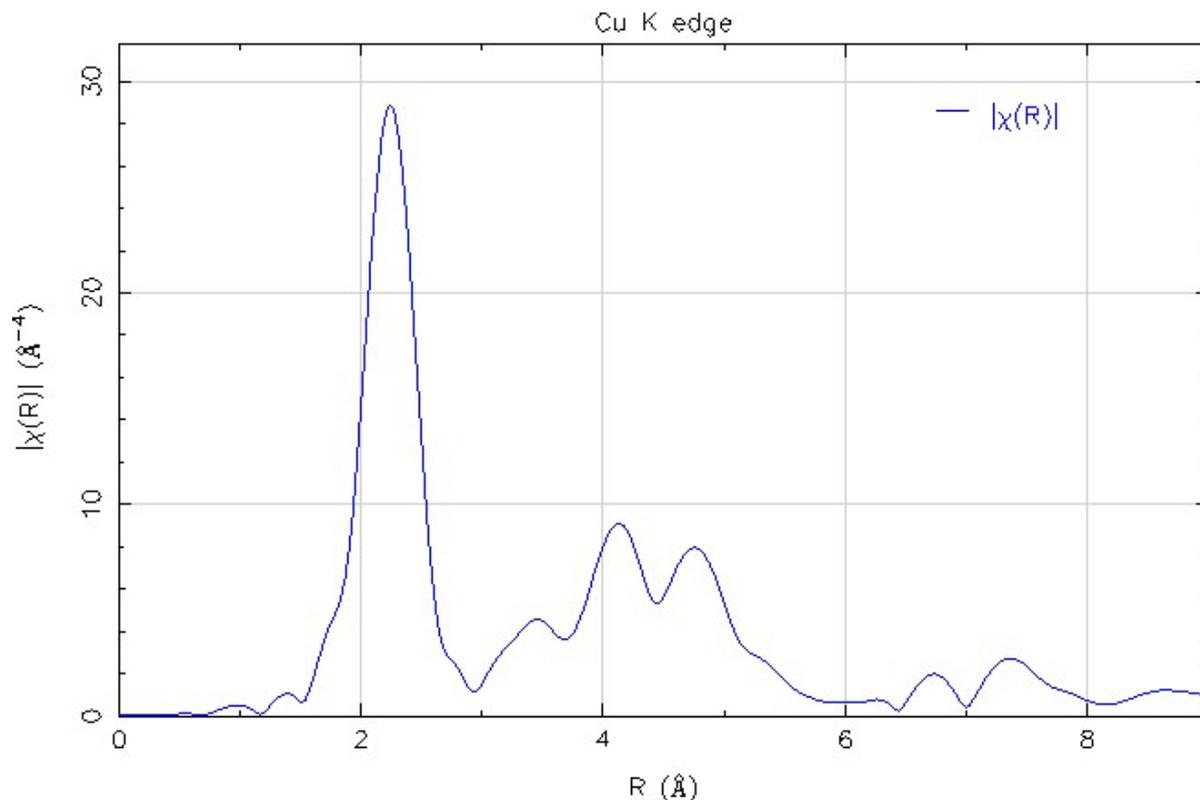


# EXAFS数据处理



## Fourier变换-R空间



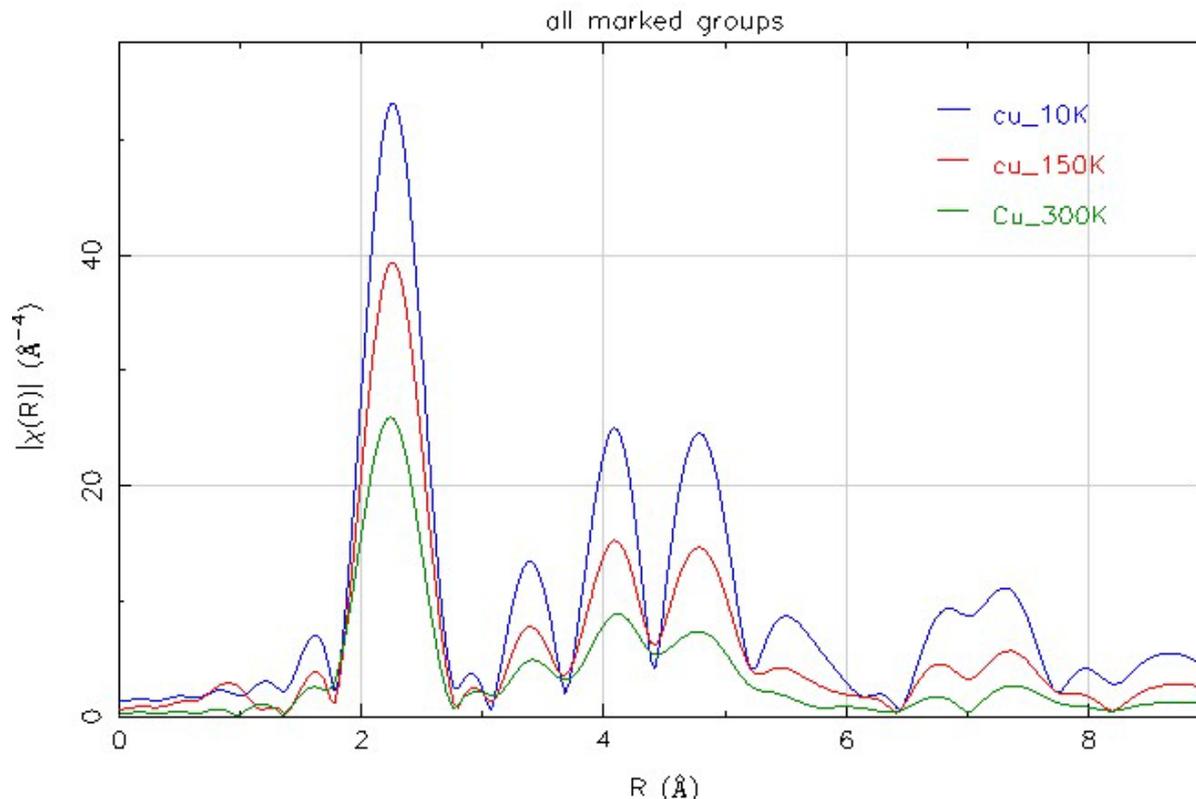
由于没有考虑相位修正，这里的R值与实际的关键长相差0.2-0.5 Å。



# EXAFS数据处理



## Fourier变换-R空间



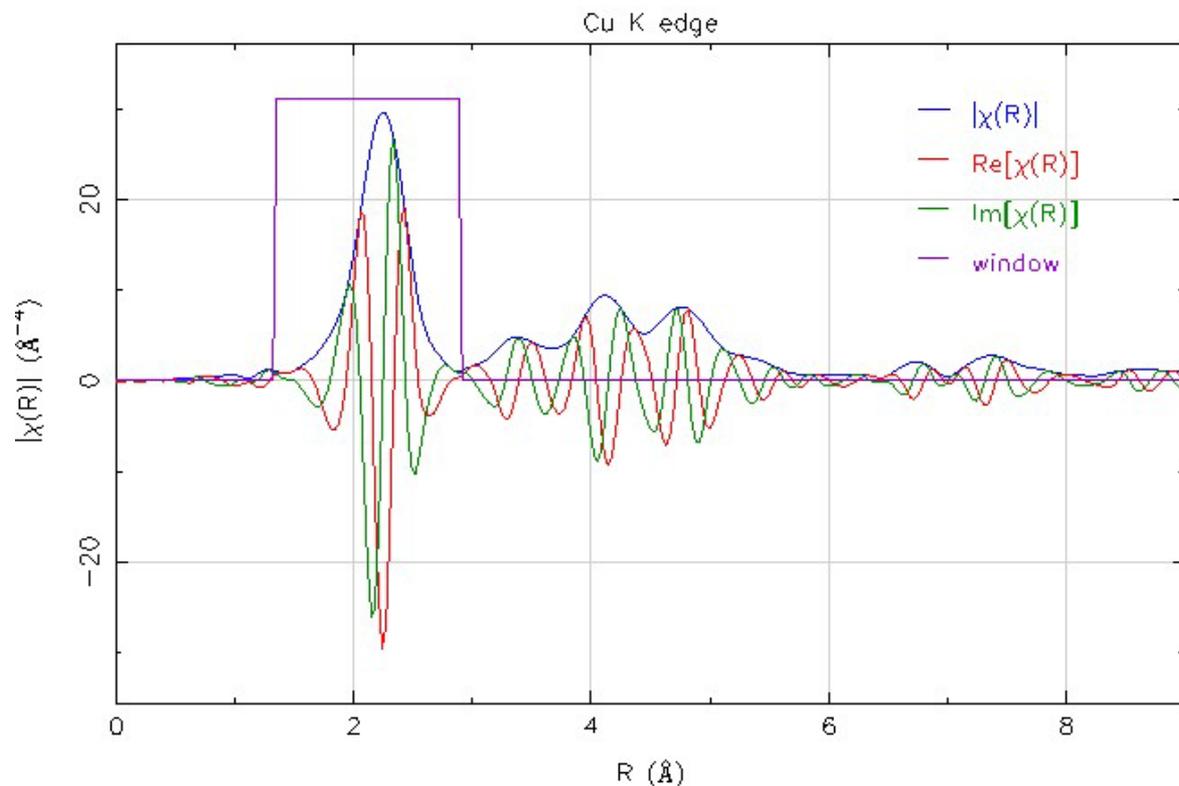
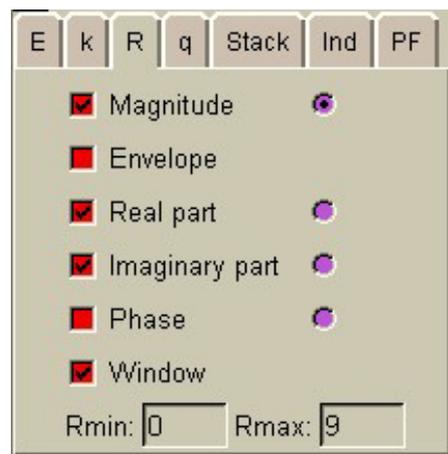
不同温度下Cu foil K边EXAFS在R空间的变化



# EXAFS数据处理



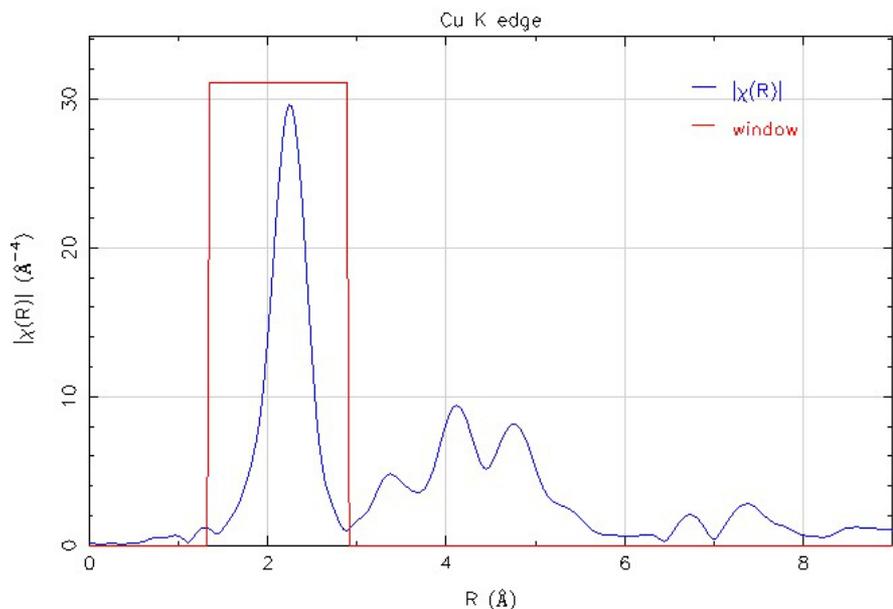
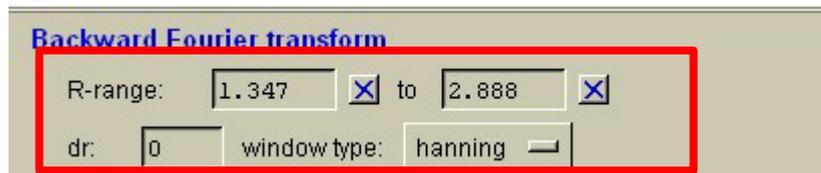
## Fourier变换-R空间



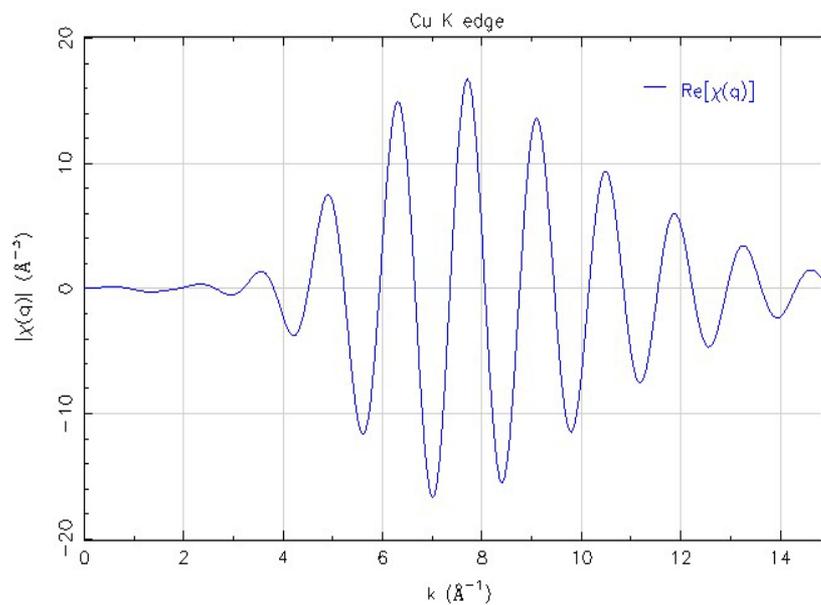
# EXAFS数据处理



## 反Fourier变换



窗函数



q空间



# EXAFS数据处理



## 技巧一：复制数据

The screenshot shows the Athena software interface. The 'Project' panel displays 'Current group: Cu K edge' and 'File: E:/paper/Cu-ST.dat'. The 'Background removal' panel shows 'E0: 8979', 'Rbkg: 1.0', 'k-weight: 2', and 'Edge step: 1.9305'. The 'Forward Fourier transform' panel shows 'k-range: 3.1 to 15.0', 'dk: 1', and 'window type: hanning'. The 'Backward Fourier transform' panel shows 'R-range: 1 to 3', 'dr: 0.0', and 'window type: hanning'. The 'Plotting parameters' panel shows 'plot multiplier: 1' and 'y-axis offset: 0'. The 'Group actions' menu is open, with 'Copy group' highlighted in red. A red arrow points from the 'Copy group' menu item to a second window showing the copied data as 'Copy of Cu K edge'.

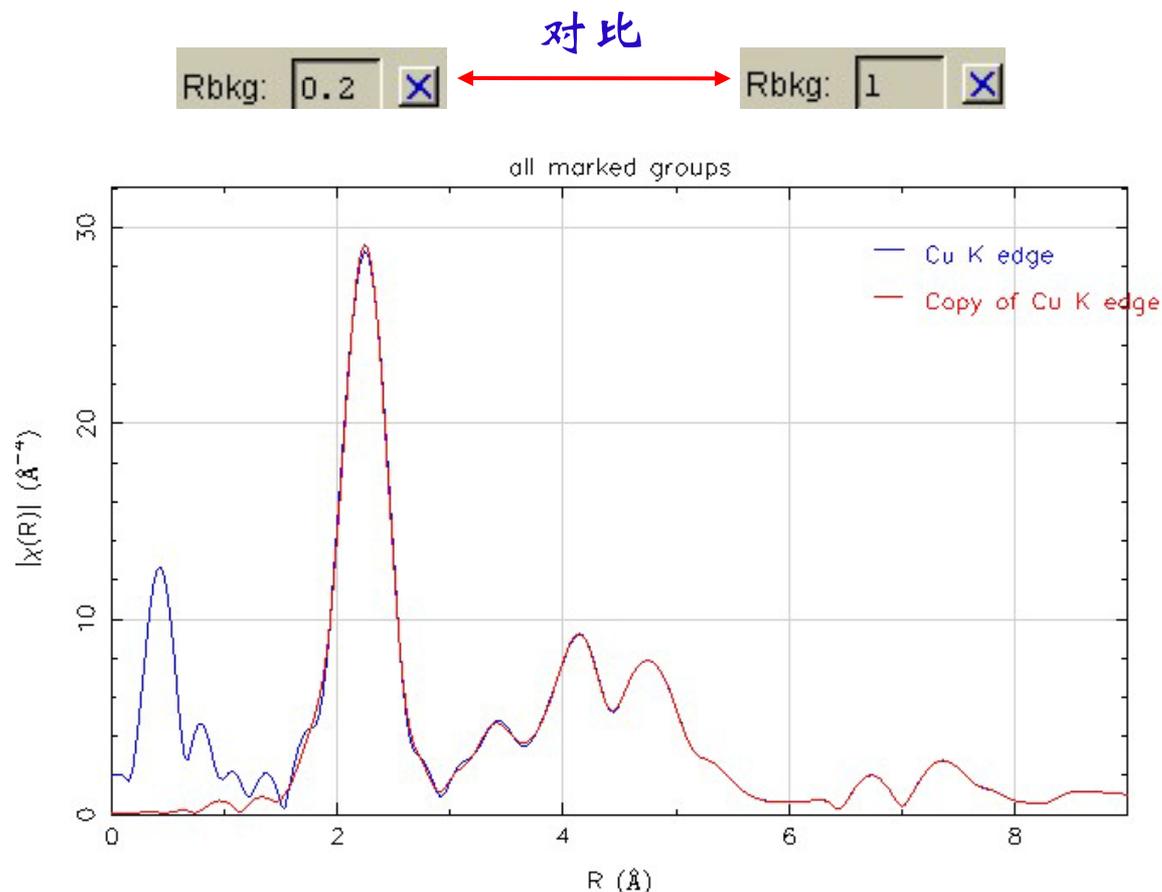
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# EXAFS数据处理



## 技巧一：复制数据

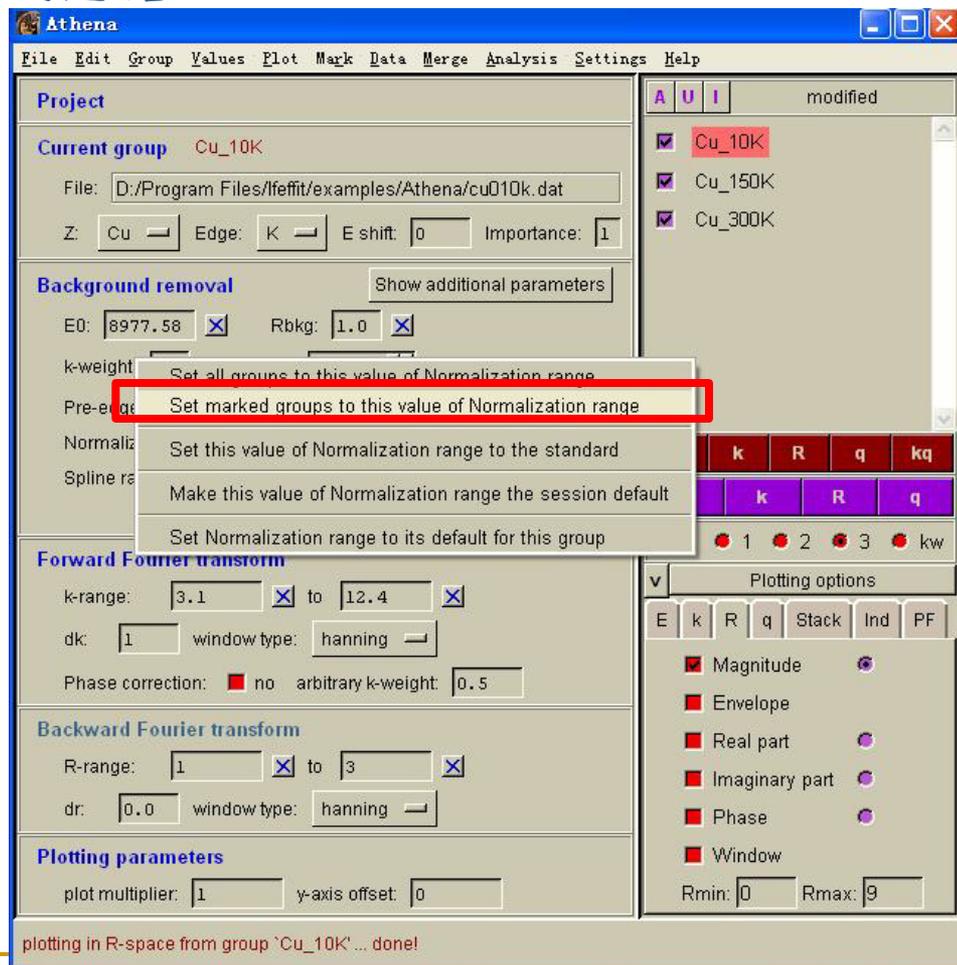


# EXAFS数据处理



## 技巧二：批量处理多组数据

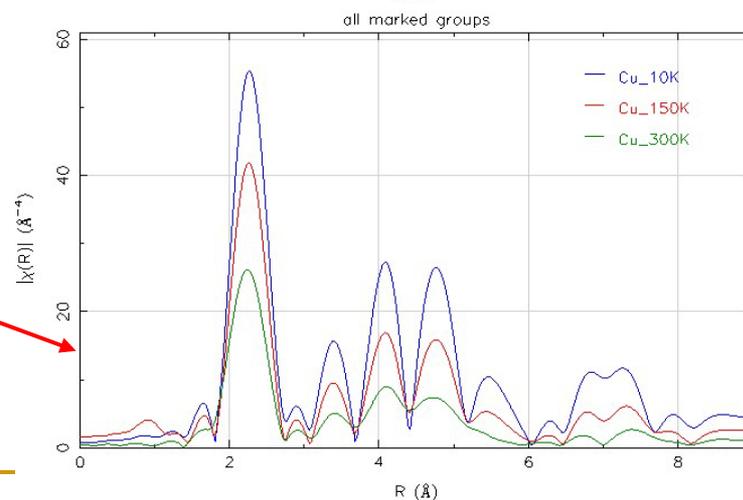
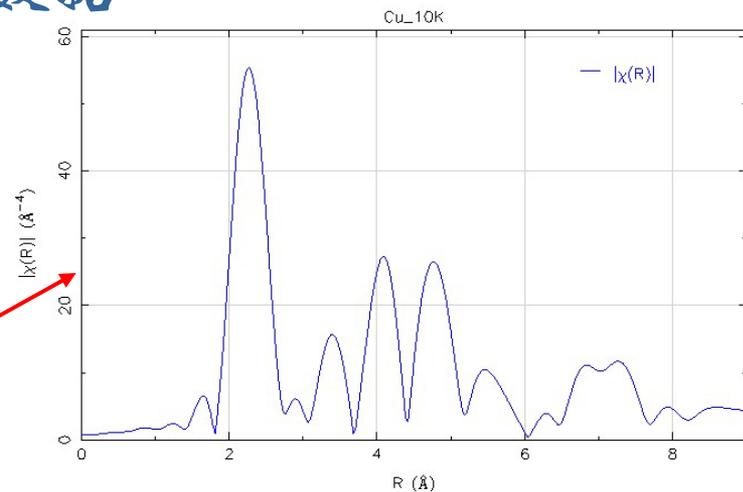
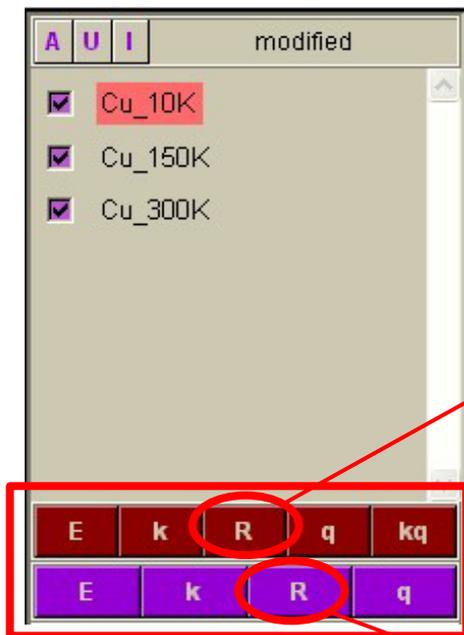
多组数据进行对比时，所有参数的设置尽量一致，例如Rbkg参数，归一化范围，样条函数范围，Fourier变换k的范围，窗函数等等。可以选择其中的一个group作为代表，优先处理，然后其他的group参数设置跟它一致。



# EXAFS数据处理



## 技巧二：批量处理多组数据



# EXAFS数据处理



## 技巧二：批量处理多组数据

Athena

File Edit Group Values Plot Mark Data Merge Analysis Settings Help

**Project**

Current group: cu\_foil.dat  
File: F:/2011/BSRFseminar/cu-foil.dat  
Z: Cu Edge: K E shift: 4.014 Importance: 1

**Background removal** Show additional parameters

E0: 8979 Rbkg: 1  
k-weight: 2 Edge step: 1.78020 fix step  
Pre-edge range: -150 to -30  
Normalization range: 50 to 920  
Spline range: k: 0.0 to 15.736  
E: 0.000 to 943.435

**Forward Fourier transform**

k-range: 2 to 15  
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 parameters**

plot multiplier: 1 y-axis offset: 0

plotting in energy from group `cu\_foil.dat' ... done!

modified

cu\_foil.dat

E k R q kq

E k R q

0 1 2 3 kw

v Plotting options

E k R q Stack Ind PF

mu(E)

background

pre-edge line

post-edge line

Normalized

Derivative

Emin: -200 Emax: 1000



# Athena图形显示

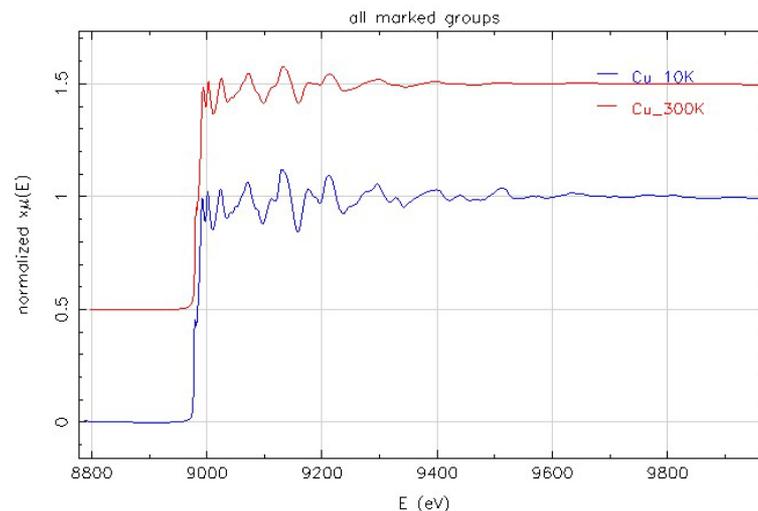


## 绘图参数 (一)

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

- Project:** Current group: Cu\_300K, File: E:/paper/Cu-ST.dat, Z: Cu, Edge: K, E shift: -1.51, Importance: 1
- Background removal:** E0: 8979, Rbkg: 1.0, k-weight: 2, Edge step: 1.98929, Pre-edge range: -150 to -30, Normalization range: 150 to 950, Spline range: k: 0.0 to 16, E: 0.000 to 975.356
- Forward Fourier transform:** k-range: 3.1 to 12.4, dk: 0.2, 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 parameters (highlighted):** plot multiplier: 1, y-axis offset: 0.5

Additional controls on the right include checkboxes for Cu\_10K, Cu\_150K, and Cu\_300K, and a 'Plotting options' section with checkboxes for mu(E), background, pre-edge line, post-edge line, Normalized, and Derivative. The Emax is set to 1000.



# Athena图形显示



## 绘图参数 (二)

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

- Project**
  - Current group: cu\_foil.dat
  - File: F:/2011/BSRFseminar/cu-foil.dat
  - Z: Cu | Edge: K | E shift: 4.014 | Importance: 1
- Background removal**
  - Show additional parameters
  - E0: 8979 | Rbkg: 1
  - k-weight: 2 | Edge step: 1.78020 |  fix step
  - Pre-edge range: -150 to -30
  - Normalization range: 50 to 920
  - Spline range: k: 0.0 to 15.736 | E: 0.000 to 943.435
- Forward Fourier transform**
  - k-range: 2 to 15
  - 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 parameters**
  - plot multiplier: 1 | y-axis offset: 0

On the right side, the **Plotting options** panel is highlighted with a red box and contains the following settings:

- Buttons: E, k, R, q, kq
- Buttons: E, k, R, q
- Buttons: 0, 1, 2, 3, kw
- Buttons: v, Plotting options
- Buttons: E, k, R, q, Stack, Ind, PF
- mu(E)
- background
- pre-edge line
- post-edge line
- Normalized
- Derivative
- Emin: -200 | Emax: 1000

At the bottom, a status bar indicates: plotting in energy from group 'cu\_foil.dat' ... done!



# Athena图形显示

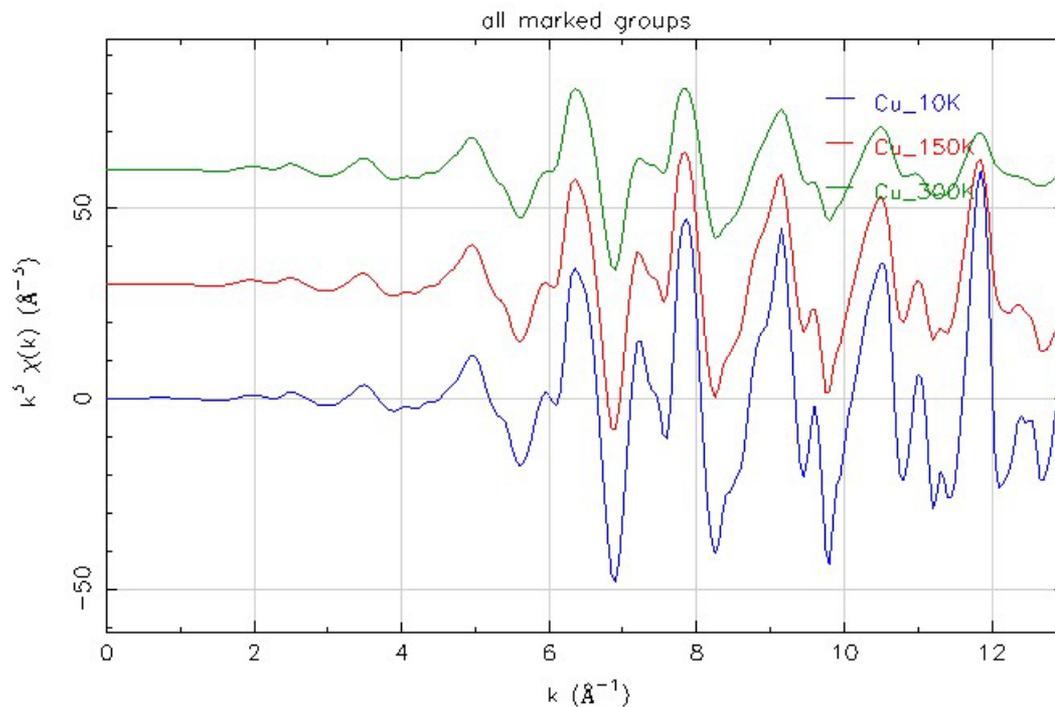
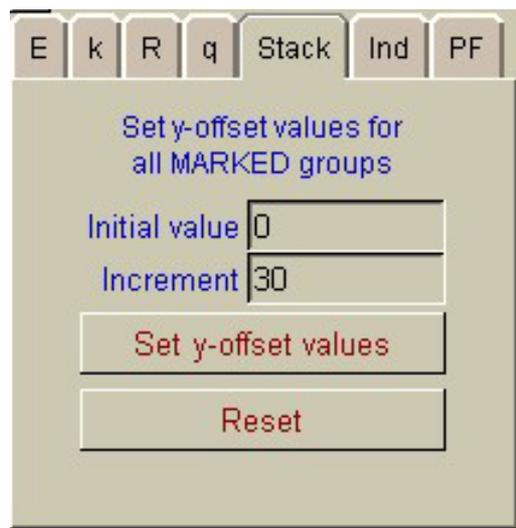


The screenshot displays six panels from the Athena software interface, arranged in two rows of three. Each panel has a header with tabs: E, k, R, q, Stack, Ind, PF.

- Top-left panel:** Controls for  $\mu(E)$  and background. Includes checkboxes for  $\mu(E)$ , background, pre-edge line, post-edge line, Normalized, and Derivative. Input fields for Emin: -200 and Emax: 1000.
- Top-middle panel:** Controls for  $\chi(E)$ . Includes checkboxes for Plot  $\chi(E)$  and Window. Input fields for kmin: 0 and kmax: 13.
- Top-right panel:** Controls for Magnitude, Envelope, Real part, Imaginary part, Phase, and Window. Includes checkboxes for Magnitude, Envelope, Real part, Imaginary part, Phase, and Window. Input fields for Rmin: 0 and Rmax: 9.
- Bottom-left panel:** "Set y-offset values for all MARKED groups". Includes input fields for Initial value (0) and Increment (0), and buttons for "Set y-offset values" and "Reset".
- Bottom-middle panel:** "Plot indicators". Includes a checked checkbox for "Display indicators" and a list of five indicators (1-5) with "R" and a checkbox.
- Bottom-right panel:** "Point finder". Includes text "The last plot was in R", input fields for X and Y, and buttons for "find Y", "find X", and "Clear".



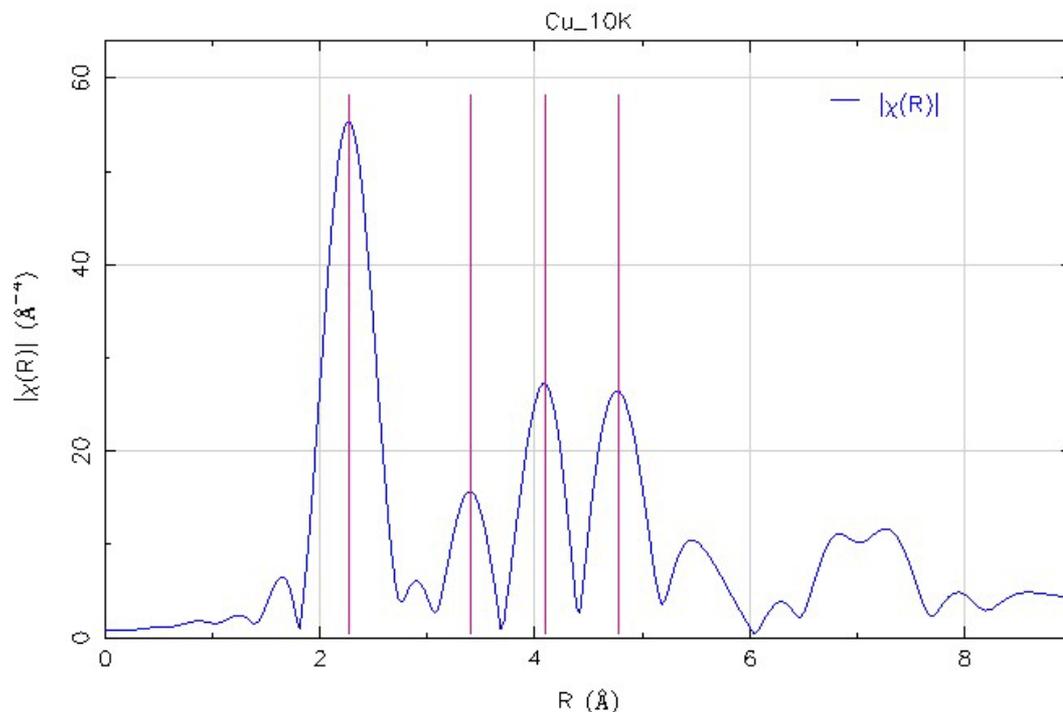
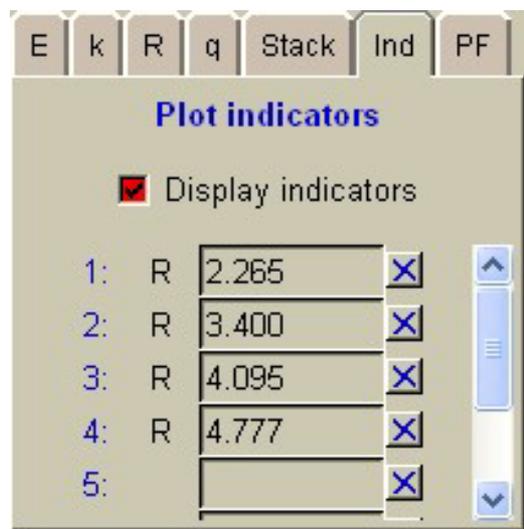
# Athena图形显示



产生堆叠效果



# Athena图形显示



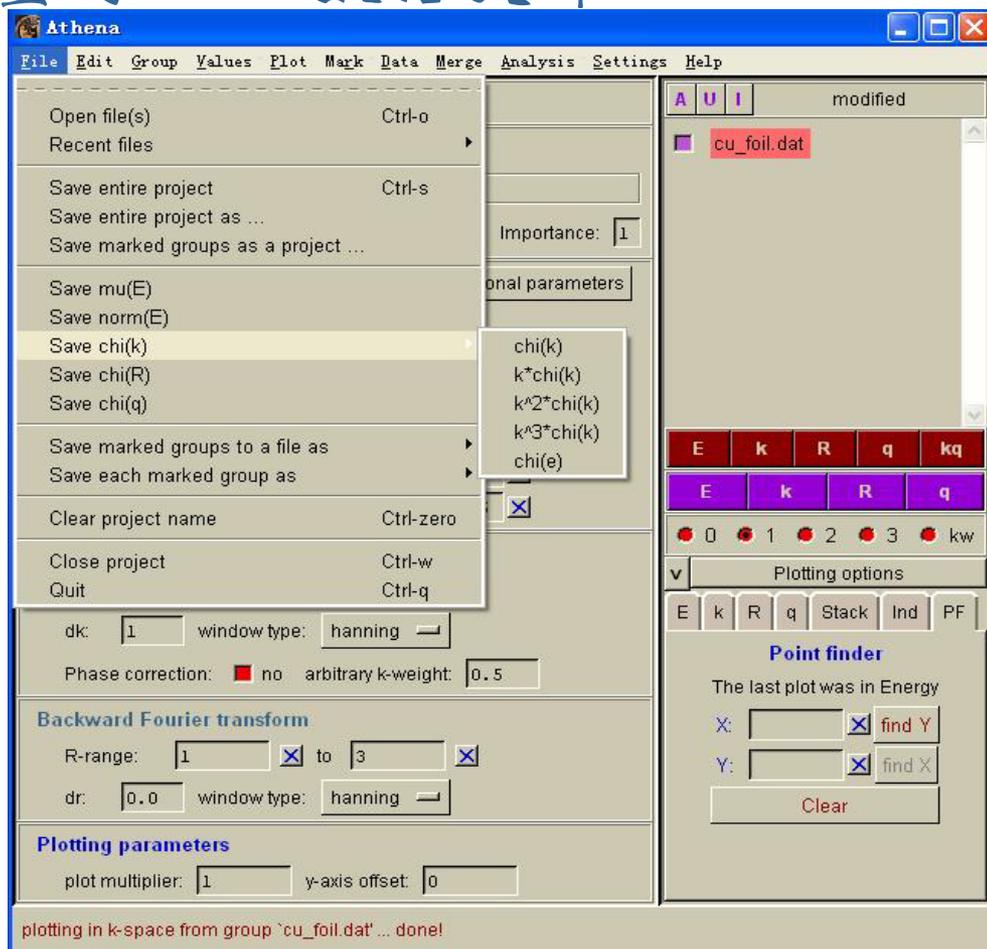
标示特殊位置

# 保存数据



## 可以保存多种类型的XAFS数据文件

- ◆ 工程文件.prj
- ◆  $\mu(E)$ ,  $\text{norm}(E)$
- ◆  $\chi(k)$ ,  $\chi(R)$ ,  $\chi(q)$



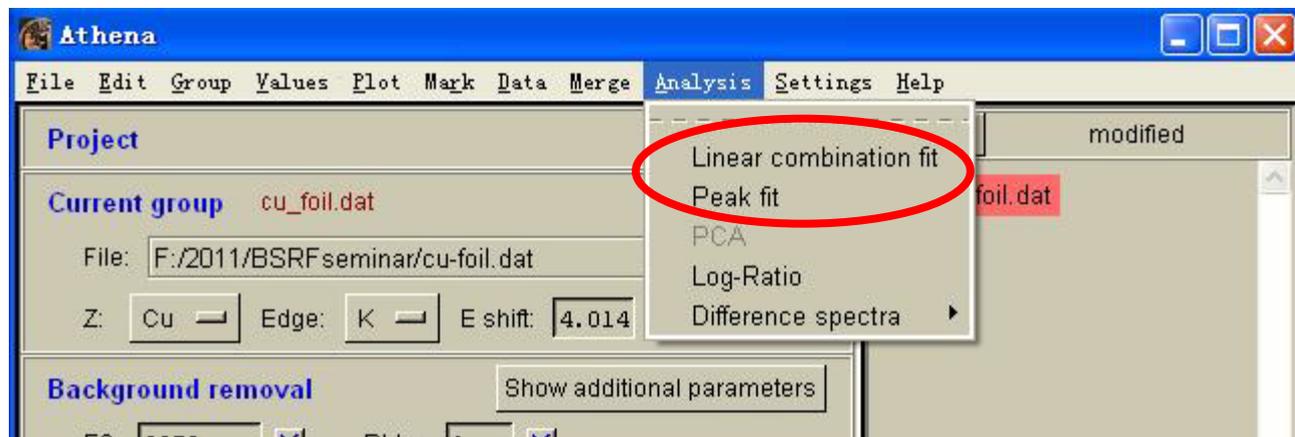
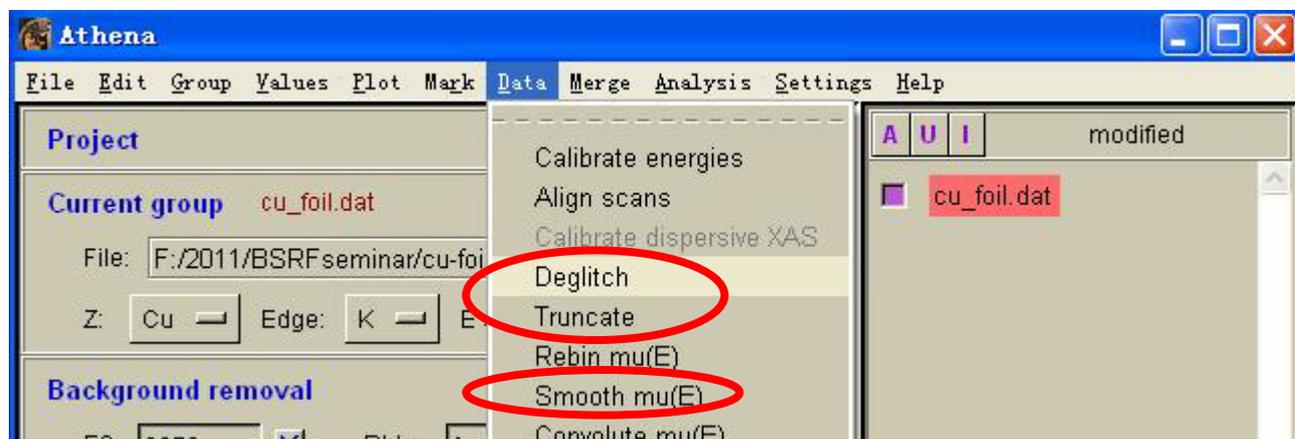
# 其他功能



- ◆ 去除glitch
- ◆ 截取数据
- ◆ 平滑数据
- ◆ 线性组合分析
- ◆ 边前峰的分峰拟合
- ◆ .....



# 其他功能



# 其他功能



## 去除glitch

Athena

File Edit Group Values Plot Mark Data Merge Analysis Settings Help

Deglitch data

Group: uhup.003

Deglitch a single point

Plot as: mu(E)

Replot Choose a point Remove point Help

Deglitch many points

Replot Remove glitches Help

Tolerance: 0.0805 Emin: 17227.472 Emax: 17668.200

Document section: deglitching data

Return to the main window

modified

- uhup.003

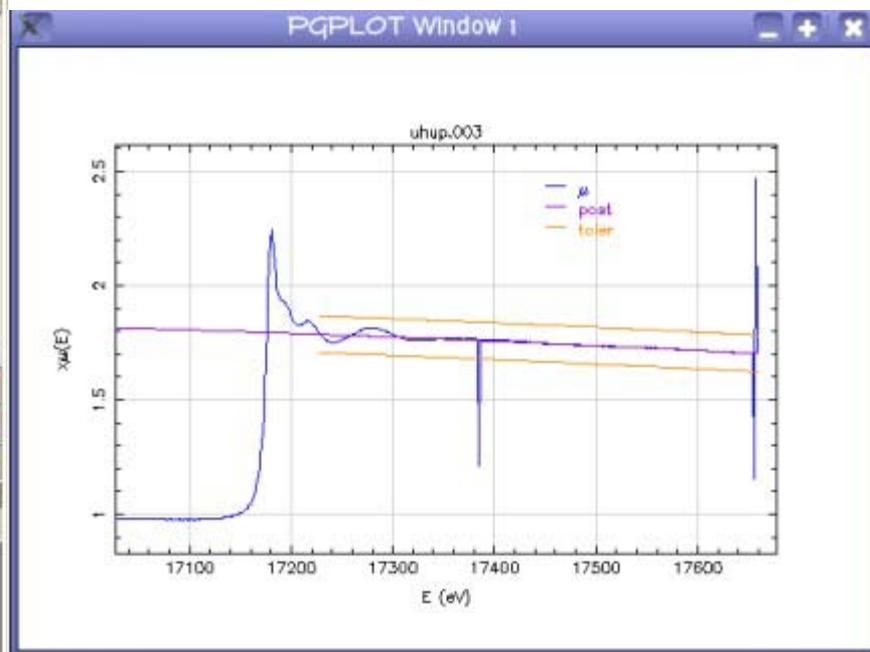
E	k	R	q	kw
E	k	R	q	
0	1	2	3	kw

Plotting options:

- mu(E)
- background
- pre-edge line
- post-edge line
- Normalized
- Derivative

Emin: -150 Emax: 500

plotting in energy from group 'uhup.003' ... done!



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# 其他功能



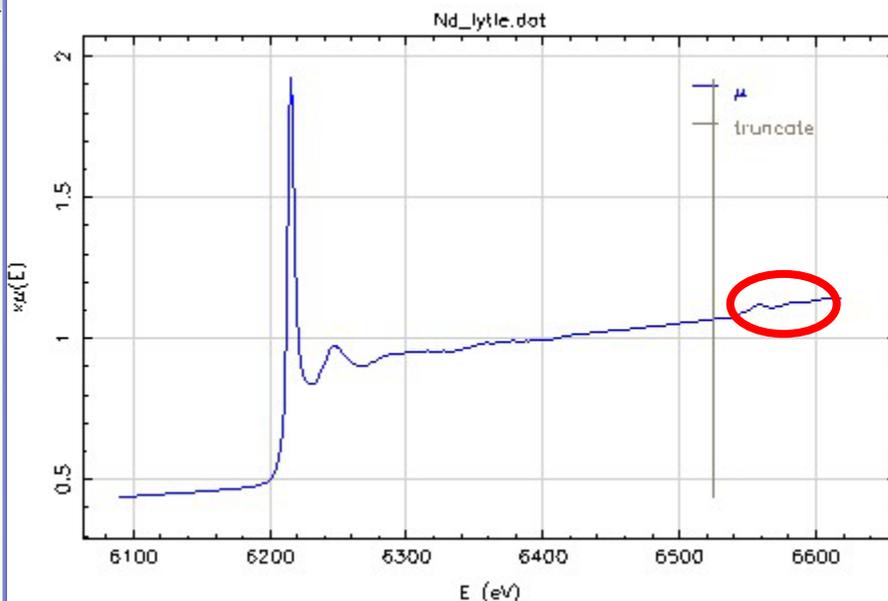
## 截取数据

The screenshot shows the Athena software interface with the 'Data truncation' dialog box open. The dialog box has a title bar 'Athena' and a menu bar 'File Edit Group Values Plot Mark Data Merge Analysis Settings Help'. The main area is titled 'Data truncation' and contains the following elements:

- Group: Nd\_lytle.dat
- Drop points: after E = 6524.917
- Buttons: Replot, Truncate data, Truncate marked groups
- Document section: truncating data
- Return to the main window

On the right side of the dialog box, there is a list of data groups with checkboxes, a set of buttons for element selection (E, k, R, q, kq), a set of buttons for edge selection (E, k, R, q), a set of buttons for edge type selection (0, 1, 2, 3, kw), a 'Plotting options' section with checkboxes for mu(E), background, pre-edge line, post-edge line, Normalized, and Derivative, and input fields for Emin (-150) and Emax (446).

At the bottom of the dialog box, it says 'Group "Cu\_10K" removed from project.'



# 其他功能



## 平滑数据

Athena

File Edit Group Values Plot Mark Data Merge Analysis Settings Help

### Data smoothing

Group: Zr-sample.dat

Interpolative smoothing Number of iterations: 5

Fourier filter smoothing Rmax: 6

Plot data and smoothed spectrum Make smoothed data group

Document section: data smoothing

Return to the main window

A U I modified

Zr-sample.dat

E k R q kq

E k R q

0 1 2 3 kw

v Plotting options

E k R q Stack Ind PF

mu(E)

background

pre-edge line

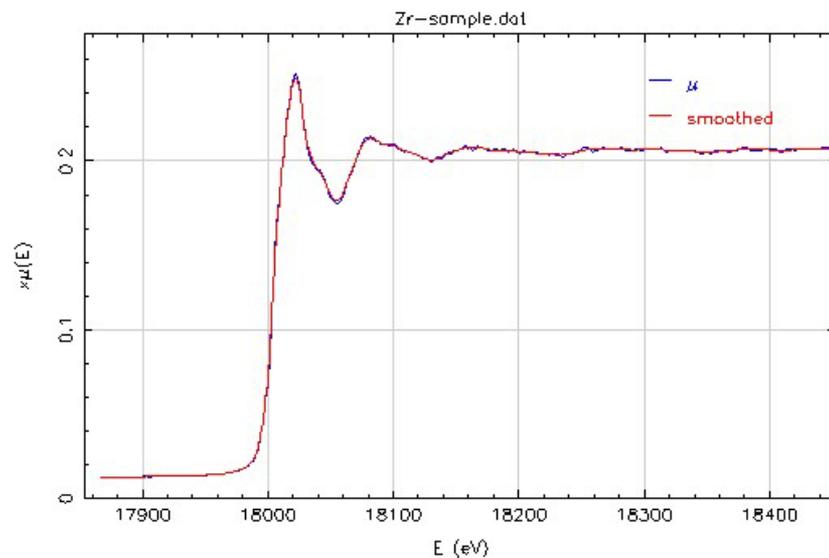
post-edge line

Normalized

Derivative

Emin: -150 Emax: 450

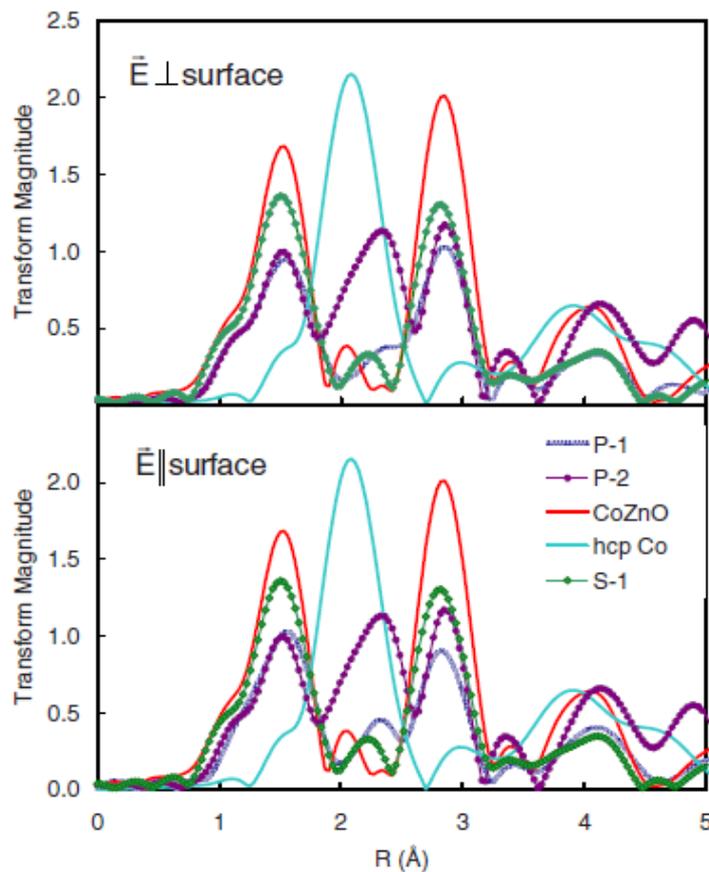
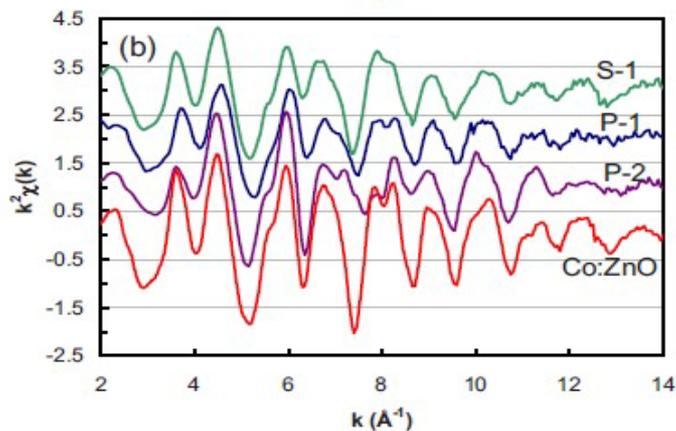
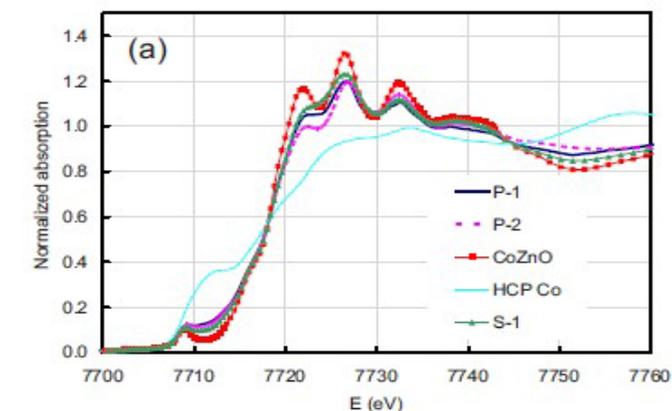
Smoothed Zr-sample.dat using 5 smoothing iterations



# 应用举例



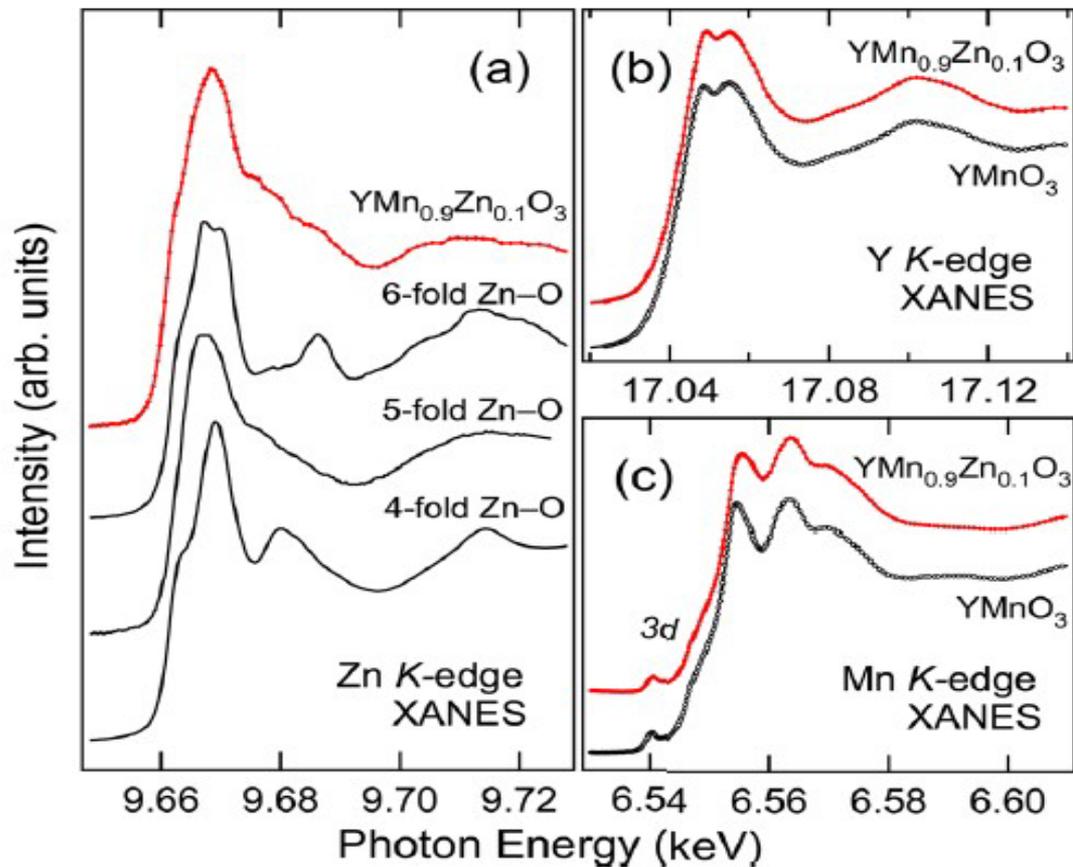
## 1 Co doped ZnO thin films



# 应用举例



## ◆ 2 Zn掺杂的多铁材料 $\text{YMnO}_3$



# 参考文献



- ◆ Athena 说明文档

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

- ◆ xafs.org

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

- ◆ 常用标样库

<http://ixs.iit.edu/database/>

<http://cars9.uchicago.edu/~newville/ModelLib/search.html>





# 谢谢!



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