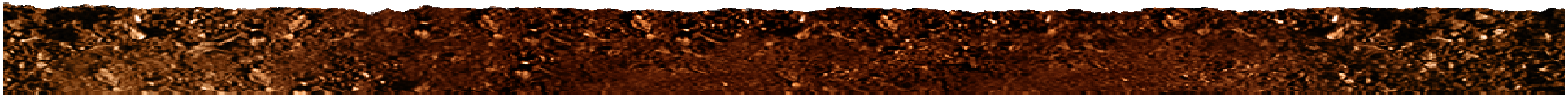
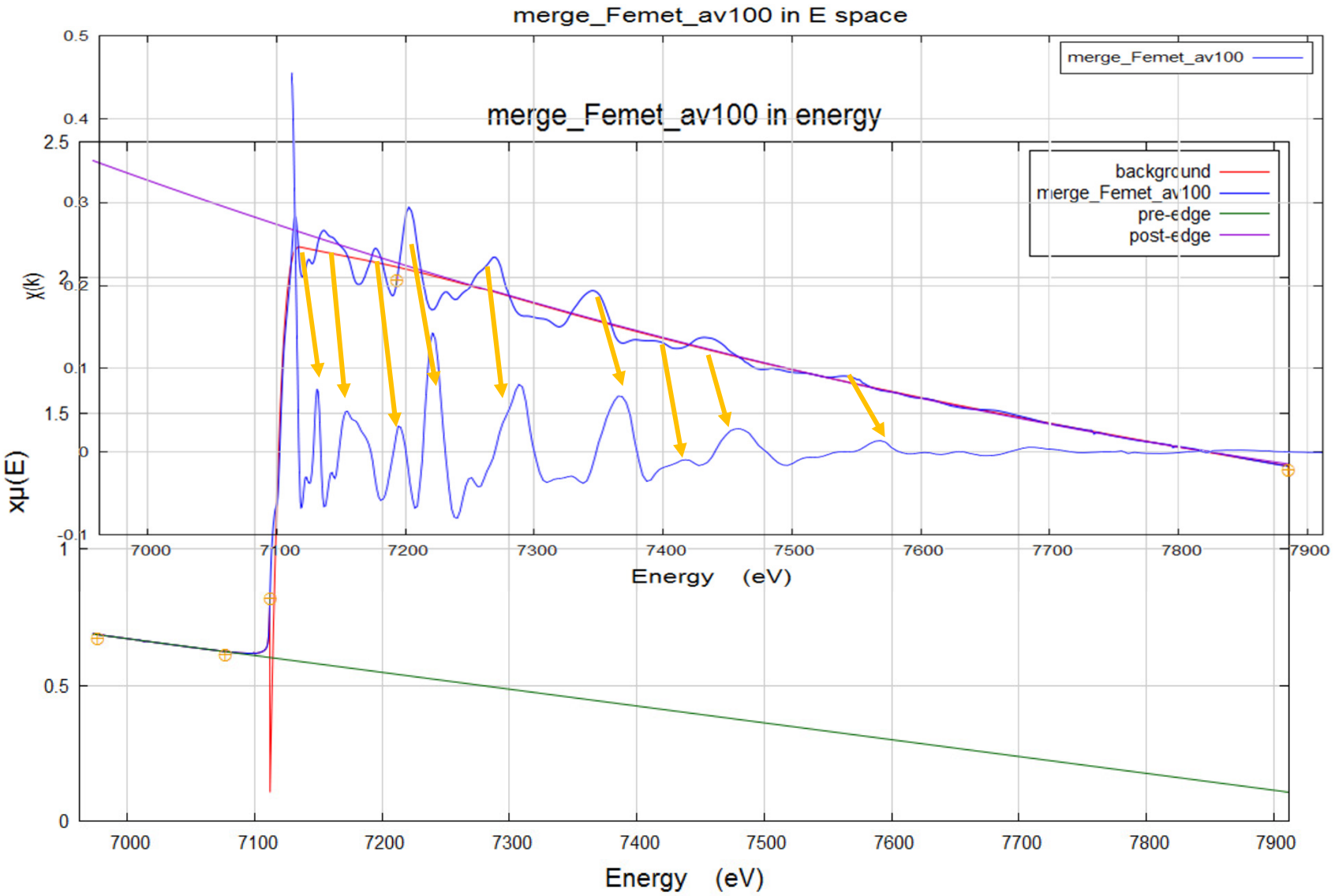
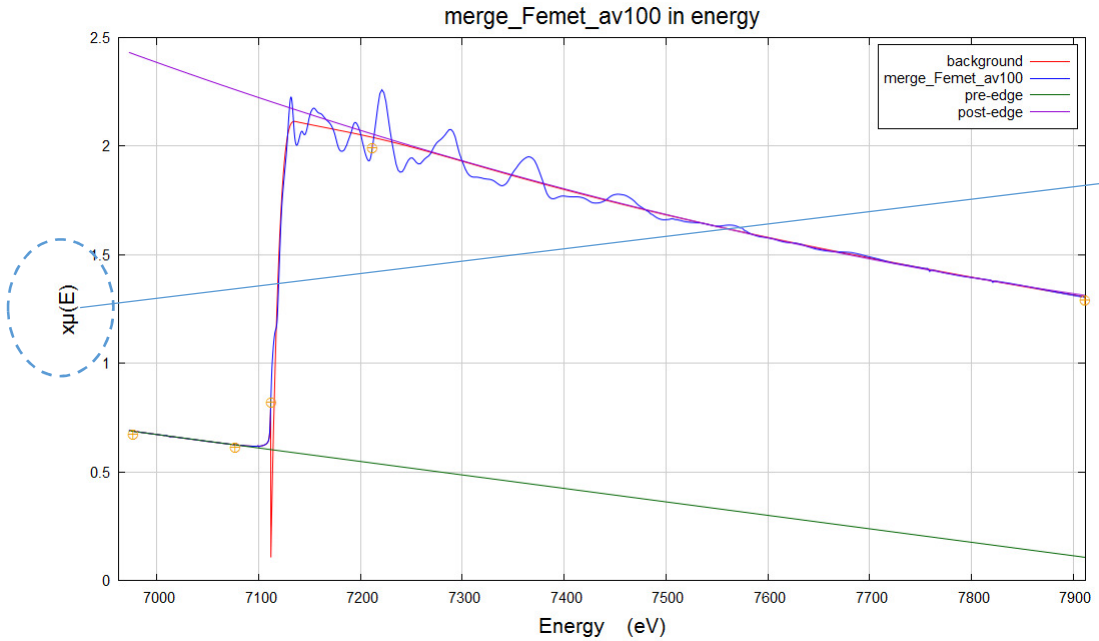
EXAFS Analysis



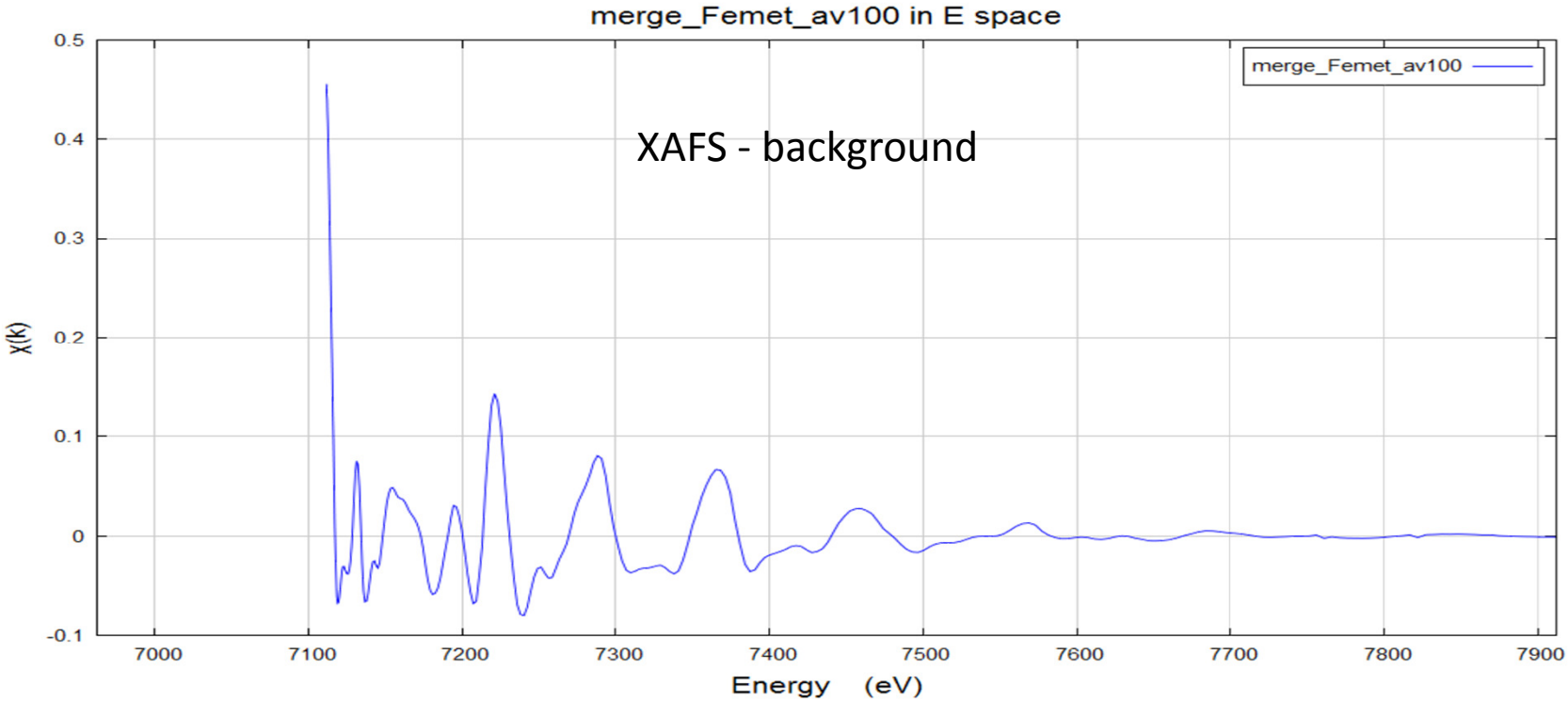
Recall

- Open file
- Calibration using reference foil
- Merging data
- Opening many files
- Data alignment
- Data normalization

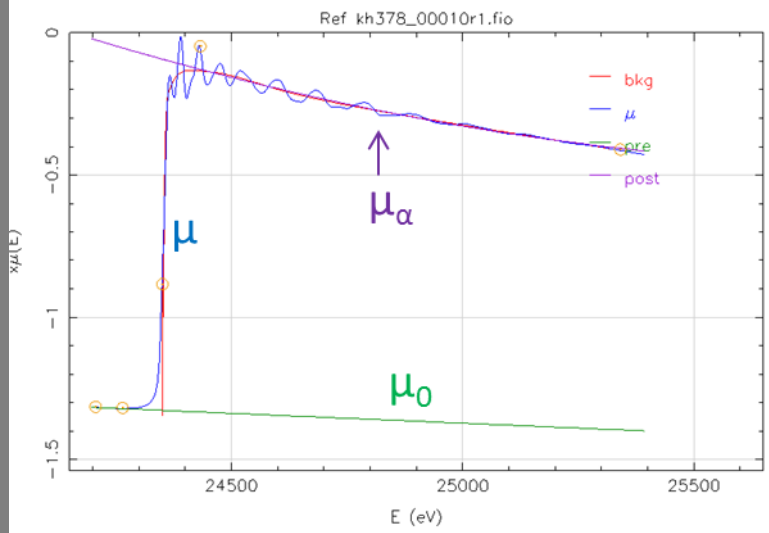

merge_Femet_av100 in E space
merge_Femet_av100
merge_Femet_av100 in energy
background
merge_Femet_av100
pre-edge
post-edge
χ(k)
Energy (eV)
xμ(E)
Energy (eV)

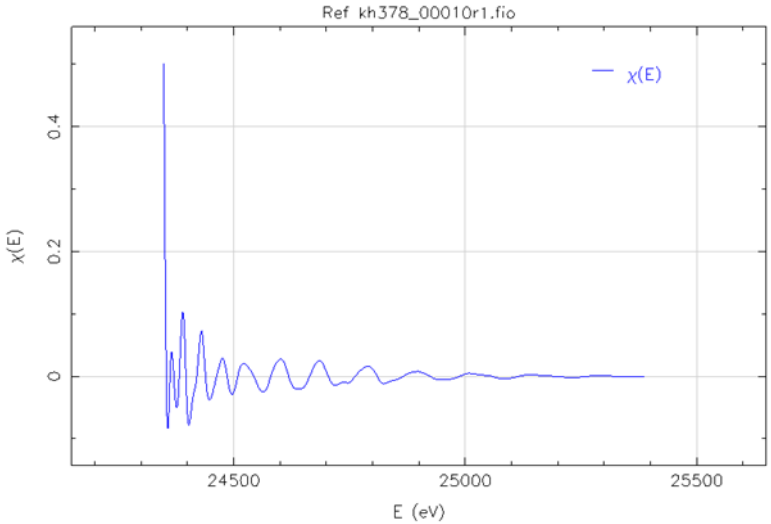

merge_Femet_av100 in energy
background
merge_Femet_av100
pre-edge
post-edge
xμ(E)
Energy (eV)

μ(E)


merge_Femet_av100 in E space
merge_Femet_av100
XAFS - background
χ(k)
Energy (eV)

Bkg subtraction



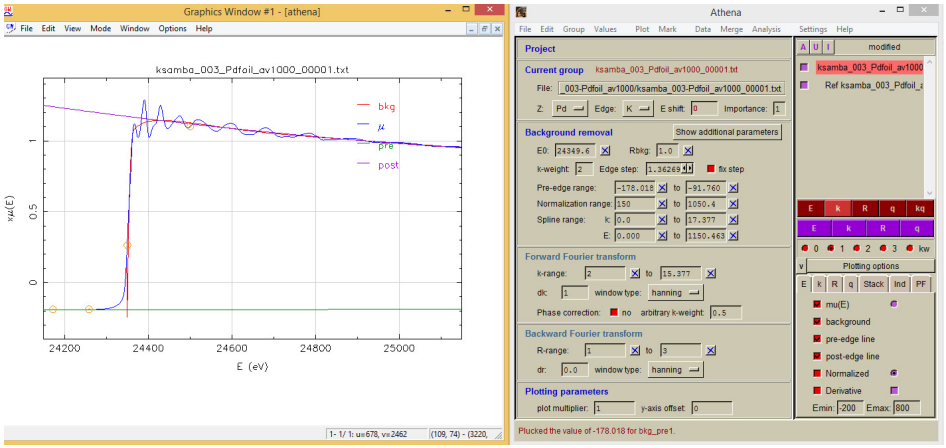


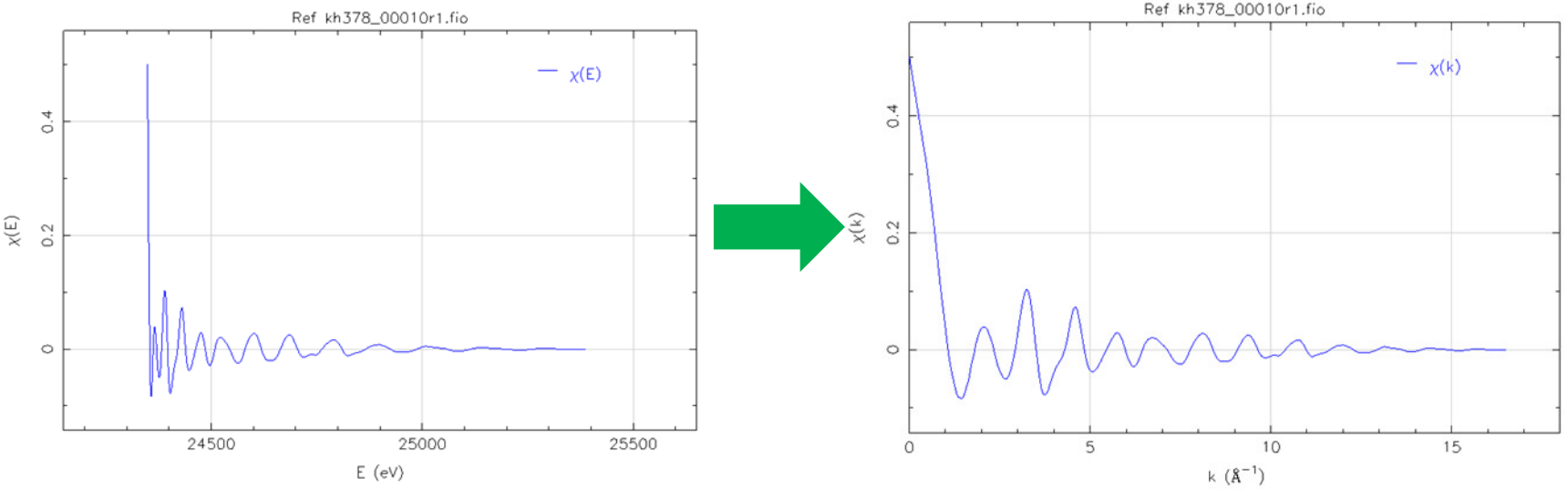
$$\chi(k) = \frac{\mu - \mu_\alpha}{\mu_\alpha - \mu_0} = \frac{\mu - \mu_{backg}}{\Delta\mu_{edge\,step}}$$

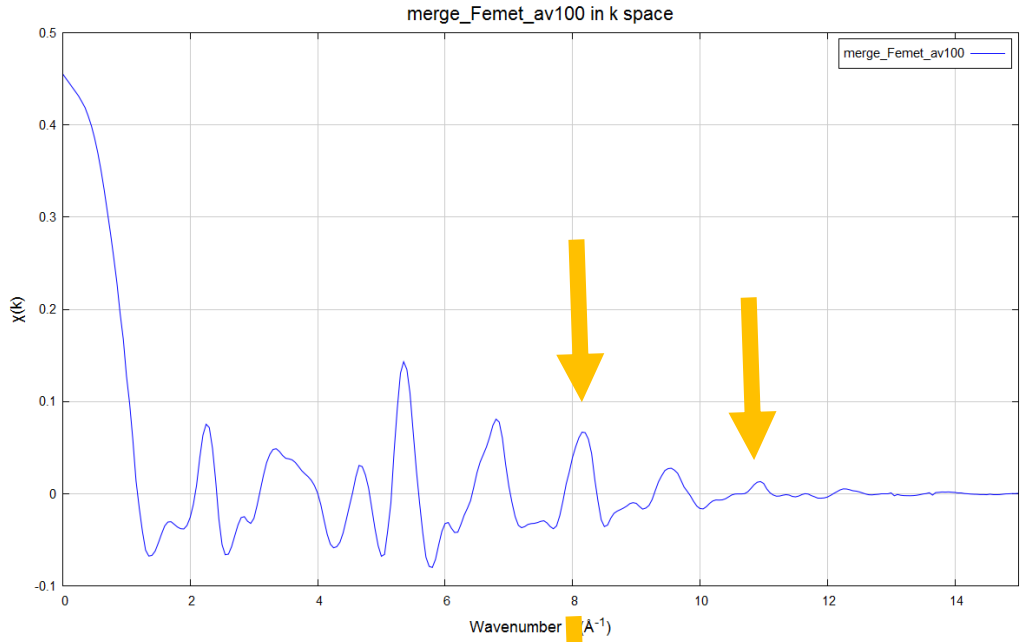
Fine structure or EXAFS!

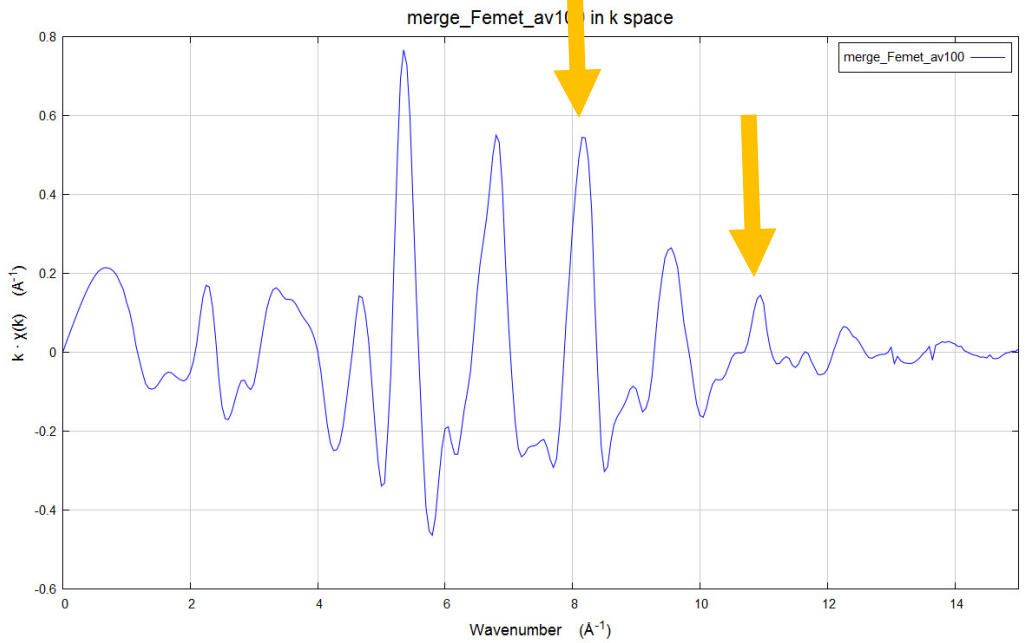
Transforming E (eV) into k(Å^{-1})

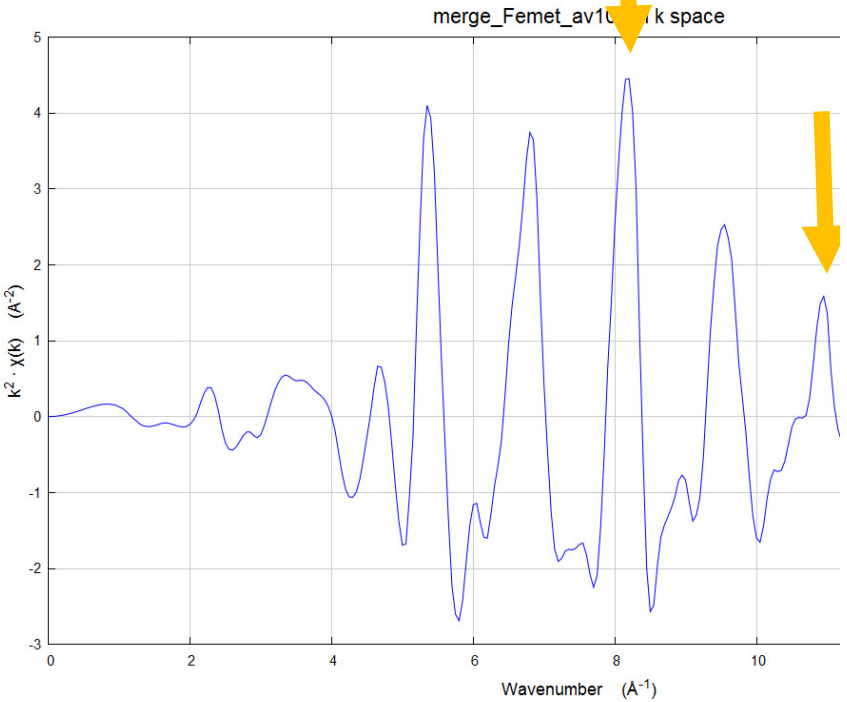
- What happens when you push the bottom?

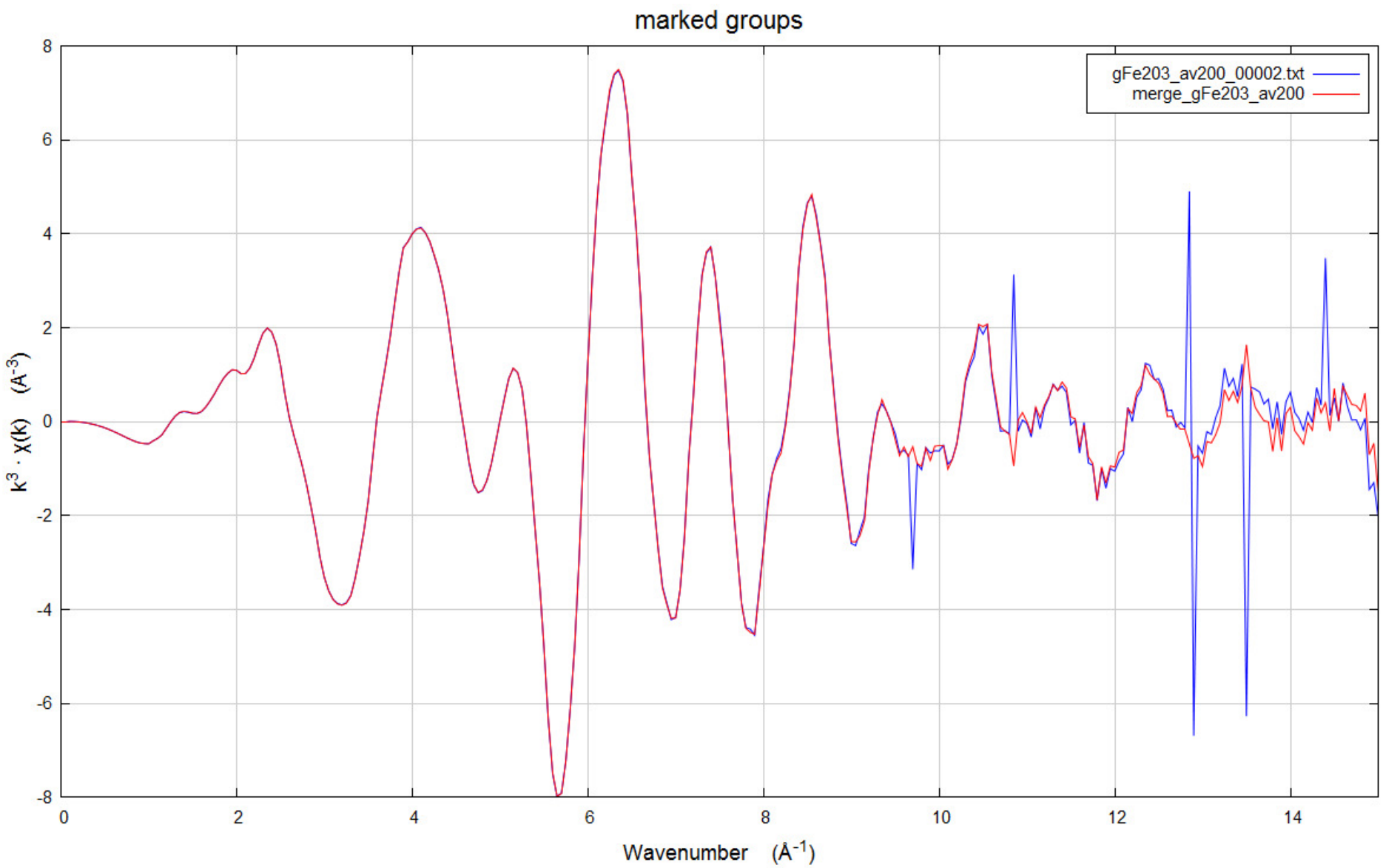


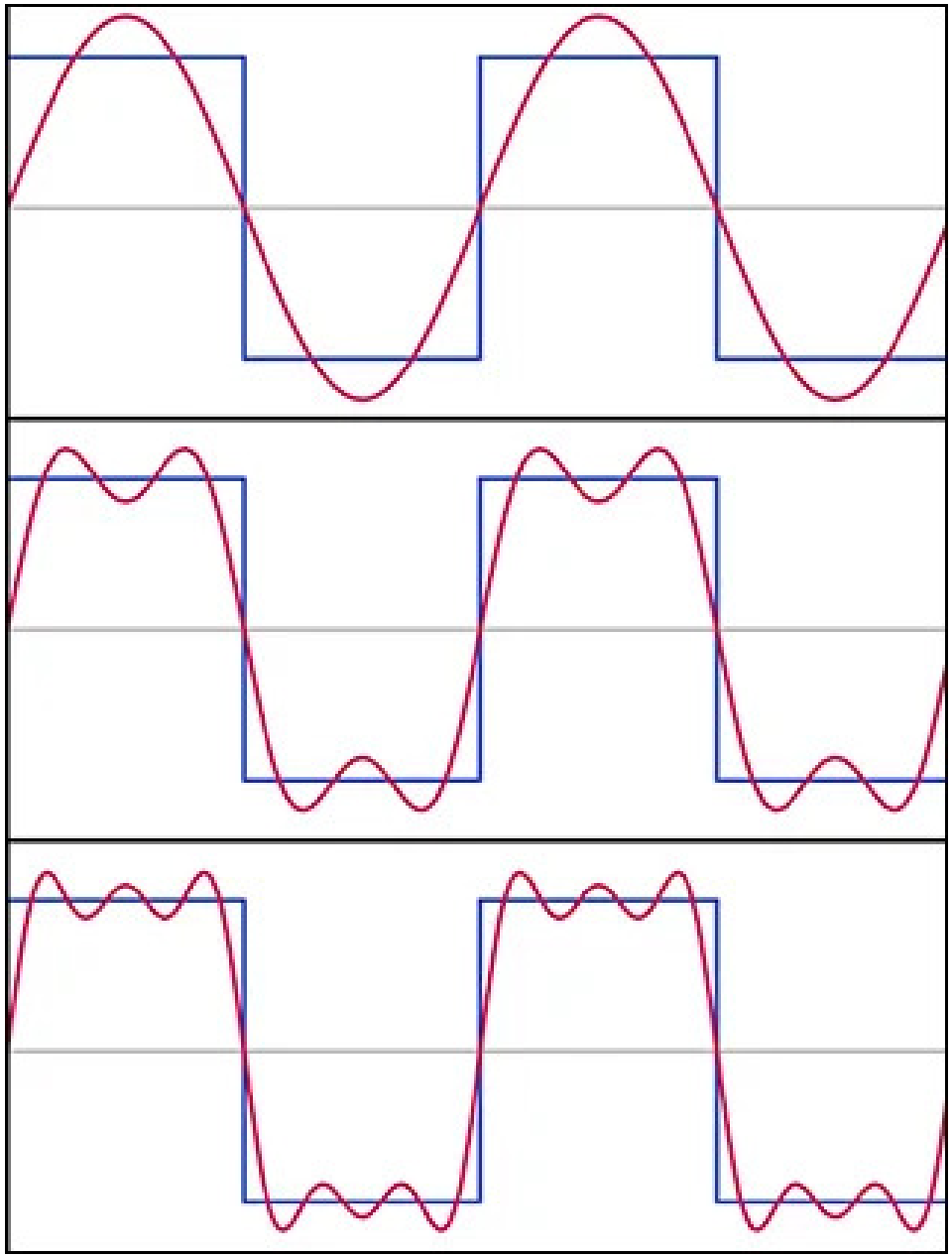


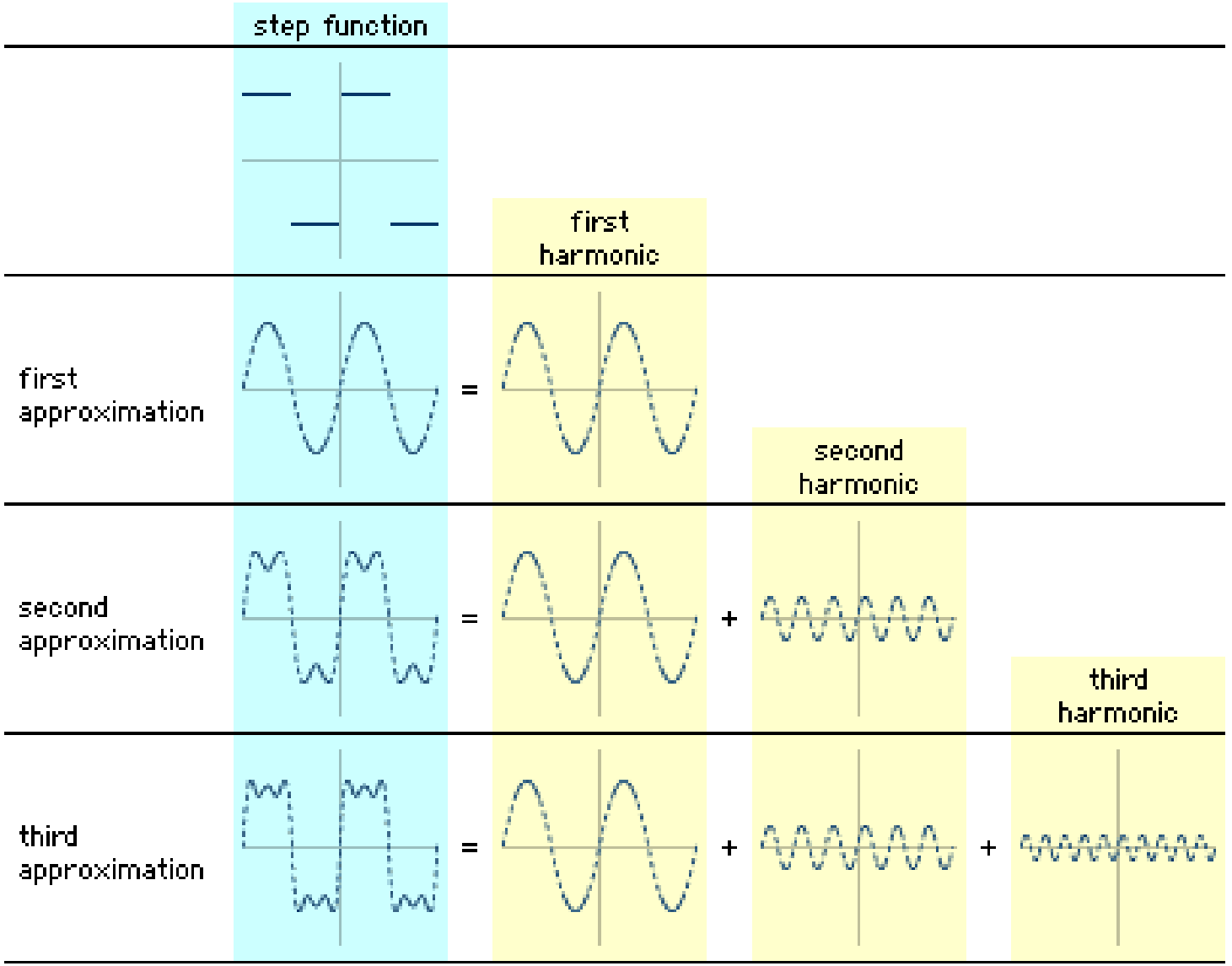

merge_Femet_av100 in k space
merge_Femet_av100
χ(k)
Wavenumber (Å-1)

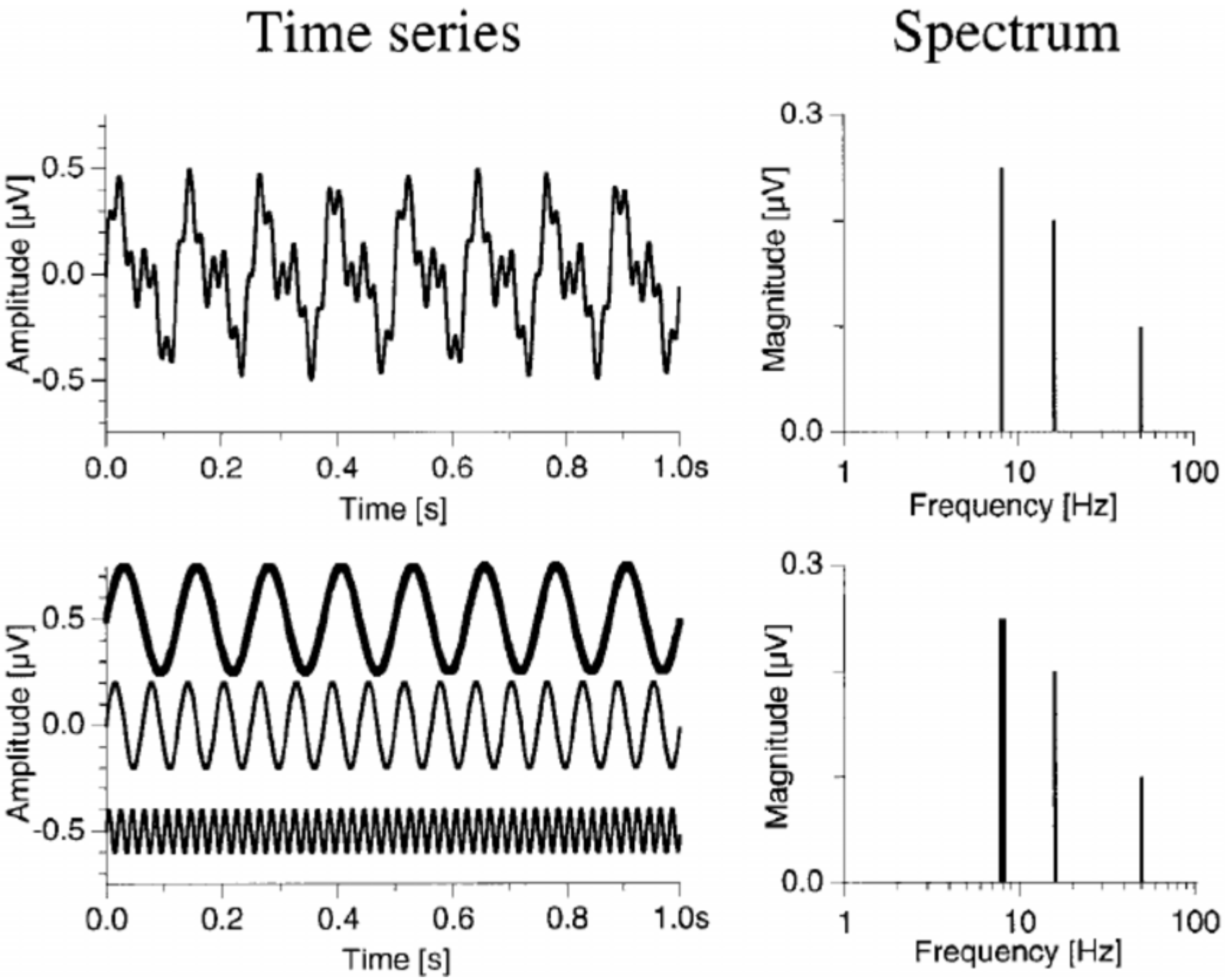

merge_Femet_av1
in k space
merge_Femet_av100
k · χ(k) (Å-1)
Wavenumber (Å-1)

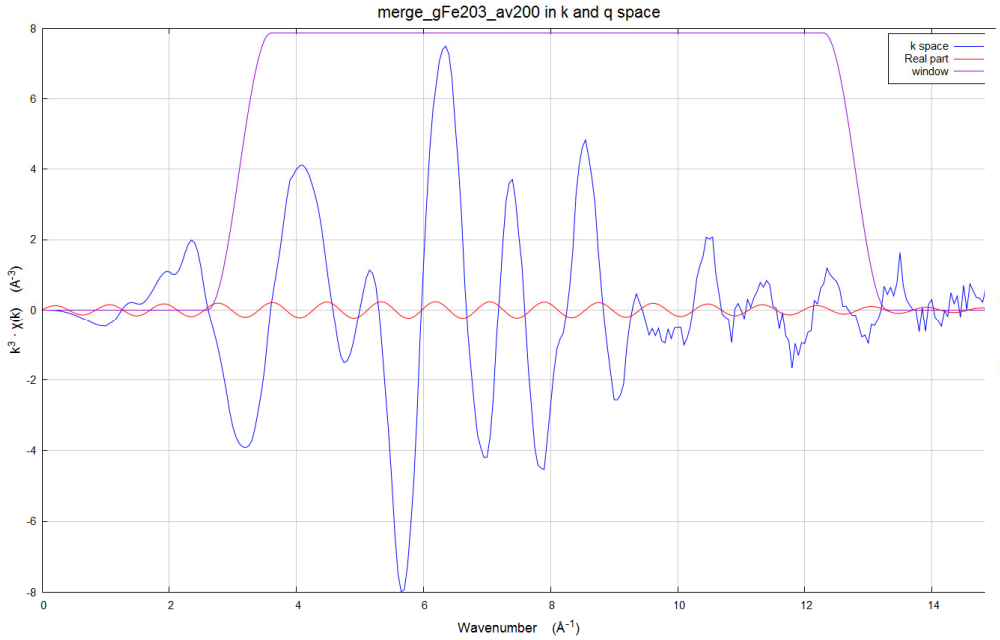

merge_Femet_av1
k space
k2 · χ(k) (Å-2)
Wavenumber (Å-1)

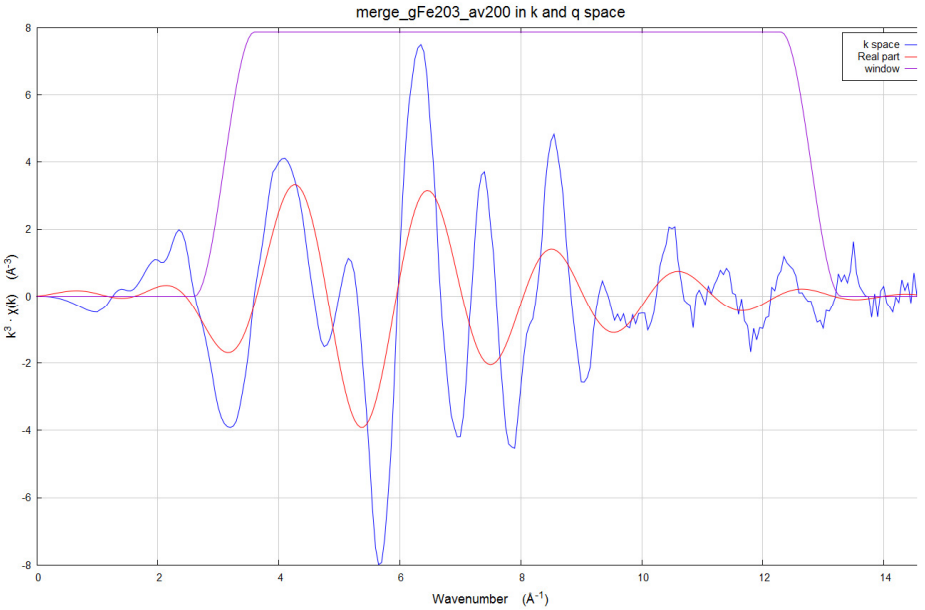

marked groups
gFe203_av200_00002.txt
merge_gFe203_av200
k3 · χ(k) (Å-3)
Wavenumber (Å-1)
8
6
4
2
0
-2
-4
-6
-8
0
2
4
6
8
10
12
14

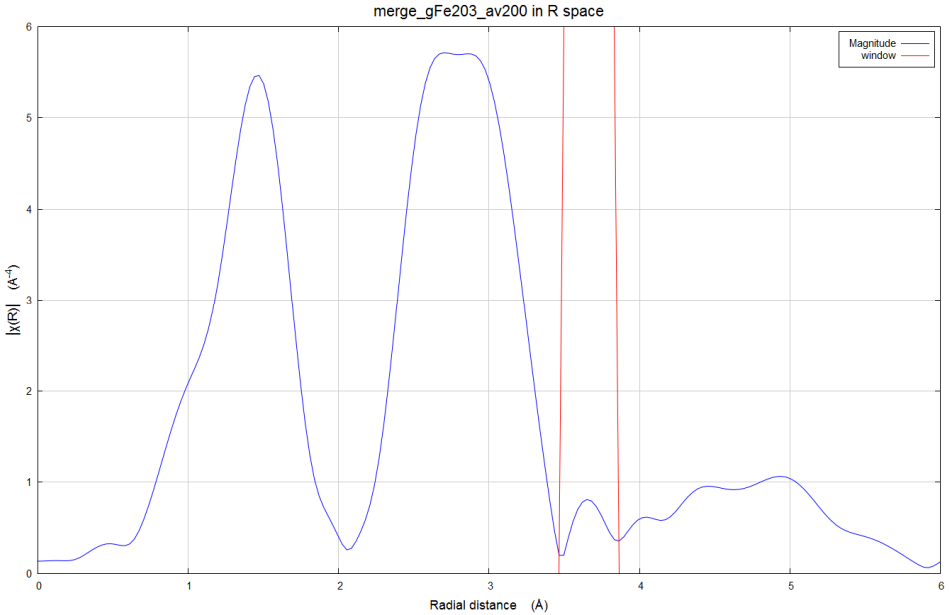


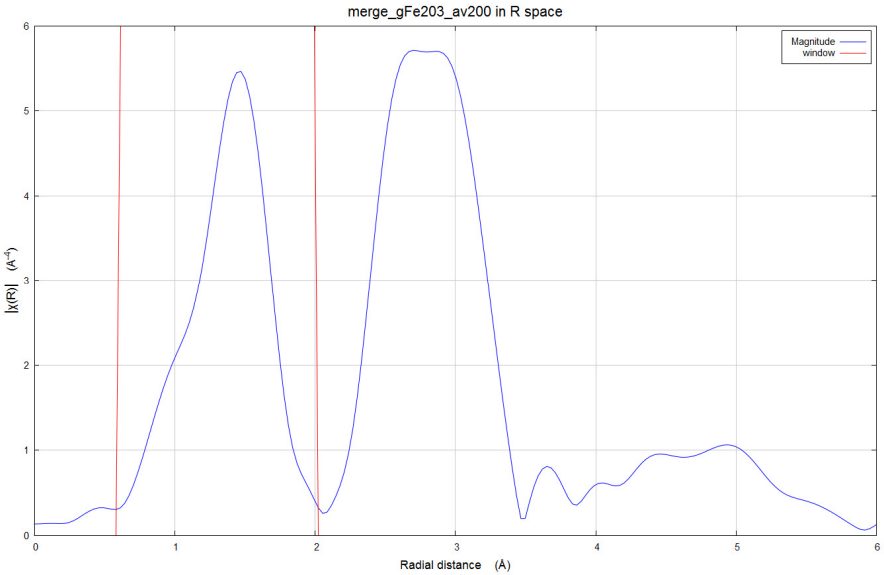



Time series
Spectrum
Amplitude [μV]
0.5
0.0
-0.5
0.0
0.2
0.4
0.6
0.8
1.0s
Time [s]
Magnitude [μV]
0.3
0.0
1
10
100
Frequency [Hz]
Amplitude [μV]
0.5
0.0
-0.5
0.0
0.2
0.4
0.6
0.8
1.0s
Time [s]
Magnitude [μV]
0.3
0.0
1
10
100
Frequency [Hz]

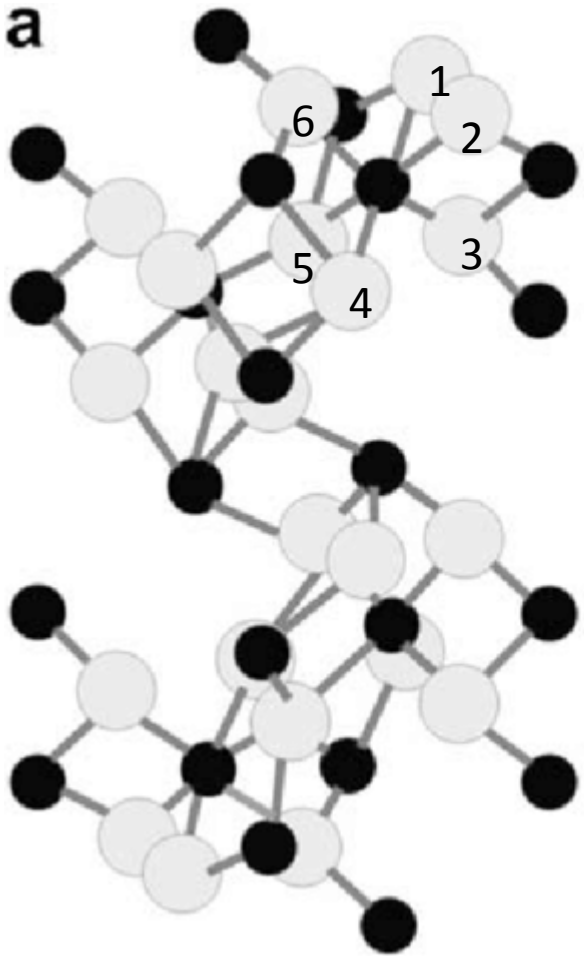

merge_gFe203_av200 in k and q space
k space
Real part
window
k³ · χ(k) (Å⁻³)
Wavenumber (Å⁻¹)


merge_gFe203_av200 in k and q space
k space
Real part
window
k⁻³ · χ(k) (Å⁻³)
Wavenumber (Å⁻¹)

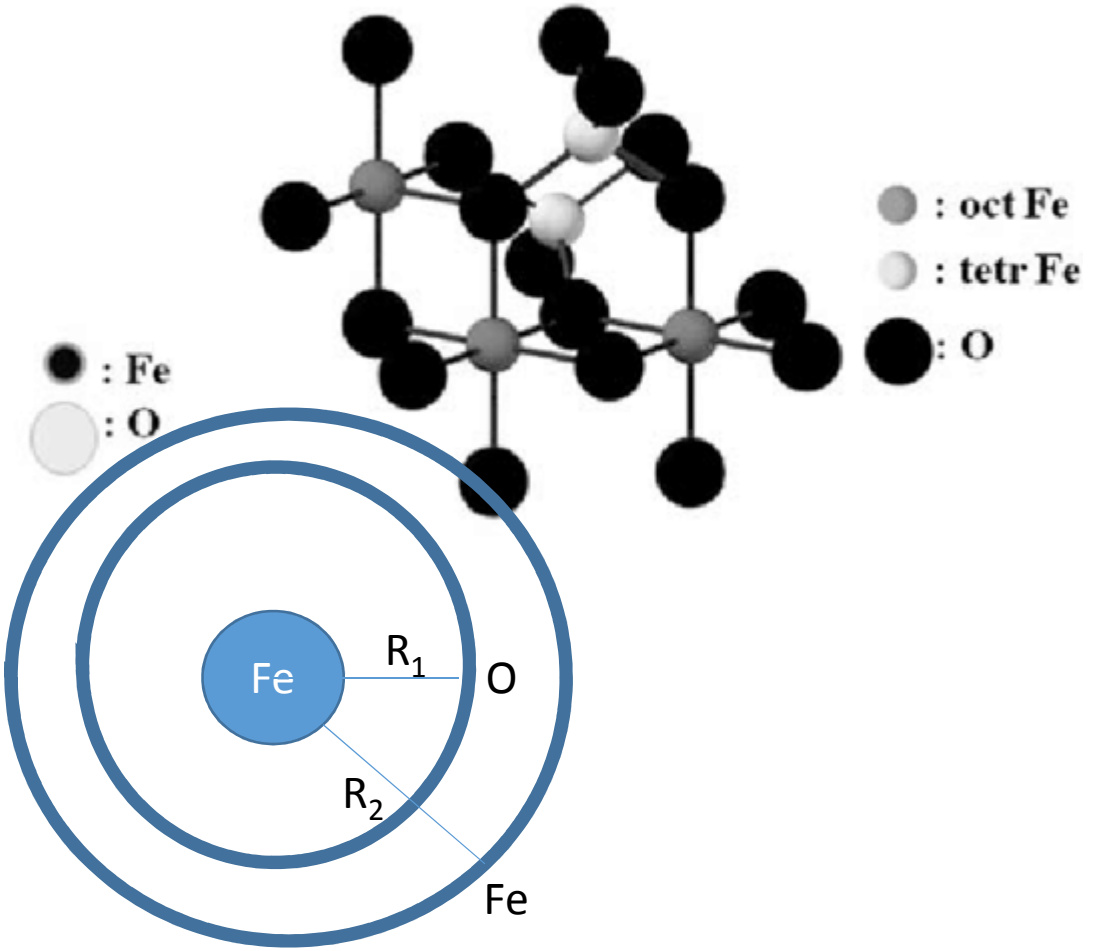

merge_gFe203_av200 in R space
Magnitude
window
|χ(R)| (Å⁻⁴)
Radial distance (Å)


merge_gFe203_av200 in R space
Magnitude
window
|χ(R)| (Å⁻⁴)
Radial distance (Å)

Hematita



magnetita



- Tarefa 1: Comparar os espectros do Fe_2O_3 e $ZnFe_2O_4$.
- Tarefa 2: Comparar o Fe e a Pt.

- Quais são as semelhanças e diferenças no espaço de k(A-1)?
- Quais são as semelhanças e diferenças em R(A)?
- Qual é causa dessas semelhanças e diferenças?
- Quantas esferas de coordenação se observa em cada caso?
- Quais seriam os átomos presentes nessas esferas de coordenação?
- Quais as distâncias atômicas aproximadas? Quais são os valores reportados na literatura? Por que eles são diferentes?
- Como podemos medir exatamente essas distâncias e identificar de forma inequívoca quais são átomos preenchendo as esferas de coordenação?

The EXAFS Equation

$$\chi_i(k) = \left(\frac{(N_i S_0^2) F_i(k)}{kR_i^2} \sin(2kR_i + \varphi_i(k)) \exp(-2\sigma_i^2 k^2) \exp(-2R_i/\lambda(k)) \right)$$

$$R_i = R_0 + \Delta R$$

$$k^2 = 2\, m_e (E - E_0)/\hbar$$

Or

EXAFS

$$\chi(k) = \sum_j A_j(k) \sin(\Phi_j(k))$$

amplitude

Interference pattern

The EXAFS Equation
Modern EXAFS Equation

- Modern EXAFS theory 1971: Lytlle, Sayers and Stern

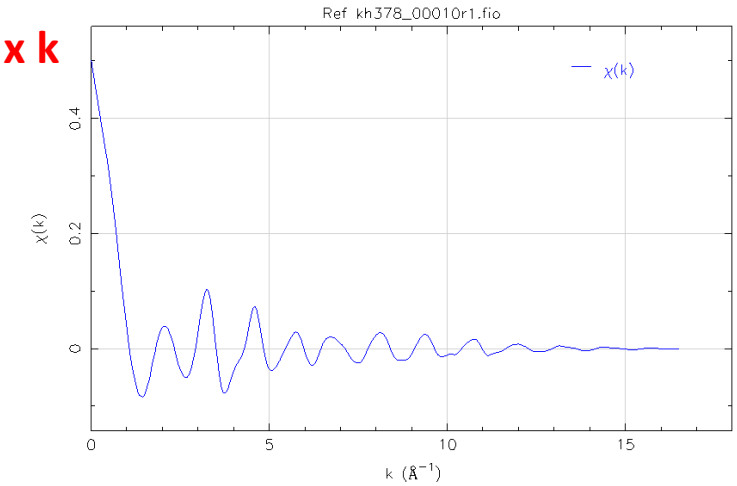
EXAFS

$$\chi(k) = \sum_j A_j(k)\sin(\Phi_j(k))$$

amplitude

Interference pattern

χ x k



Regular wave eq. solution

$$u = A \sin(\vec{k}\,\vec{r} - wt)$$

A = amplitude
k= wave vector
r= position
w= 2πf= angular freq
t= time