Data reduction and background removal

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What is included in this talk

- How is XAFS data is collected at the beamline
- How to calculate the absorption spectra for transmission and fluorescence measurements
- Why we need to normalize and remove background from absorption spectra
- Data reduction steps: Pre-edge and post-edge background subtraction
- Data reduction steps: compute background function to extract *chi* spectra
- Data reduction steps: Fourier Transform of *chi* spectra to get representative radial distribution

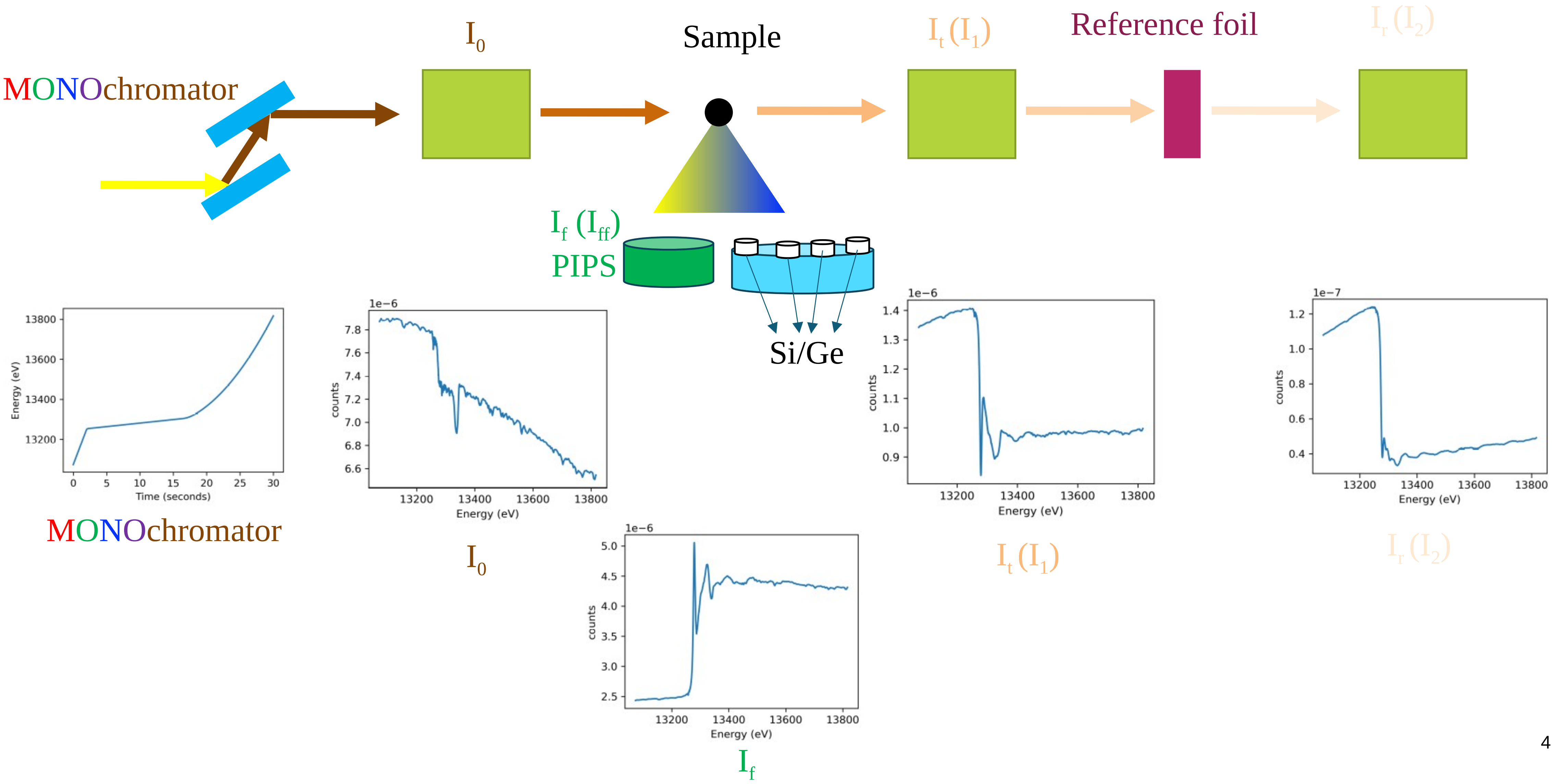
XAFS books

Introduction to XAFS: A Practical Guide to X-ray Absorption Fine Structure Spectroscopy
Grant Bunker

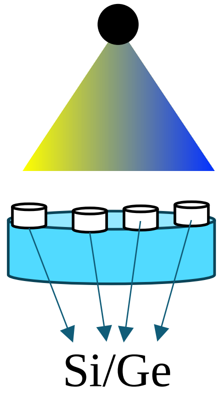
EXAFS: Basic Principles and Data Analysis
Dr. Boon K. Teo

XAFS for Everyone
Scott Calvin

Data collection

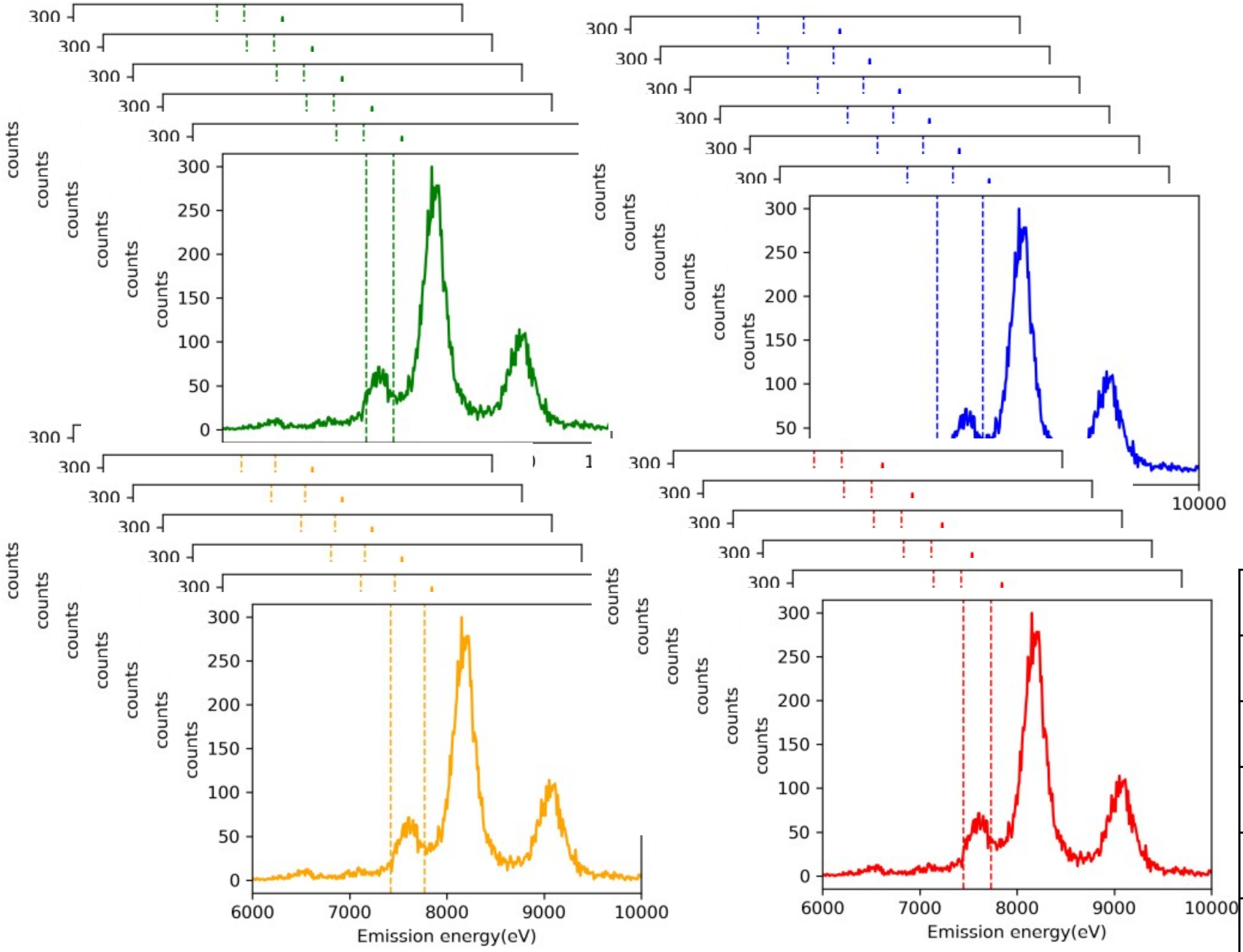


Si/Ge detector data



Channel 1

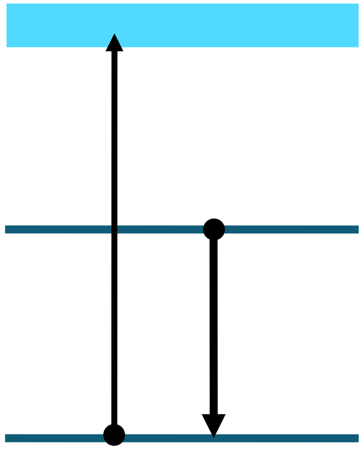
Channel 2



Channel 3

Channel 4

Energy Level



Energy	Ch1	Ch2	Ch3	Ch4
E1	45	44	45	46
E2	42	41	40	42
E3	20	23	25	20
E4	21	21	21	21
E5	23	20	21	22

Data File

```
# energy            i0            it            ir           iff           xs_roi01     xs_ch01_roi01 xs_ch02_roi01 xs_ch03_roi01 xs_ch04_roi01
13073.000000 -3.972144e-06 -1.405205e-07 -1.108702e-08 -2.481562e-07 1.622849e-02 4.025056e-03 4.057912e-03 3.530254e-03 4.615269e-03
13078.000000 -3.987104e-06 -1.411195e-07 -1.117292e-08 -2.494934e-07 1.638280e-02 4.028765e-03 4.117364e-03 3.528756e-03 4.707913e-03
13083.000000 -4.007183e-06 -1.421063e-07 -1.126769e-08 -2.511177e-07 1.649624e-02 4.073405e-03 4.140805e-03 3.540213e-03 4.741813e-03
13088.000000 -3.985857e-06 -1.418912e-07 -1.128669e-08 -2.500882e-07 1.633222e-02 4.058421e-03 4.052907e-03 3.541270e-03 4.679625e-03
13093.000000 -3.987541e-06 -1.424549e-07 -1.134783e-08 -2.504947e-07 1.640753e-02 4.098472e-03 4.056191e-03 3.525928e-03 4.726942e-03
13098.000000 -4.003168e-06 -1.434870e-07 -1.147684e-08 -2.520052e-07 1.623098e-02 4.071138e-03 4.027229e-03 3.554777e-03 4.577840e-03
```

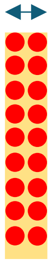
```
# Facility.name: NSLS-II
# Facility.mode: Beam available
# Facility.current: 399.7092291335699
# Facility.current: 3 GeV
# Facility.year: 2023
# Facility.cycle: 3
# Facility.GUP: 313873
# Facility.SAF: 312125
# Experimenter.name: Akhil Tayal
# Beamline.name: ISS (8-ID)
# Beamline.x-ray_source: damping wiggler
# Beamline.collimation_mirror1.material: Si
# Beamline.collimation_mirror2.material: Pt
# Beamline.collimation_mirror2.bender_loading: -259.0
# Beamline.focusing: toroidal mirror
# Beamline.focusing.material: Pt
# Beamline.focusing.bender_loading: -398.0
# Beamline.harmonic_rejection: Rh
# Mono.scan_mode: Si(111)
# Mono.d_spacing: 3.1354951
# Mono.scan_mode: pseudo-channel cut
# Mono.scan_type: fly_scan
# Mono.trajectory_name: 647b56c3-e11a.txt
# Mono.direction: None
# Mono.angle_offset: 0.69726544
# Mono.angle_offset: 39.95 deg
# Mono.encoder_resolution: 48.0 nrad
# Detector.I0: ion chamber
# Detector.I1: ion chamber
# Detector.I2: ion chamber
# Detector.IF: PIPS
# Detector.I0.length: 15 cm
# Detector.I1.length: 28 cm
# Detector.I2.length: 15 cm
# Detector.IF.thickness: 300 um
# Detector.I0.gas.N2: 50.0%
# Detector.I1.gas.N2: 50.0%
# Detector.I2.gas.N2: 50.0%
# Detector.I0.gas.He: 50.0%
# Detector.I1.gas.He: 50.0%
# Detector.I2.gas.He: 50.0%
```

```
# Detector.aux: {'Xspress3': {'config': {}}}
# Element.symbol: Pt
# Element.edge: L2
# Element.line: None
# Scan.transient_id: 395793
# Scan.uid: 47eb3f72-47c2-4132-bcc6-0d293a2b9627
# Scan.edge_energy: 13273.0
# Scan.start_time: 09/23/2023  21:15:46.030720
# Scan.end_time: 09/23/2023  21:17:22.651740
# Scan.name: Pt0p05_rep RT cool Pt-L2 90sec 0002
# Scan.comment:
# Sample.name: Pt0p05_rep
# Sample.comment:
# Sample.position.x: 7.666231008499999
# Sample.position.y: -89.5050982975
# Sample.position.z: -12.988999999999995
# Sample.position.theta: 0.0
# SampleHeater.temperature1.setpoint: 300.0
# SampleHeater.temperature1.readback: 1372.0
# SampleHeater.current.setpoint: 0.0
# SampleHeater.current.readback: 0.0
# SampleHeater.temperature2.setpoint: 25.0
# SampleHeater.temperature2.readback: 33.7
# SampleHeater.voltage.setpoint: 0.0
# SampleHeater.voltage.readback: 0.0
# SampleHeater.PID.P: 0.025
# SampleHeater.PID.I: 0.07
# SampleHeater.PID.D: 0.0
# SampleGasCart.MFC.CH4.setpoint: 0.0
# SampleGasCart.MFC.CH4.readback: 0.0
# SampleGasCart.MFC.CO.setpoint: 0.0
# SampleGasCart.MFC.CO.readback: 0.0
# SampleGasCart.MFC.H2.setpoint: 0.0
# SampleGasCart.MFC.H2.readback: 0.0
# SampleGasCart.MFC.exhaust.setpoint: 100.0
# SampleGasCart.MFC.exhaust.readback: 25.67
# SampleSwitchValve.GHS.readback: 1
# SampleSwitchValve.GasCart.readback: 0
# SampleSwitchValve.Inert.readback: 0
# Potentiostat.Voltage.readback: 0
# Potentiostat.Current.readback: 0
# SampleGasHandlingSystem.gas_a.name: None
# SampleGasHandlingSystem.gas_b.name: None
# SampleGasHandlingSystem.gas_c.name: Ethylene
# SampleGasHandlingSystem.gas_d.name: None
# SampleGasHandlingSystem.gas_e.name: He
# SampleGasHandlingSystem.MFC1.setpoint: 25.0
# SampleGasHandlingSystem.MFC1.readback: 25.0
# SampleGasHandlingSystem.MFC2.setpoint: 0.0
```

Important terms

Strength of absorption is “cross section” σ (cm^2)

x (cm)



σ_{total} (cm^2/g)

ϱ (density g/cm^3)

Probability of absorption = $x\varrho\sigma_{total} = x\mu$ (μ is linear absorption coefficient)

Bouguer’s Law:

$$I_t \text{¿} I_0 e^{-\mu x}$$

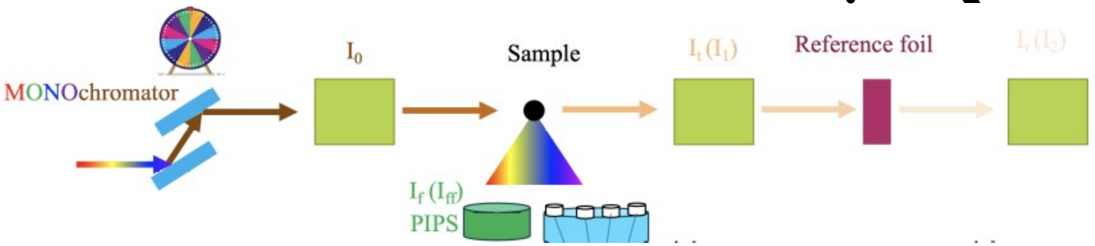
Absorption coefficient for transmission

$$\mu x = log\left(\frac{I_0}{I_t}\right)$$

Absorption coefficient for fluorescence

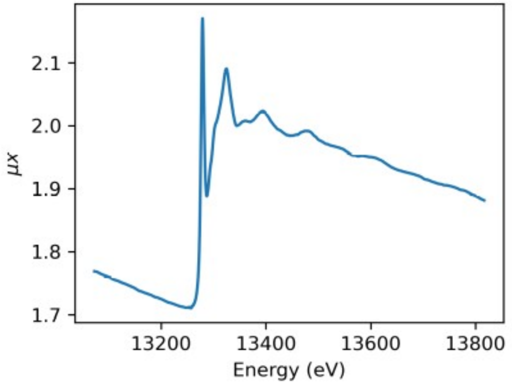
$$\mu x = \left(\frac{I_f}{I_0}\right)$$

Calculation of μ (absorption coefficient)

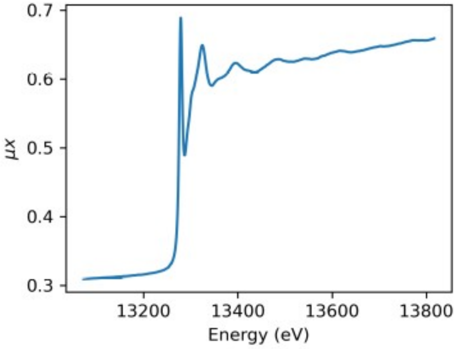


# energy	i0	it	ir	iff	xs_roi01	xs_ch01_roi01	xs_ch02_roi01	xs_ch03_roi01	xs_ch04_roi01
13073.000000	-3.972144e-06	-1.405205e-07	-1.108702e-08	-2.481562e-07	1.622849e-02	4.025056e-03	4.057912e-03	3.530254e-03	4.615269e-03
13078.000000	-3.987104e-06	-1.411195e-07	-1.117292e-08	-2.494934e-07	1.638280e-02	4.028765e-03	4.117364e-03	3.528756e-03	4.707913e-03
13083.000000	-4.007183e-06	-1.421063e-07	-1.126769e-08	-2.511177e-07	1.649624e-02	4.073405e-03	4.140805e-03	3.540213e-03	4.741813e-03
13088.000000	-3.985857e-06	-1.418912e-07	-1.128669e-08	-2.500882e-07	1.633222e-02	4.058421e-03	4.052907e-03	3.541270e-03	4.679625e-03
13093.000000	-3.987541e-06	-1.424549e-07	-1.134783e-08	-2.504947e-07	1.640753e-02	4.098472e-03	4.056191e-03	3.525928e-03	4.726942e-03
13098.000000	-4.003168e-06	-1.434870e-07	-1.147684e-08	-2.520052e-07	1.623098e-02	4.071138e-03	4.027229e-03	3.554777e-03	4.577840e-03

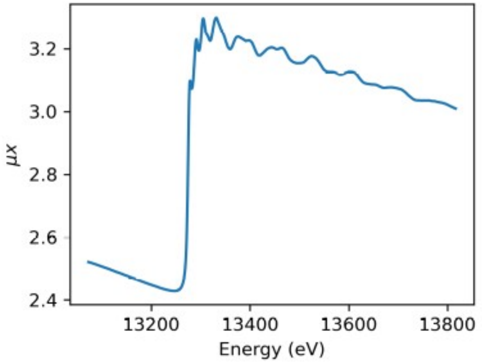
Absorption coefficient for sample transmission: $\mu x = log\left(\frac{i_0}{i_t}\right)$



Absorption coefficient for sample fluorescence:



Absorption coefficient for reference transmission: $\mu x = log\left(\frac{i_r}{i_t}\right)$



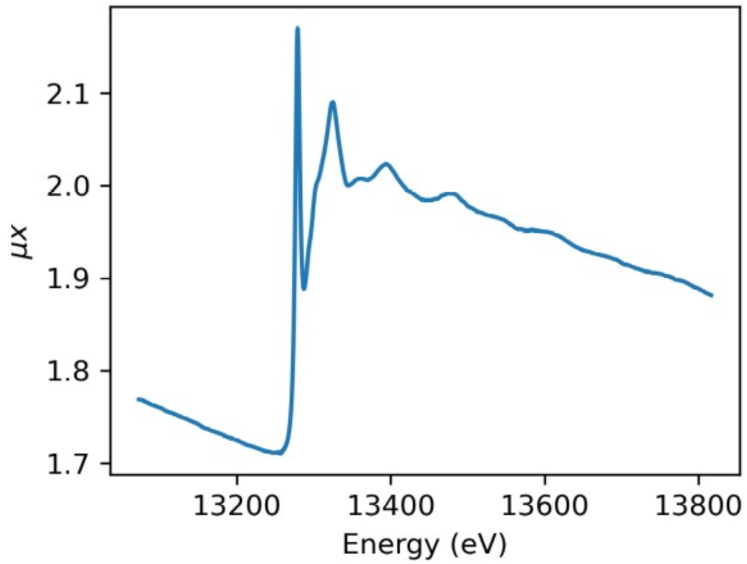
Before processing some common steps

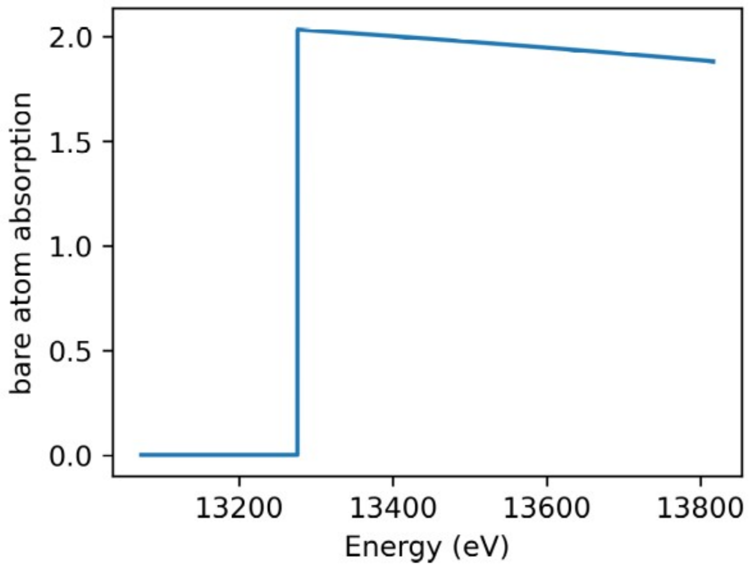
- Rebinning
- Energy alignment
- Merging

Some background

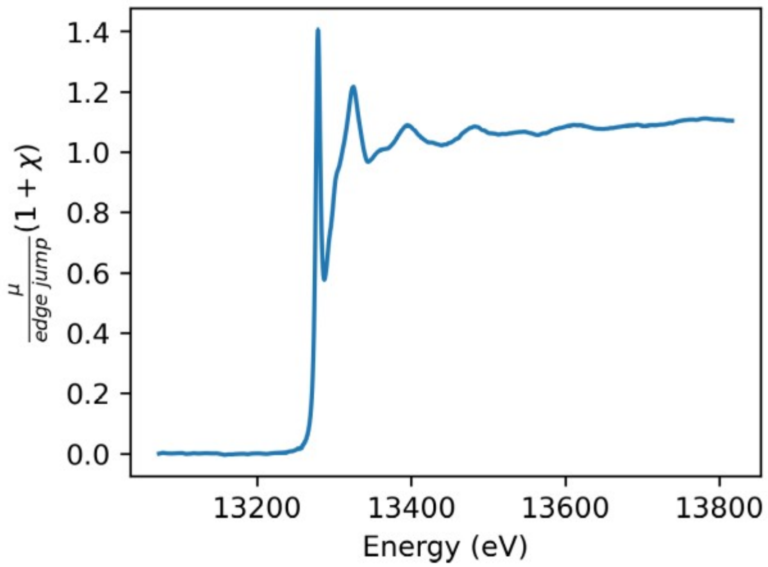
XAFS analysis based on comparison

- Fingerprinting
- Linear Combination Analysis
- Curve Fitting with Theoretical standards





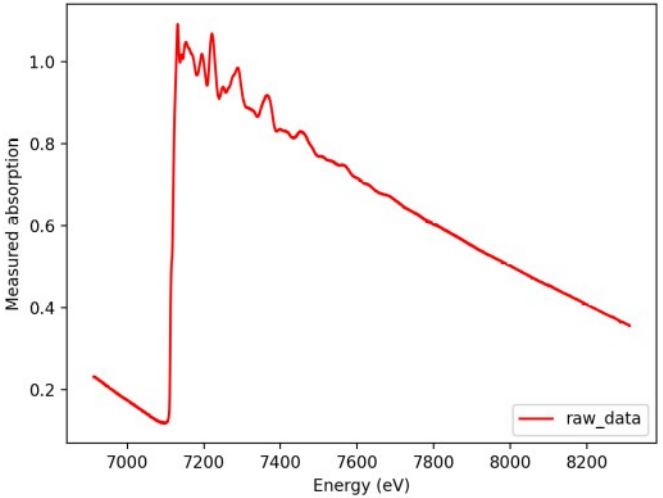
μ_0

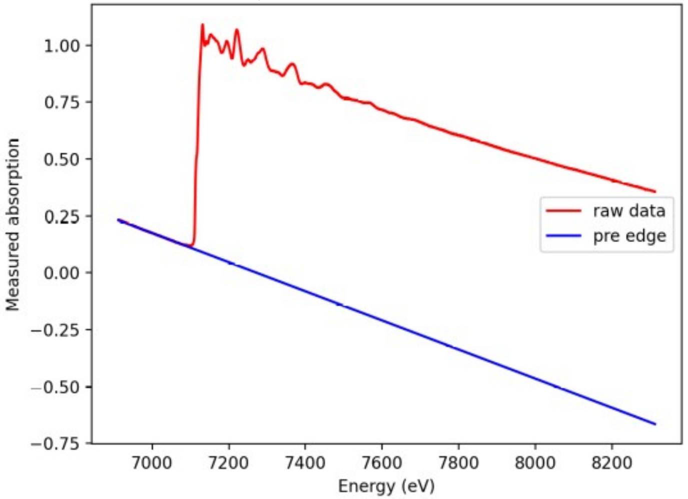


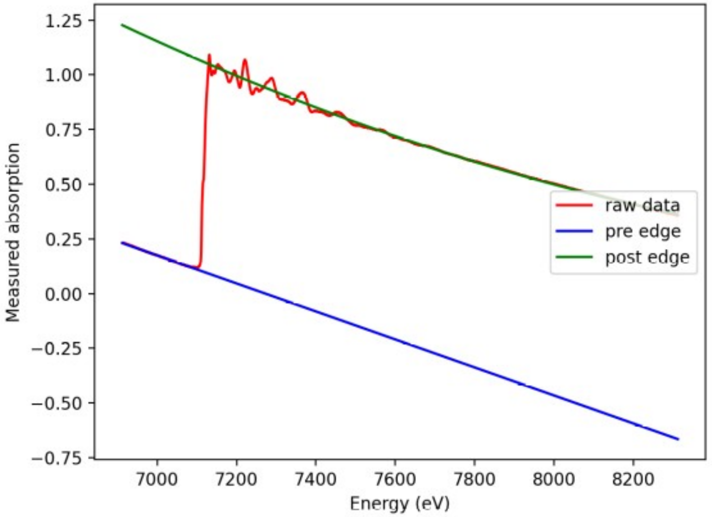
$$\frac{\mu}{edge\,jump}(1+\chi)$$

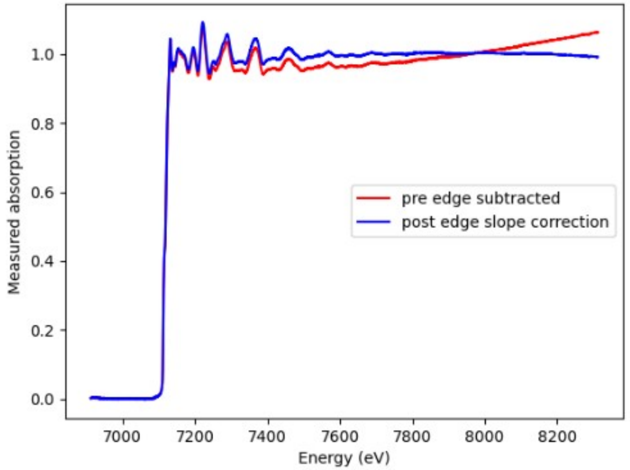
Pre and Post-edge background subtraction

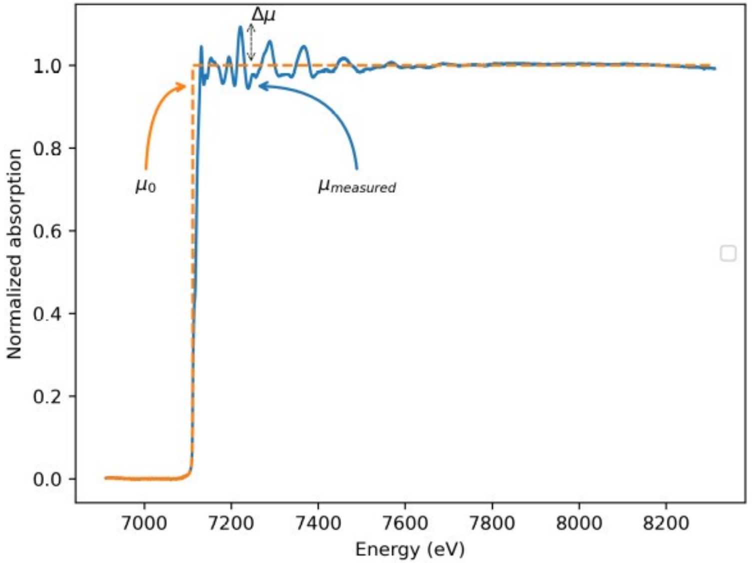
$$\mu = C\,E^3 - D\,E^4 (Victoreen\,Equation\,imperical)$$

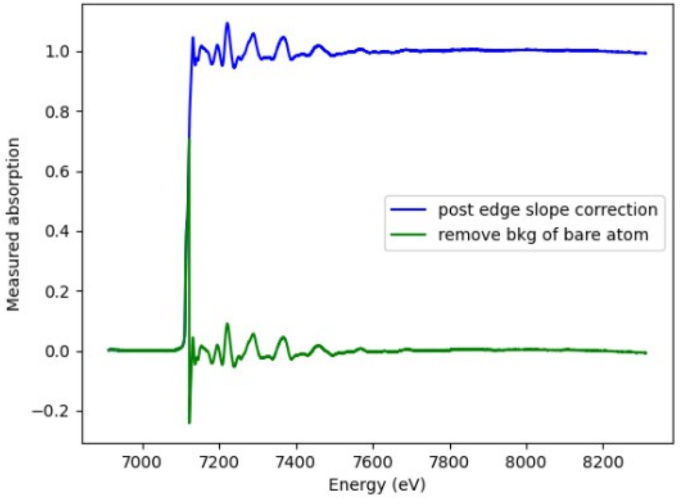








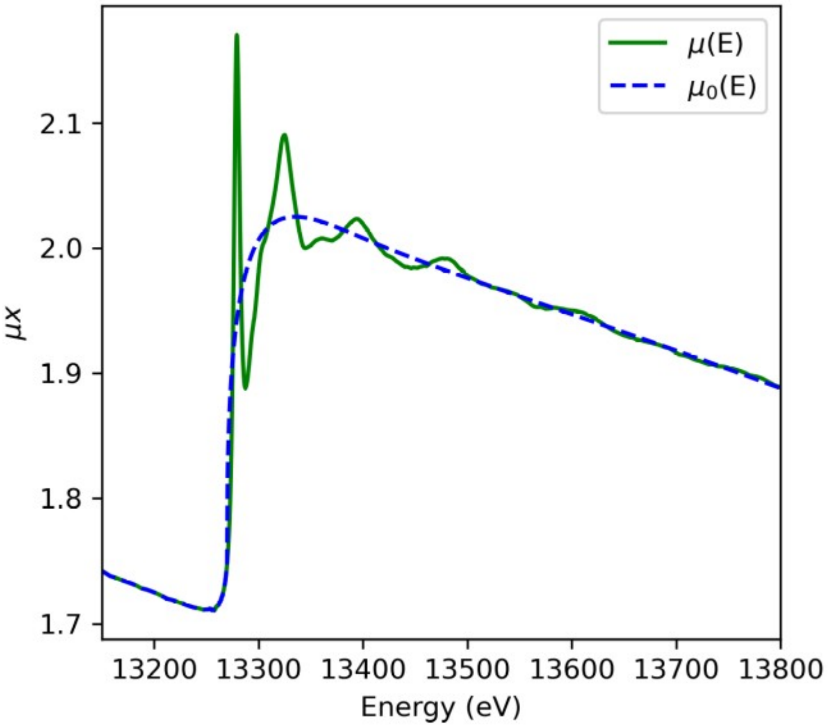


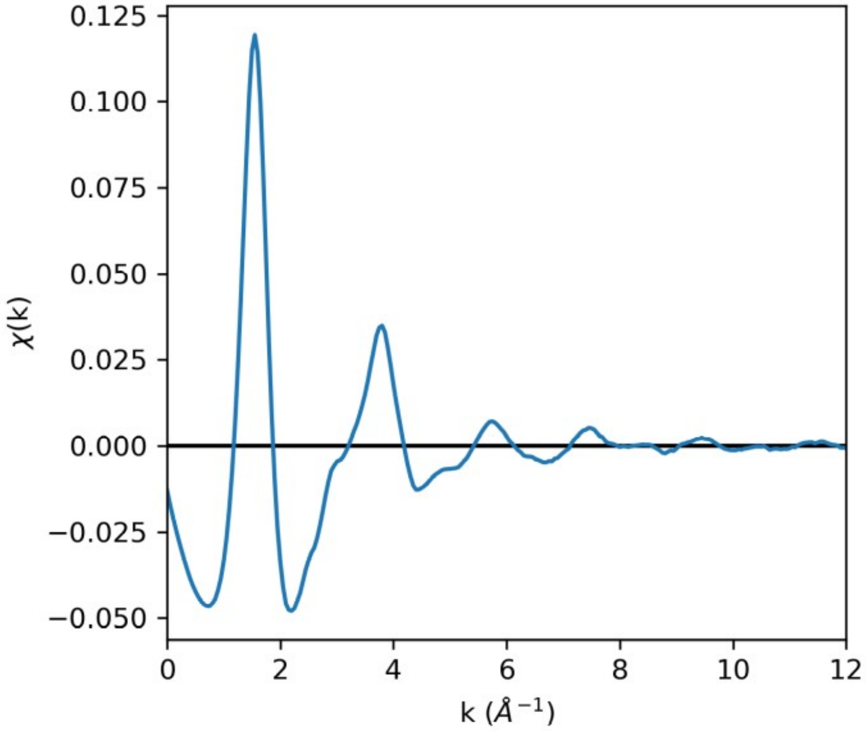


Conversion of E to k

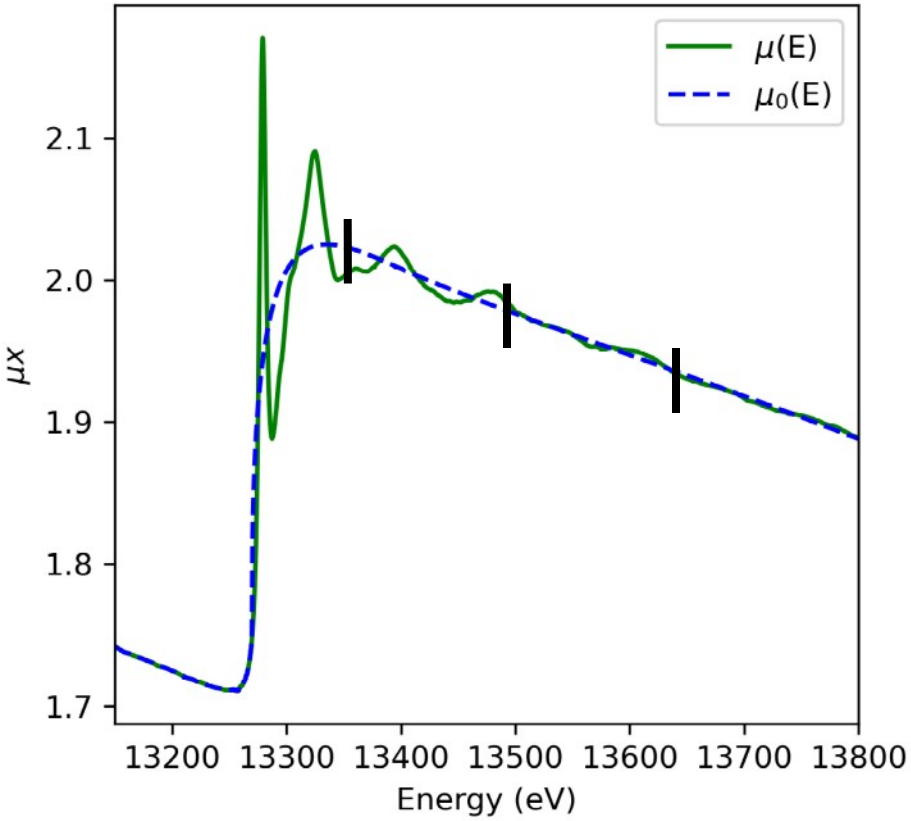
$$k=\sqrt{\frac{2m\left(E-E_0^{ex}\right.}{\hbar^2}}$$

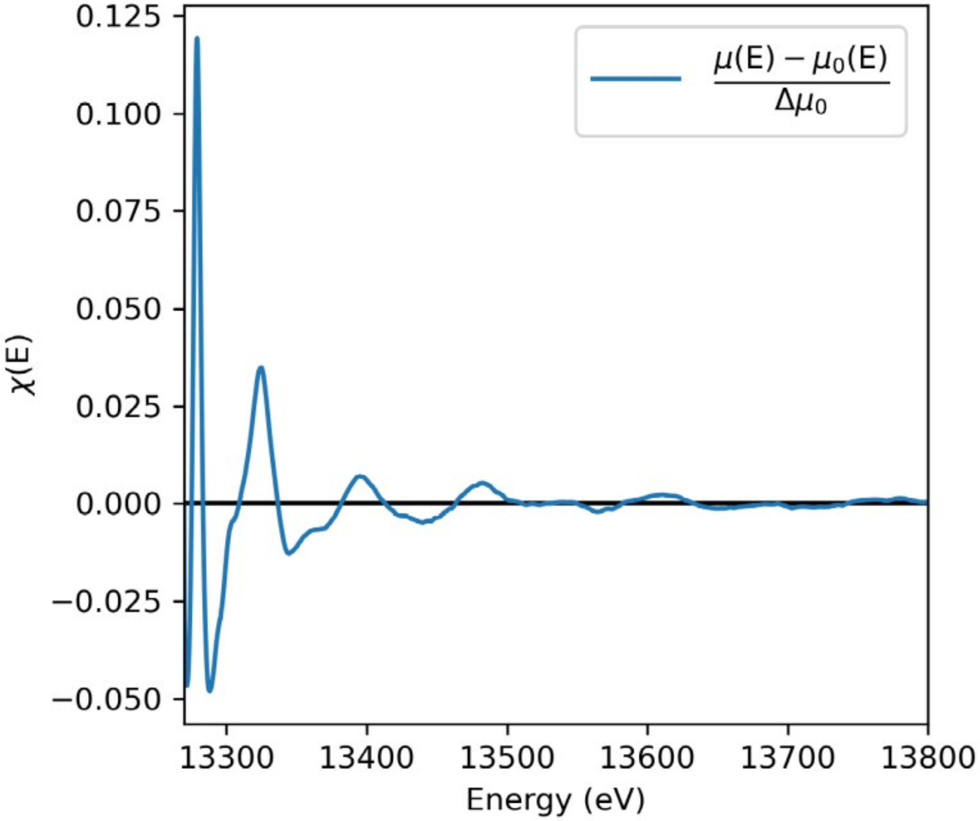
$$k=\sqrt{0.2625\left(E-E_0^{e}\right.}$$



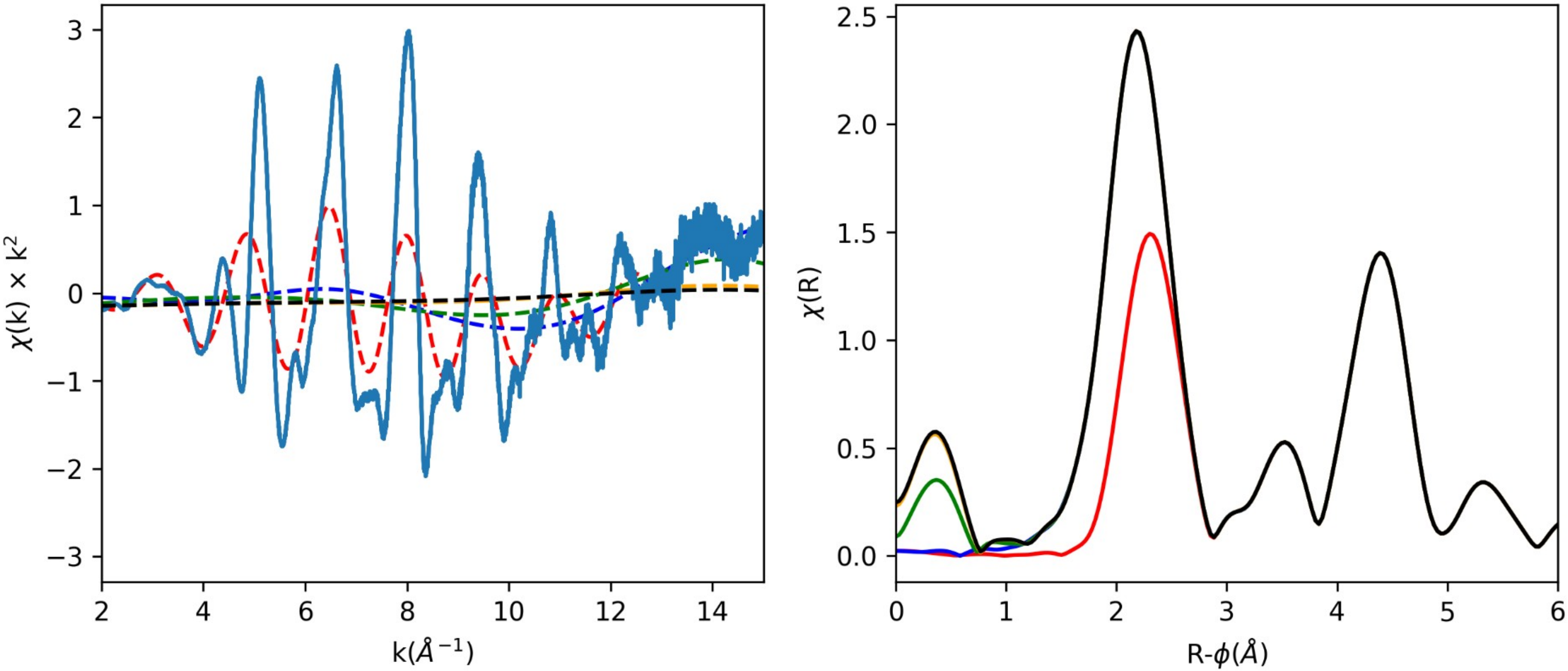


EXAFS extraction

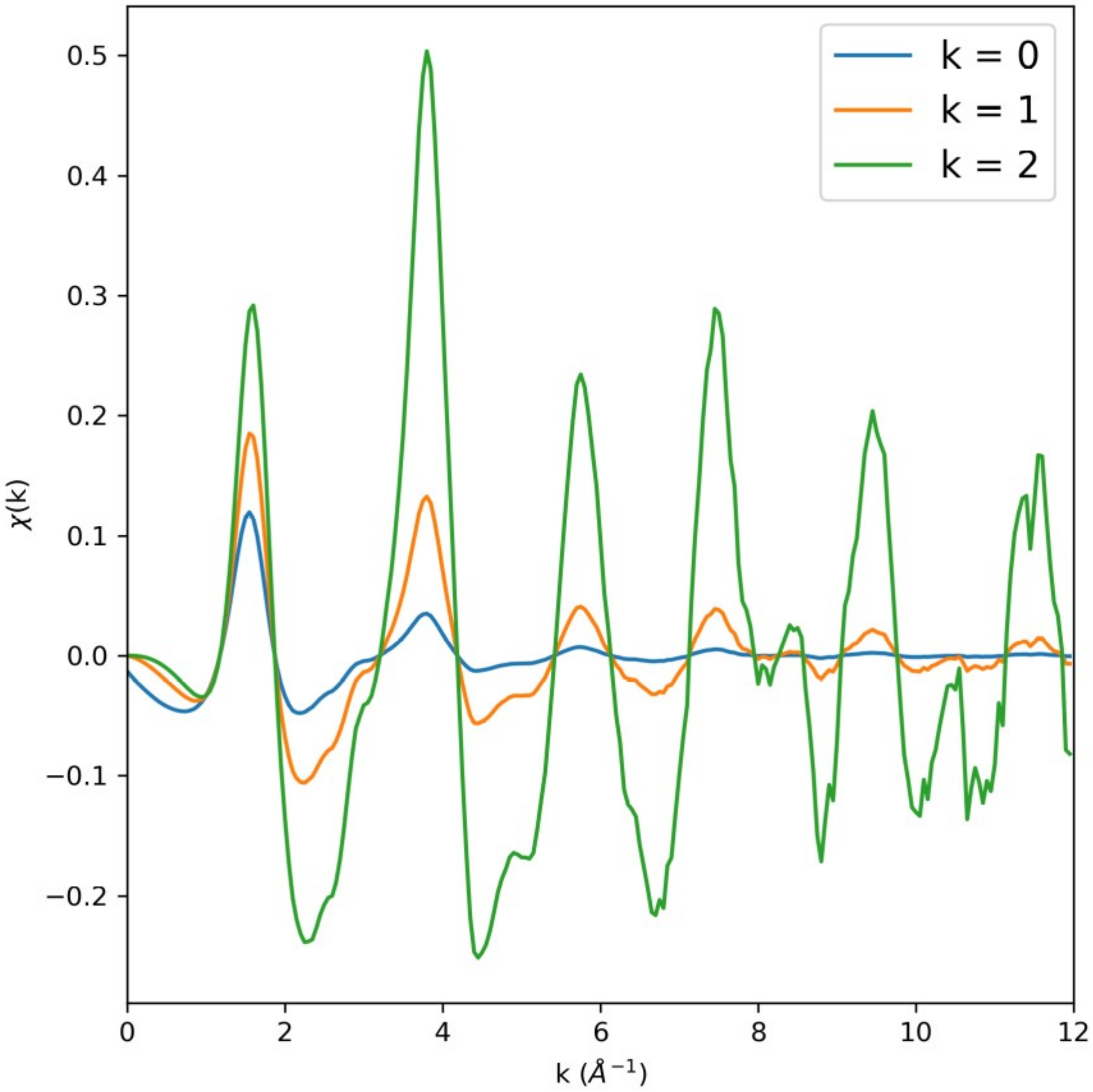




EXAFS extraction



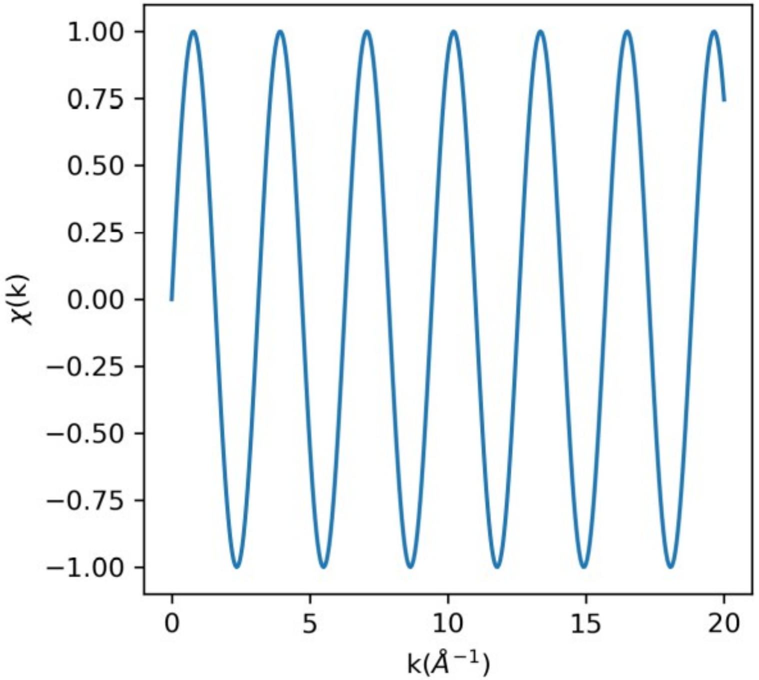
k weighting 1, 2, 3



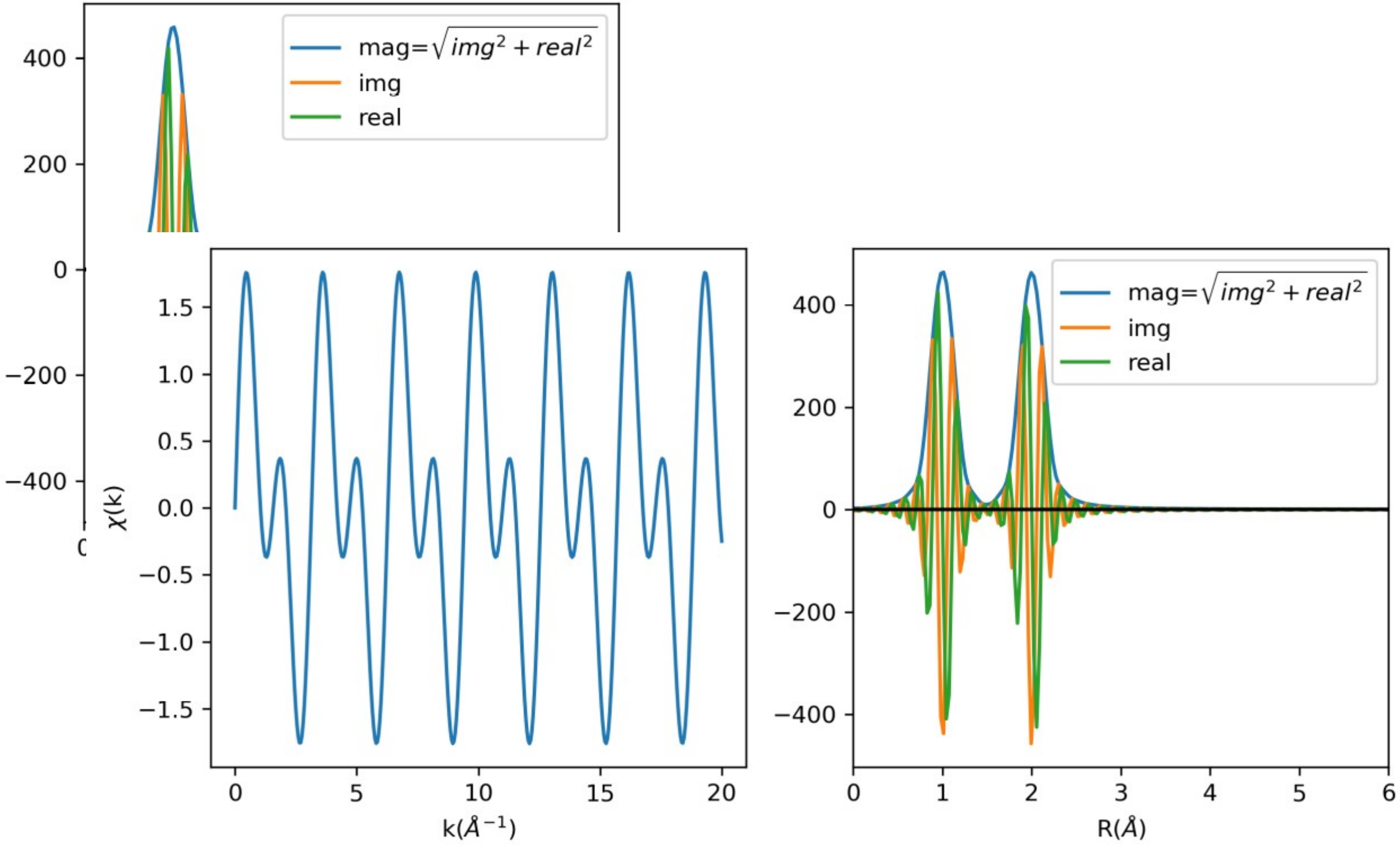
This procedure is important to prevent the larger amplitude oscillations from dominating the smaller ones in determining interatomic distances, which depends only on the frequency and not the amplitude.

k weight 1, 2, 3 for Z > 57, 36 < Z < 57 and Z > 36
Teo and Lee (1979)

Fourier Transform



FT of a sine wave with phase 2k



FT of two sine waves

Fourier Transform of PtO_2