



Data reduction and background removal

Akhil Tayal

10-10-2023



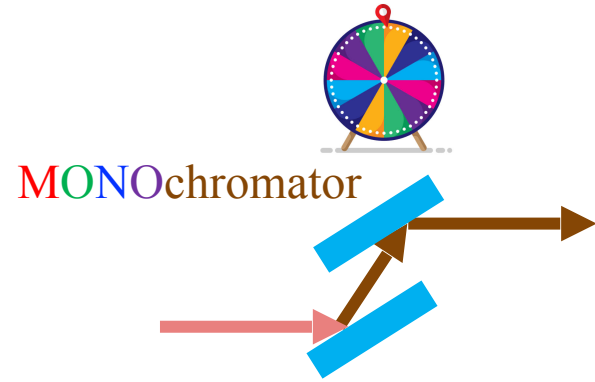
XAFS books

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

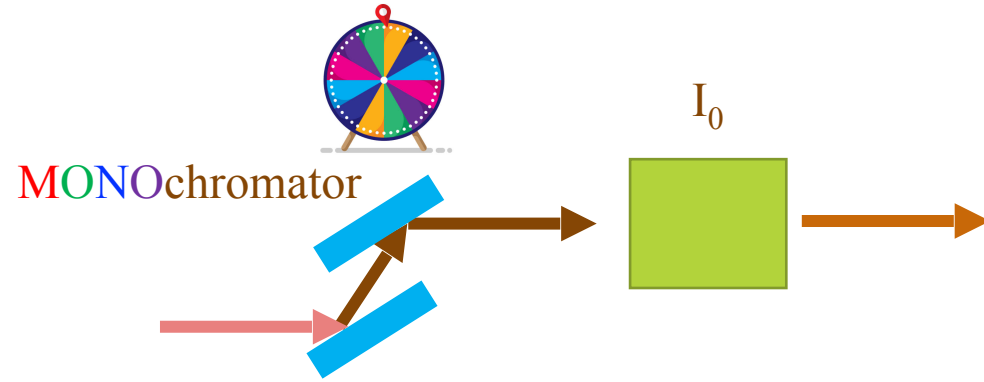
EXAFS: Basic Principles and Data Analysis
Dr. Boon K. Teo

XAFS for Everyone
Scott Calvin

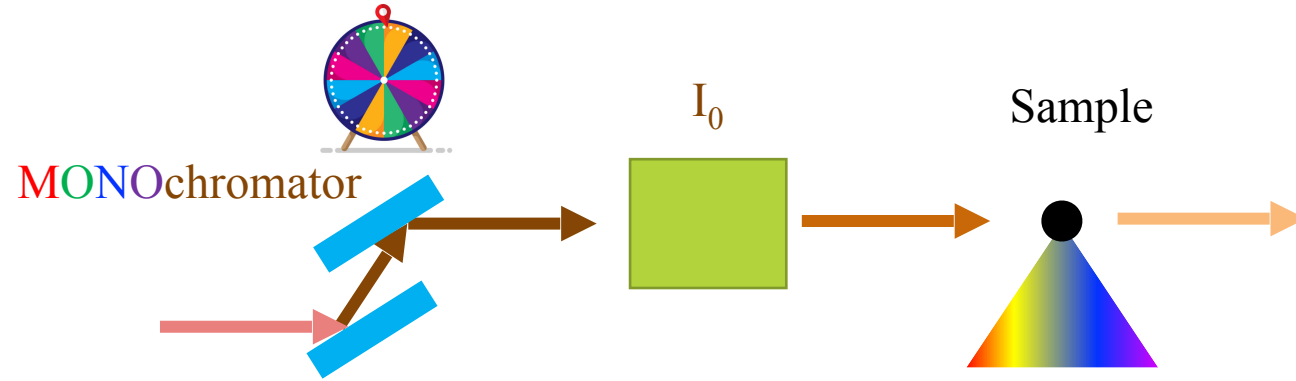
Data collection



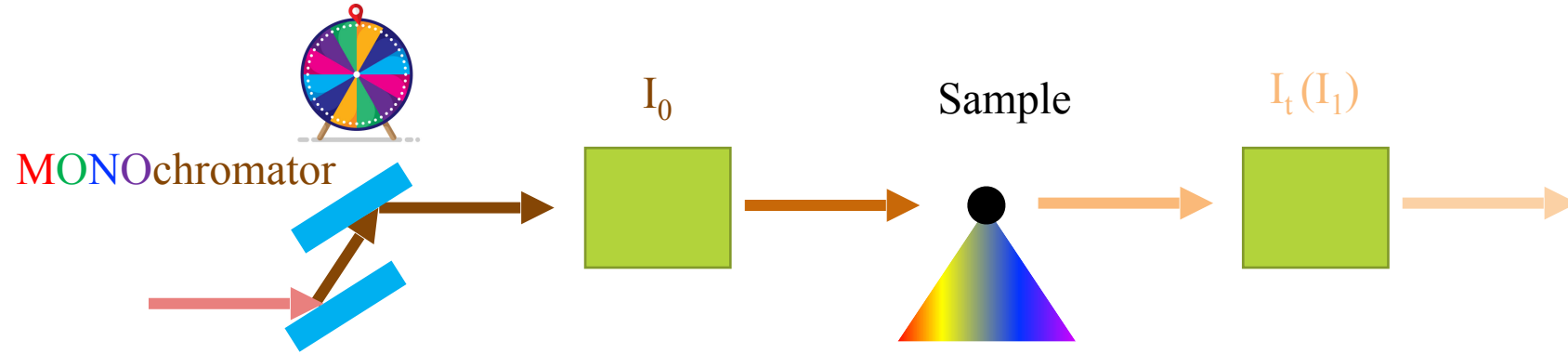
Data collection



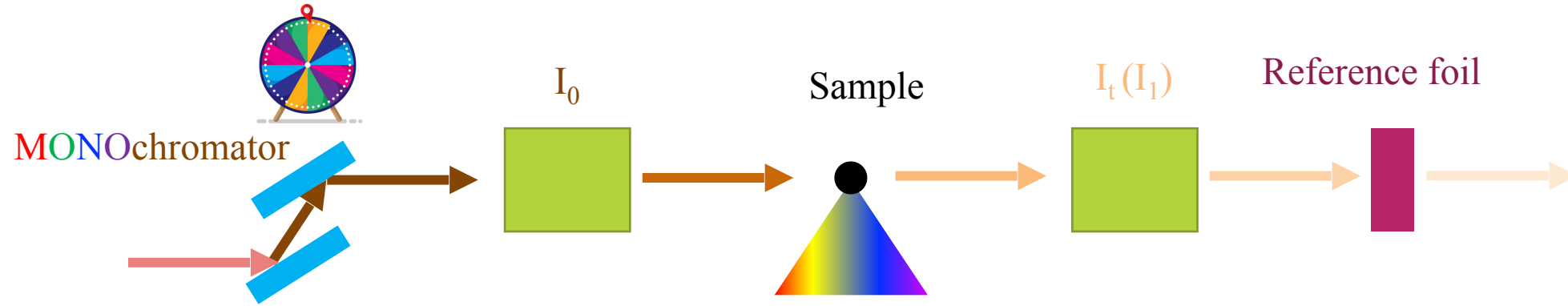
Data collection



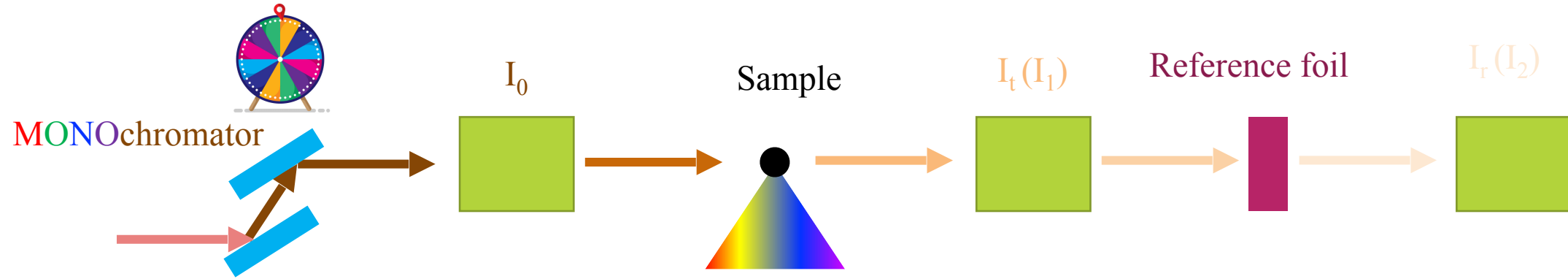
Data collection



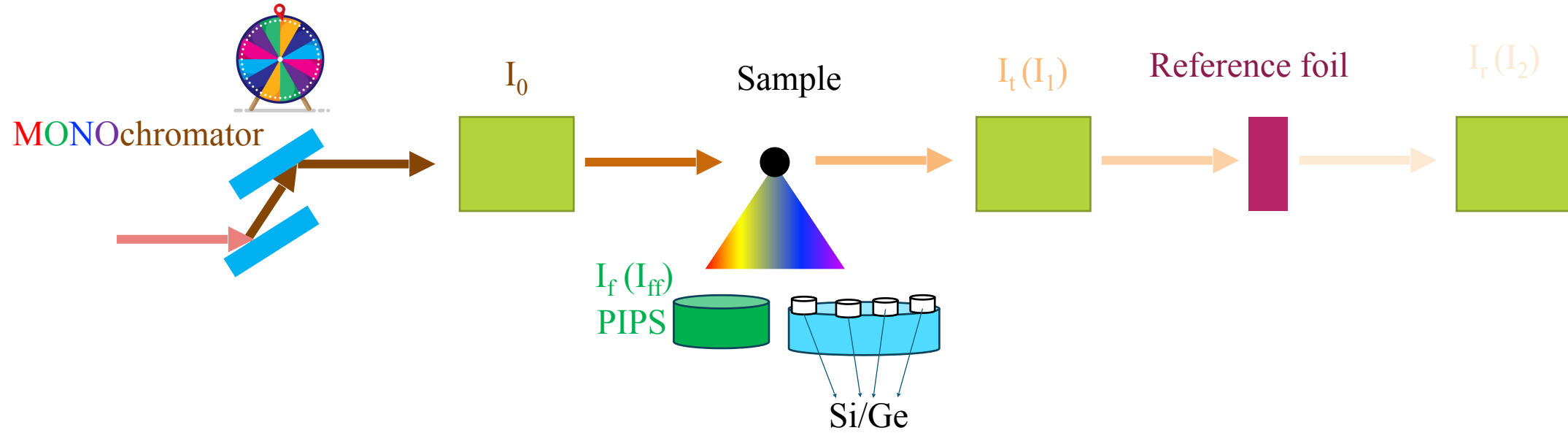
Data collection



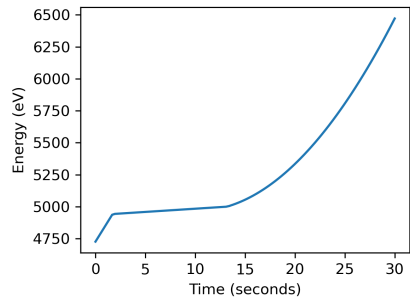
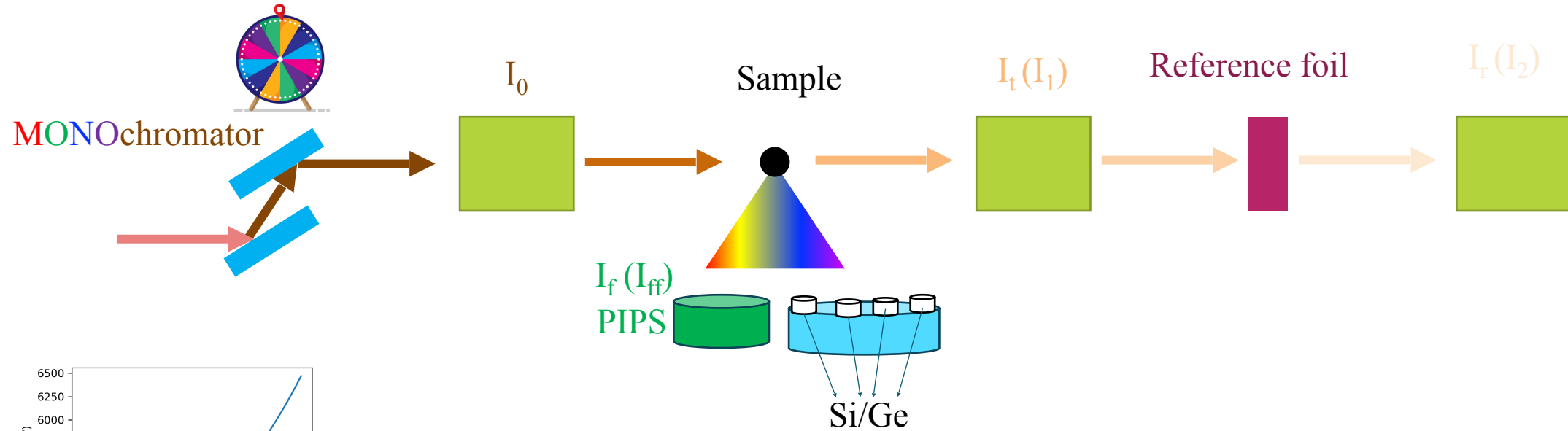
Data collection



Data collection

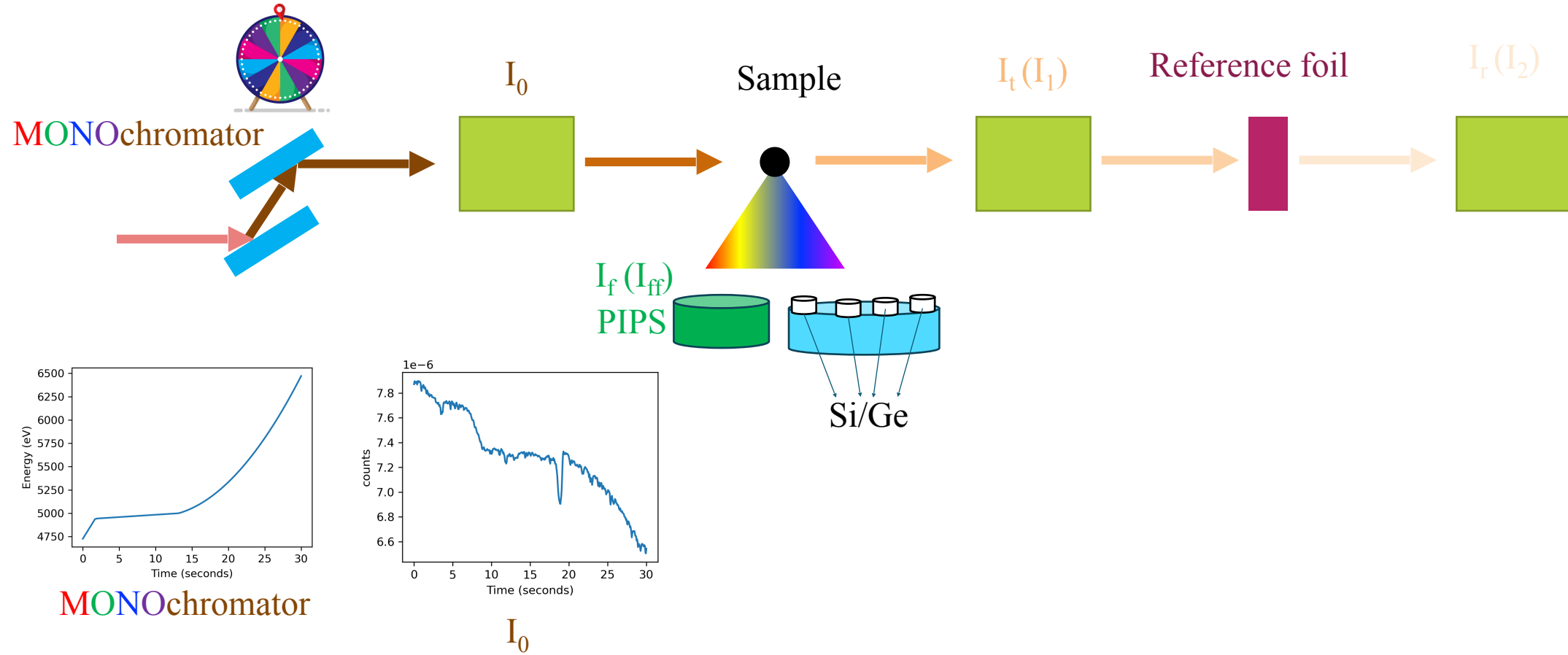


Data collection

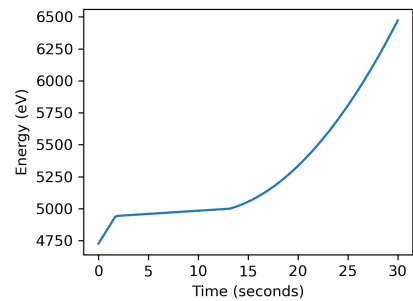
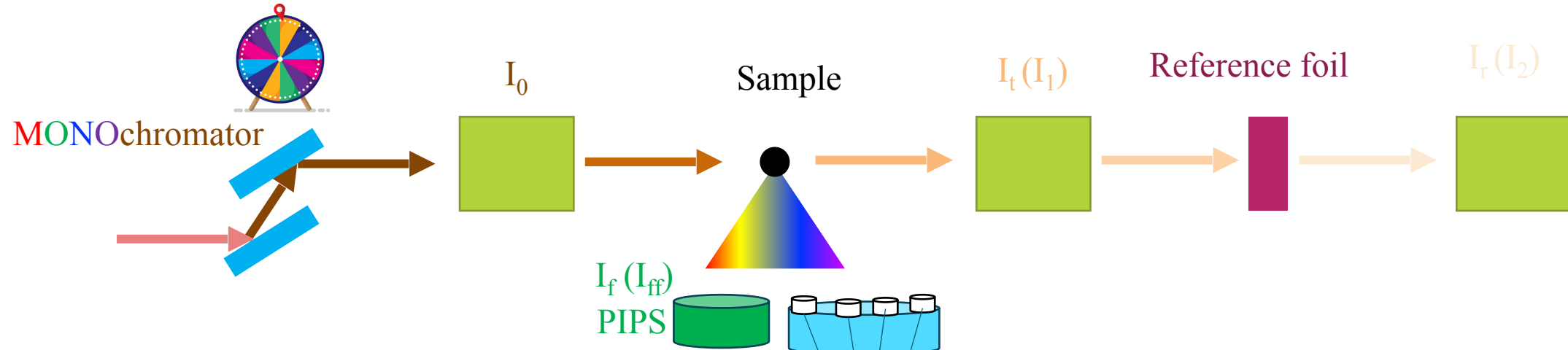


MONOchromator

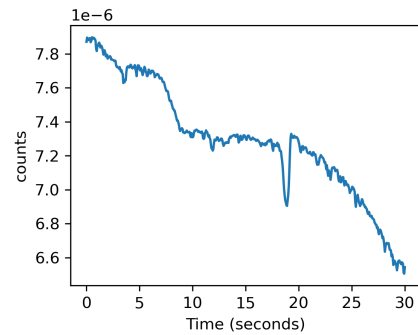
Data collection



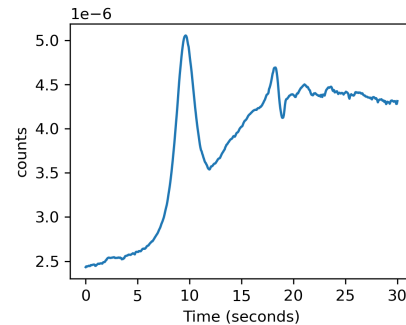
Data collection



MONOchromator

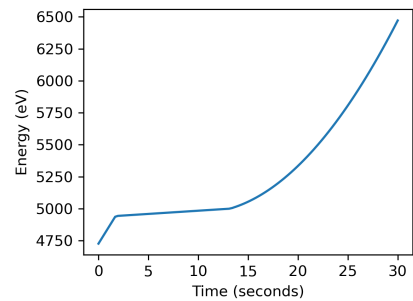
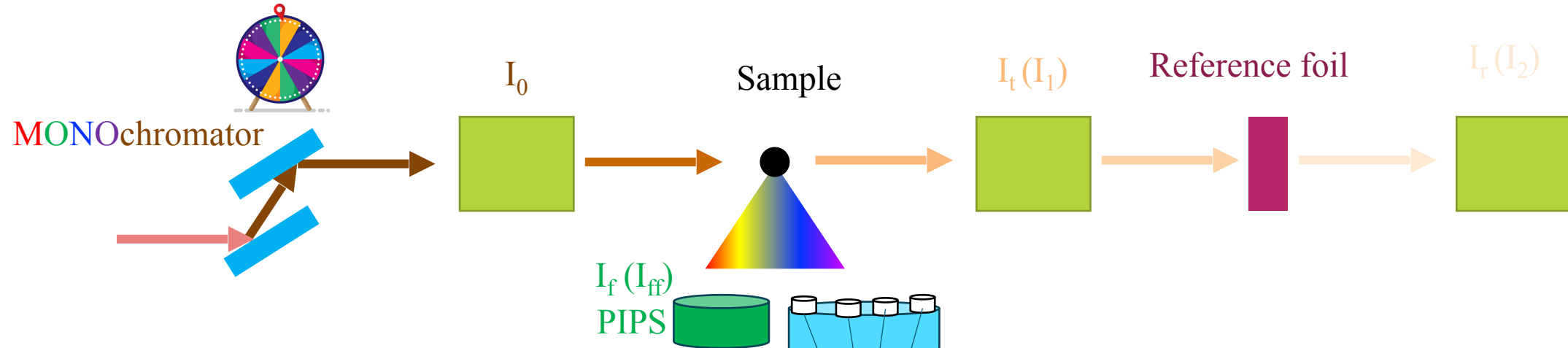


I_0

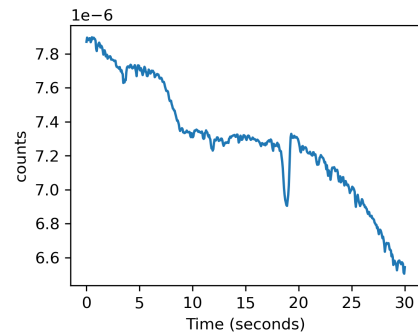


I_f

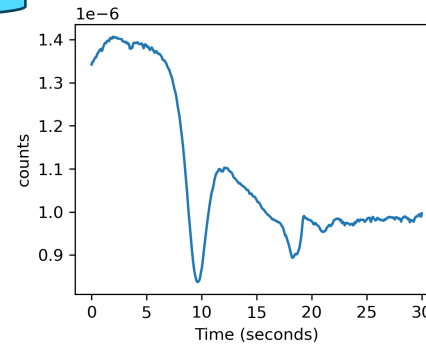
Data collection



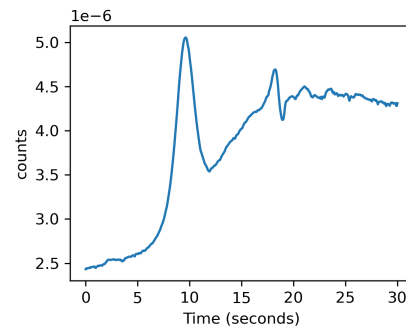
MONOchromator



I_0

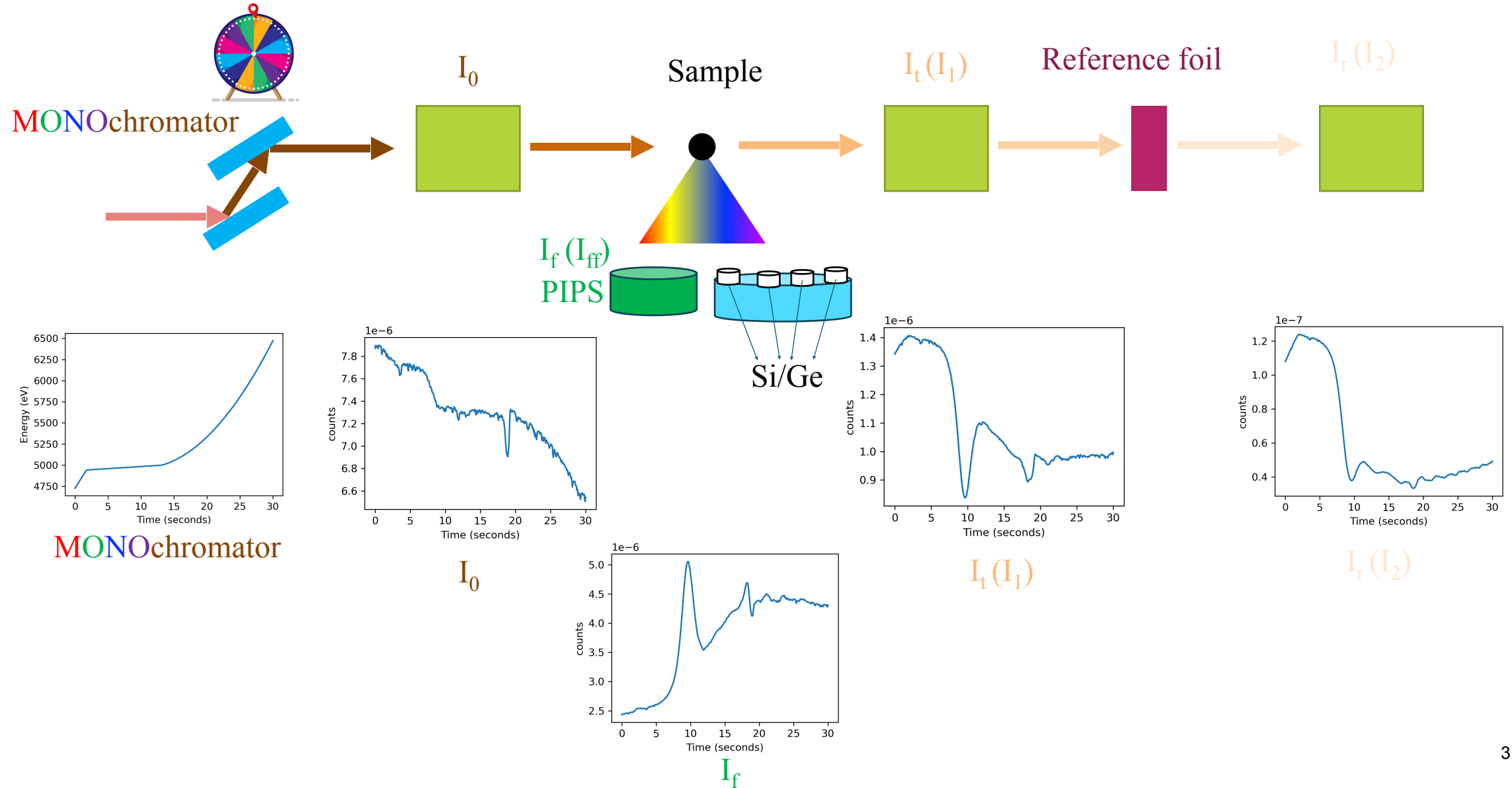


$I_t(I_1)$

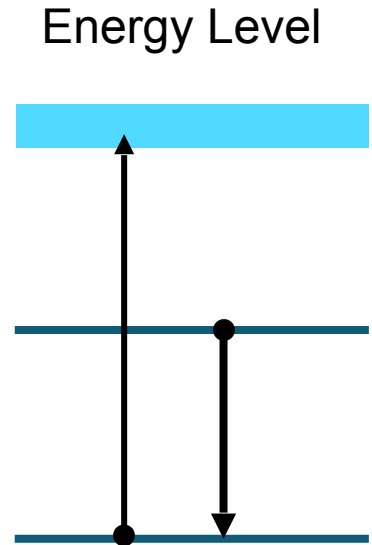
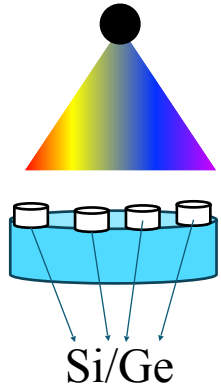


I_f

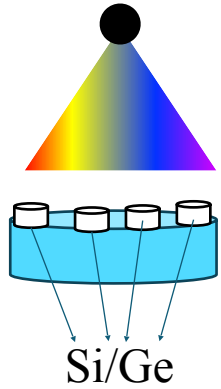
Data collection



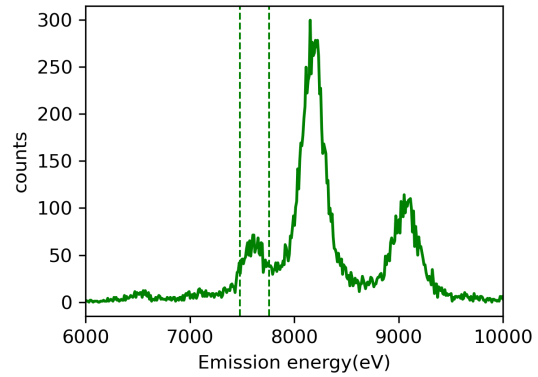
Si/Ge detector data



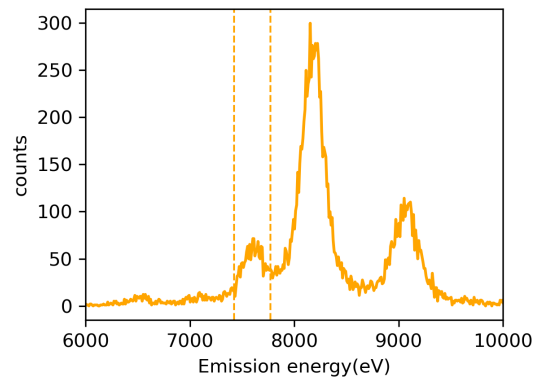
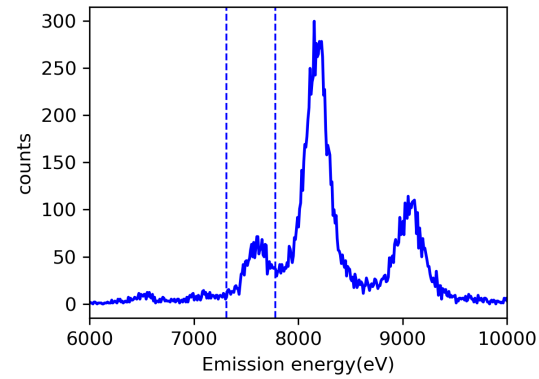
Si/Ge detector data



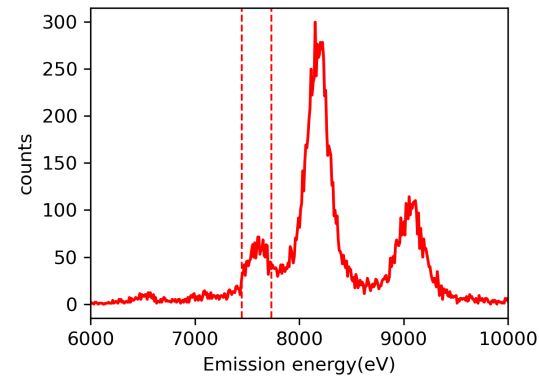
Channel 1



Channel 2

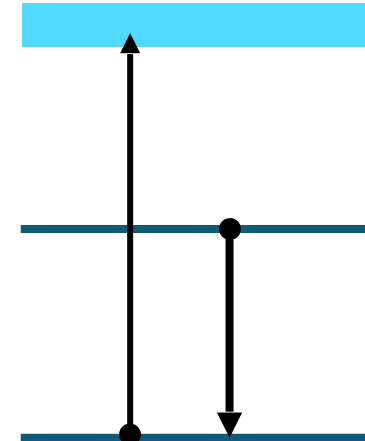


Channel 3

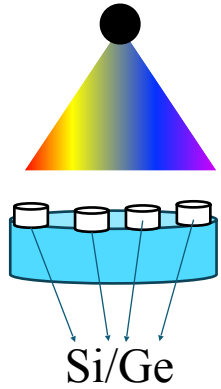


Channel 4

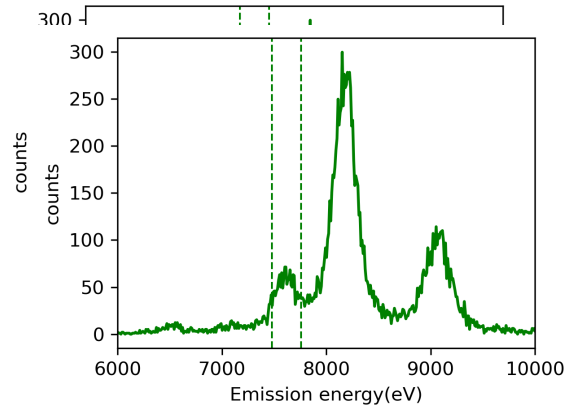
Energy Level



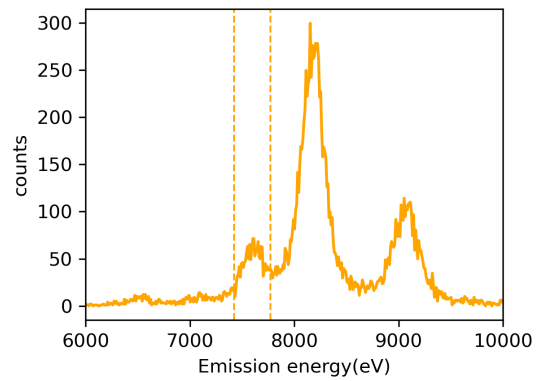
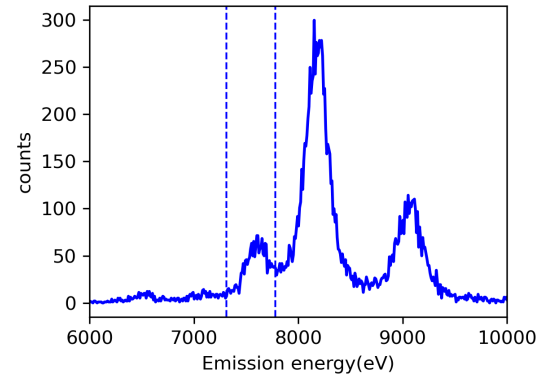
Si/Ge detector data



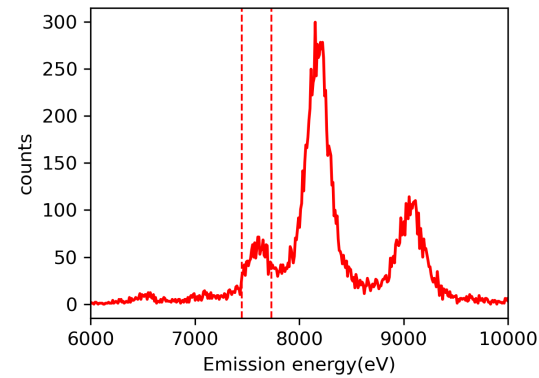
Channel 1



Channel 2

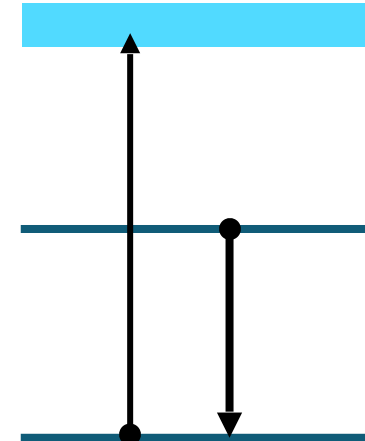


Channel 3

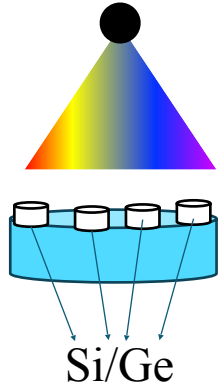


Channel 4

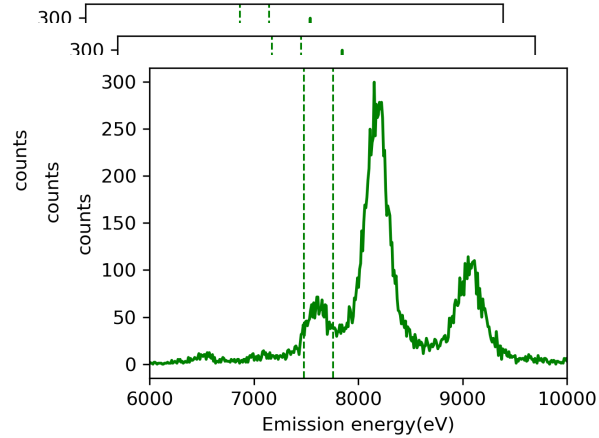
Energy Level



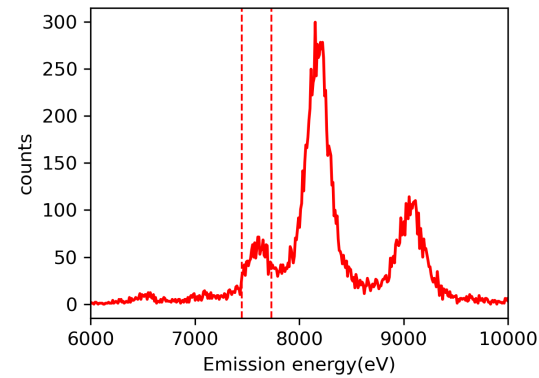
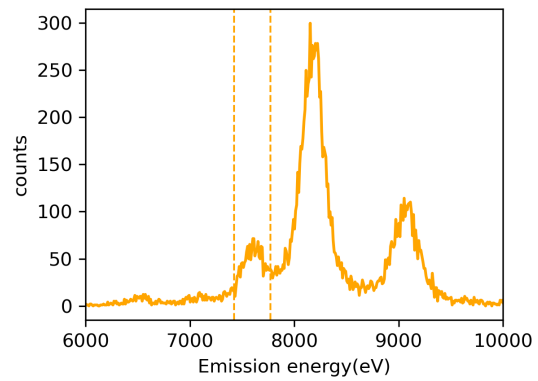
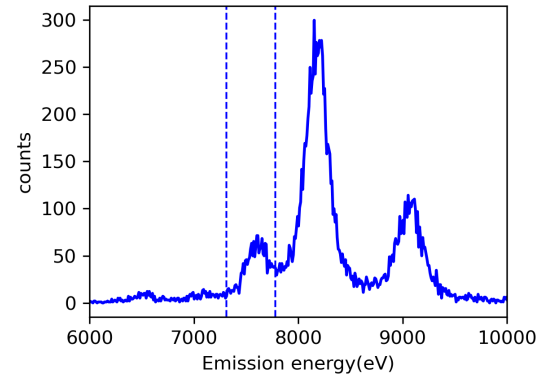
Si/Ge detector data



Channel 1



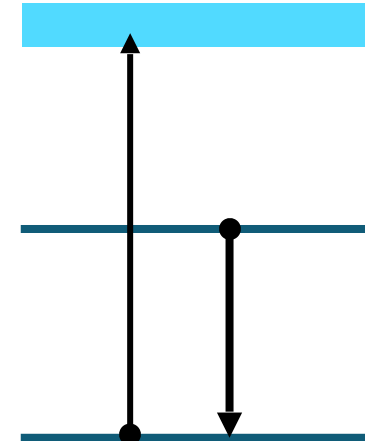
Channel 2



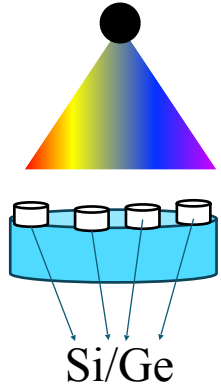
Channel 3

Channel 4

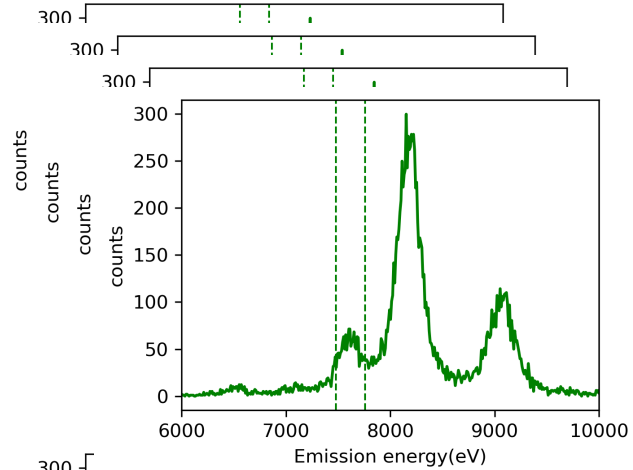
Energy Level



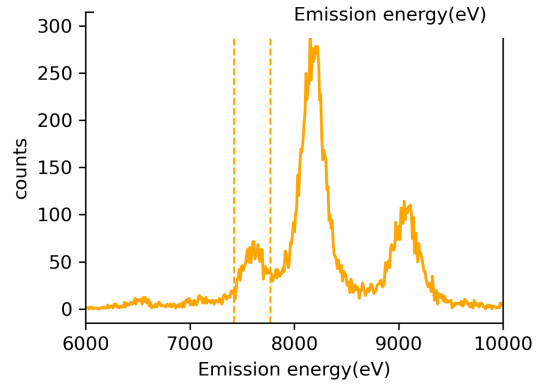
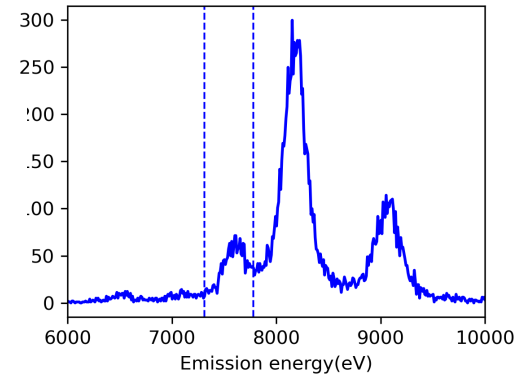
Si/Ge detector data



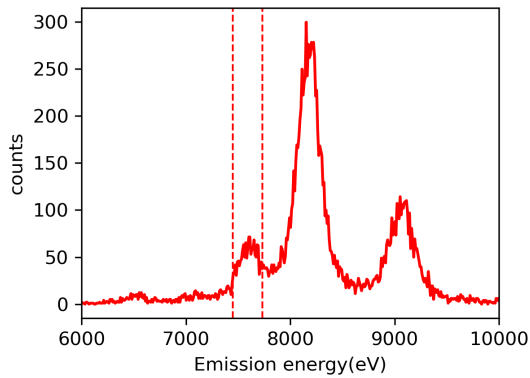
Channel 1



Channel 2

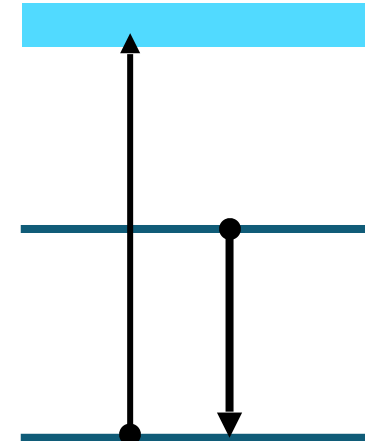


Channel 3

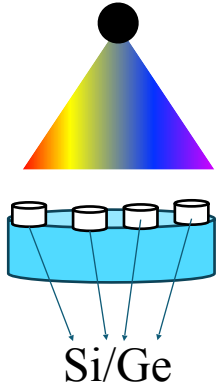


Channel 4

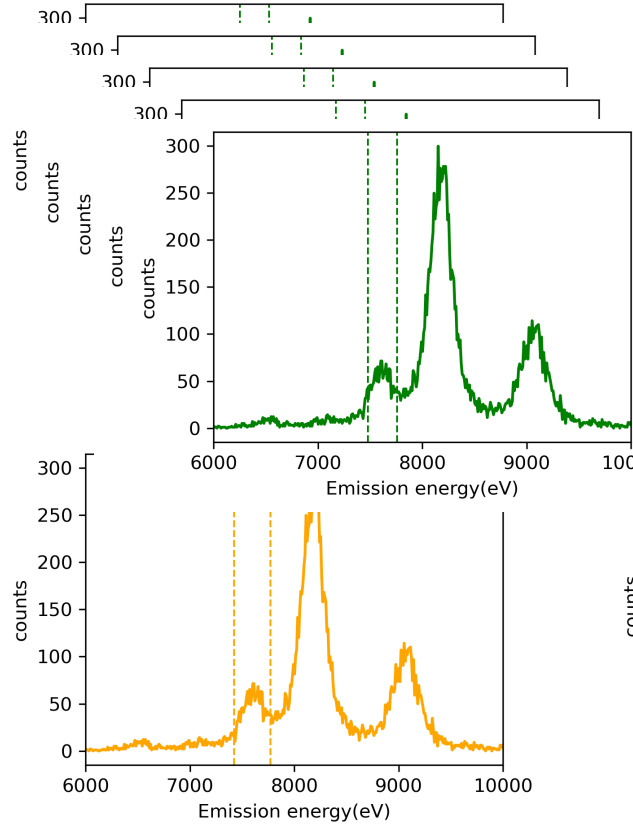
Energy Level



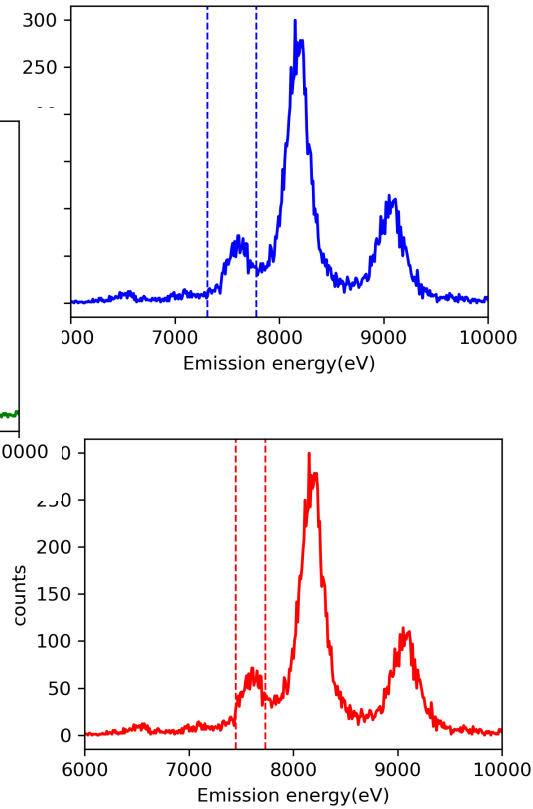
Si/Ge detector data



Channel 1



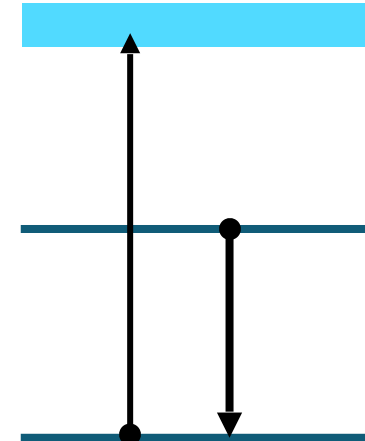
Channel 2



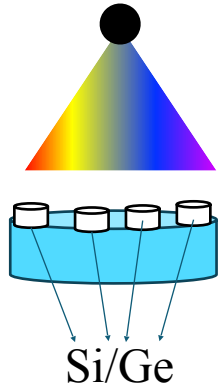
Channel 3

Channel 4

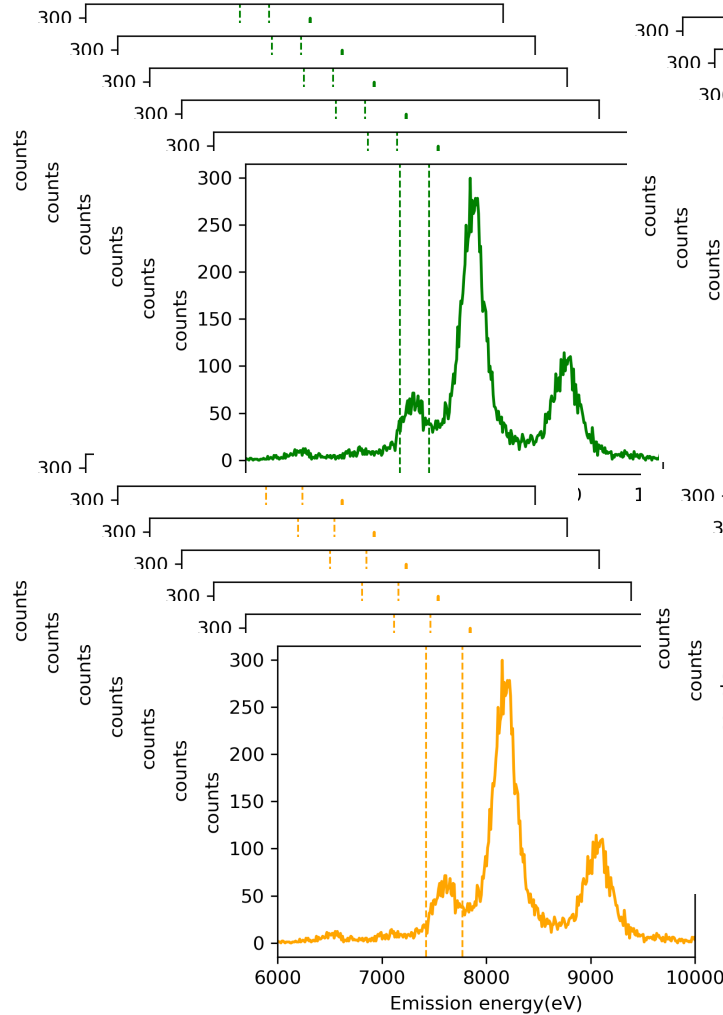
Energy Level



Si/Ge detector data

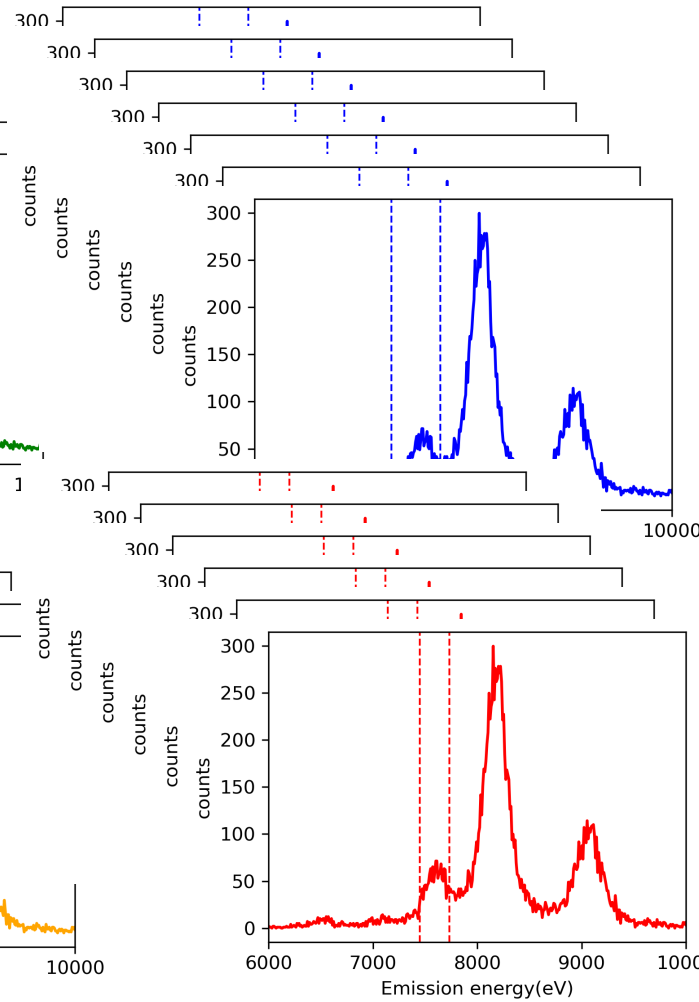


Channel 1



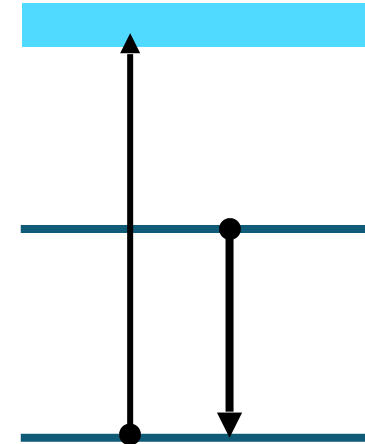
Channel 3

Channel 2



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 |

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: -12.98899999999995
# 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 (cm²)

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x (cm)



σ_{total} (cm²/g)




ρ (density g/cm³)

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ρ (density g/cm³)

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

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x (cm)



σ_{total} (cm²/g)



ρ (density g/cm³)

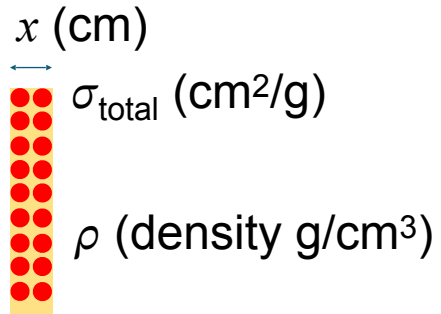
Probability of absorption = $x\rho\sigma_{\text{total}} = x\mu$ (μ is linear absorption coefficient)

Bouguer's Law:

$$I_t = I_0 e^{-\mu x}$$

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

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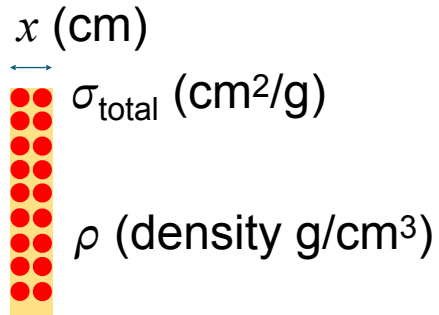
$$I_t = I_0 e^{-\mu x}$$

Absorption coefficient for transmission

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

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

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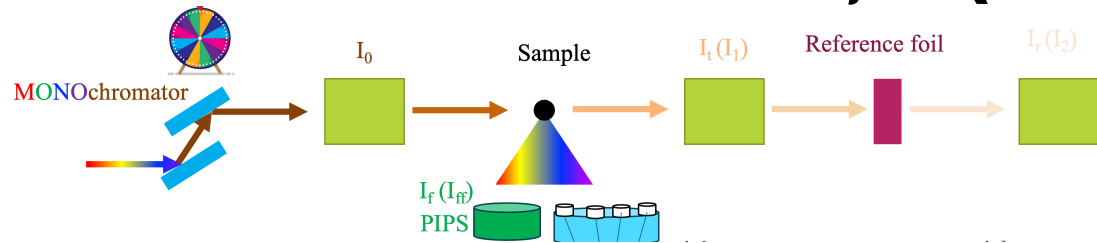
Absorption coefficient for transmission

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

Absorption coefficient for fluorescence

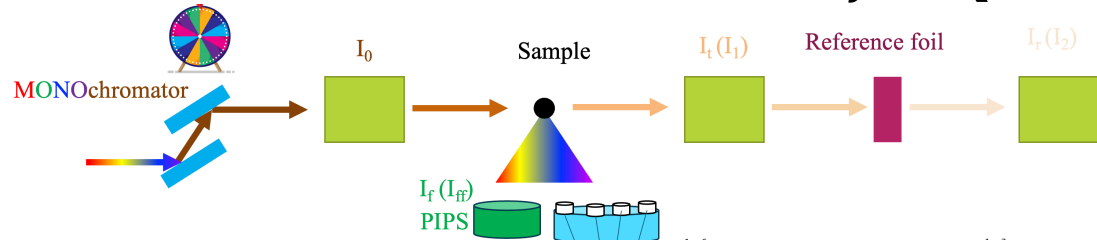
$$\mu x = \left(\frac{I_f}{I_0}\right)$$

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. | 0.000000 | -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. | 0.000000 | -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. | 0.000000 | -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. | 0.000000 | -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. | 0.000000 | -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. | 0.000000 | -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 |

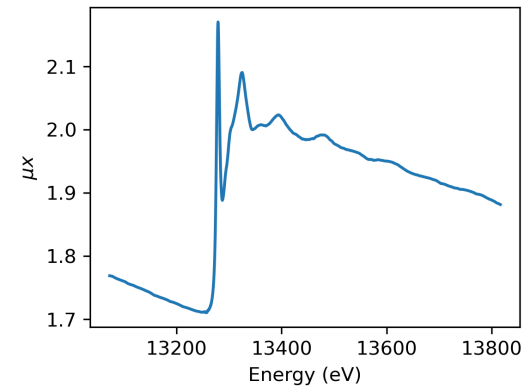
Calculation of μ (absorption coefficient)



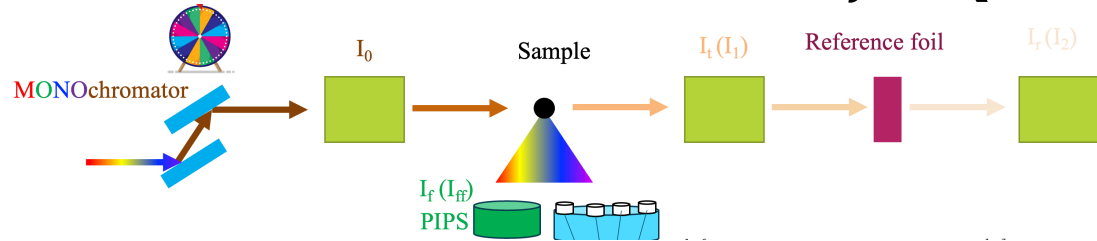
| # | energy | i0 | it | ir | iff | xs_roi01 | xs_ch01_roi01 | xs_ch02_roi01 | xs_ch03_roi01 | xs_ch04_roi01 |
|--------------|---------------|---------------|---------------|---------------|--------------|--------------|---------------|---------------|---------------|---------------|
| 13073.000000 | -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:

$$\mu x = \log\left(\frac{i_0}{i_t}\right)$$



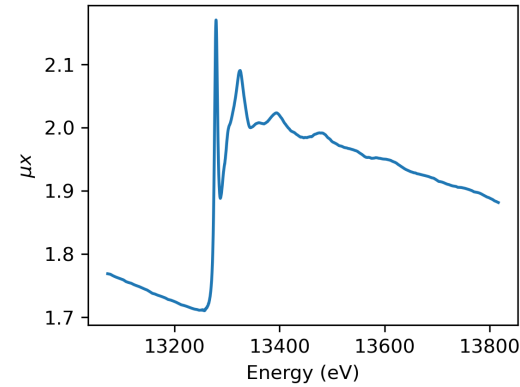
Calculation of μ (absorption coefficient)



| # | energy | i_0 | i_t | i_r | i_{ff} | xs_roi1 | xs_ch01_roi1 | xs_ch02_roi1 | xs_ch03_roi1 | xs_ch04_roi1 |
|--------------|---------------|---------------|---------------|---------------|--------------|--------------|------------------|------------------|------------------|------------------|
| 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:

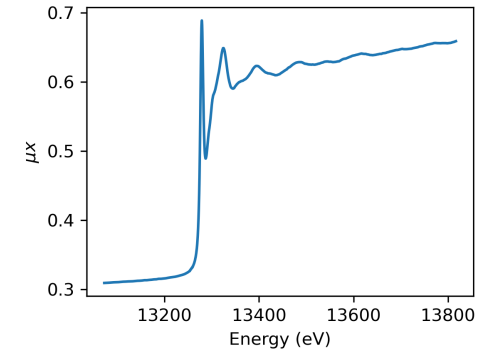
$$\mu x = \log\left(\frac{i_0}{i_t}\right)$$



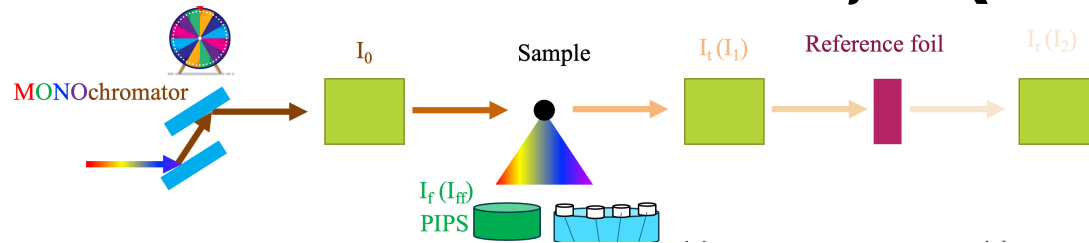
Absorption coefficient for sample fluorescence:

$$\mu x = \left(\frac{i_{ff}}{i_0}\right)$$

$$; \mu x = \left(\frac{xs_roi1}{i_0}\right)$$



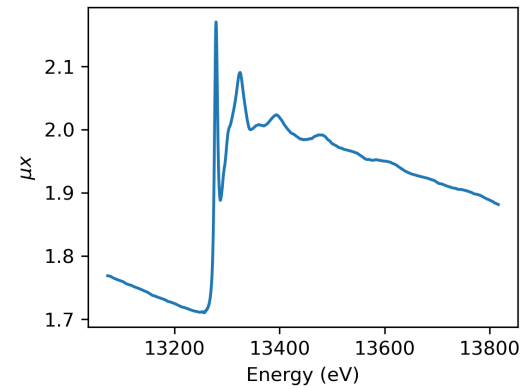
Calculation of μ (absorption coefficient)



| # | energy | i0 | it | ir | iff | xs_roi1 | xs_ch01_roi1 | xs_ch02_roi1 | xs_ch03_roi1 | xs_ch04_roi1 |
|--------------|--------|---------------|---------------|---------------|---------------|--------------|--------------|--------------|--------------|--------------|
| 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:

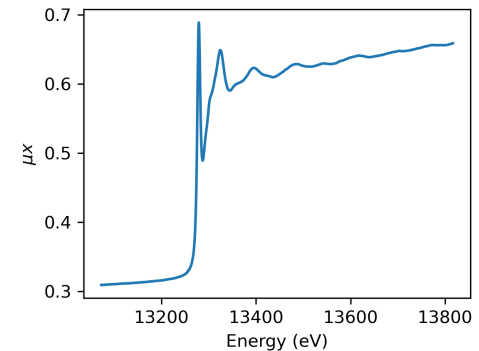
$$\mu x = \log\left(\frac{i_0}{i_t}\right)$$



Absorption coefficient for sample fluorescence:

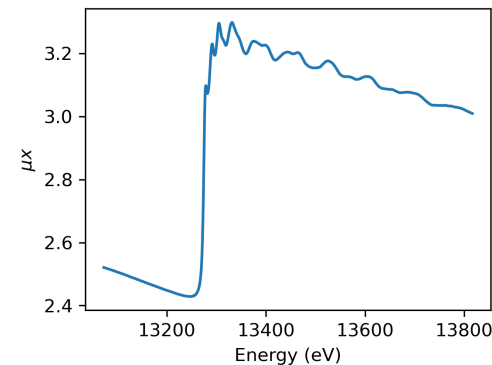
$$\mu x = \left(\frac{i_{ff}}{i_0}\right)$$

$$; \mu x = \left(\frac{xs_roi1}{i_0}\right)$$

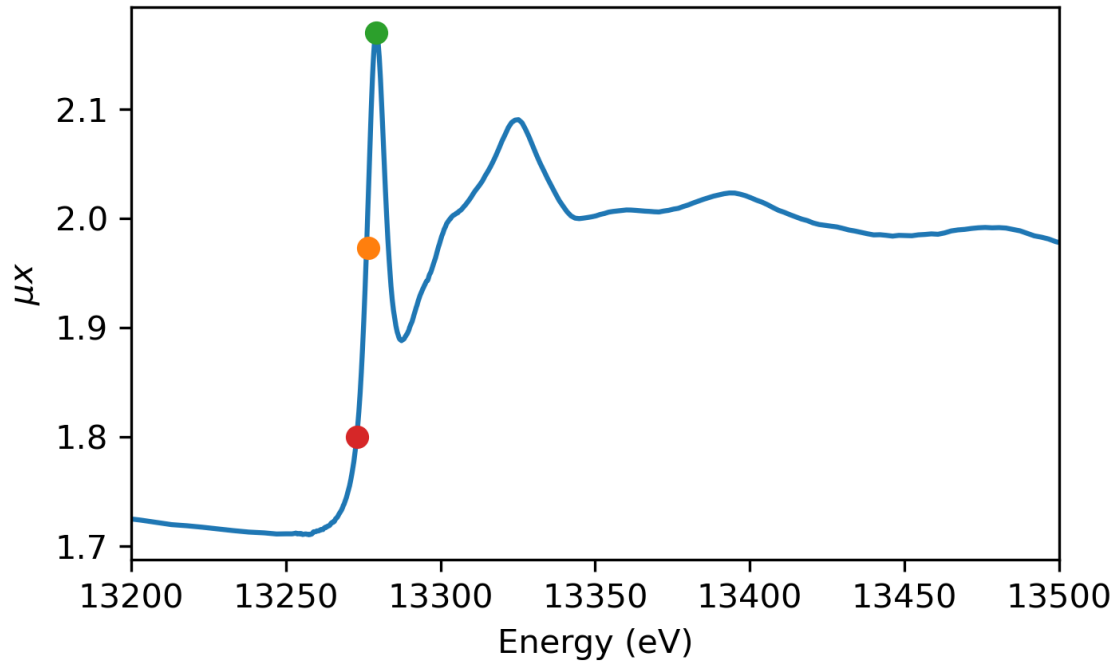


Absorption coefficient for reference transmission:

$$\mu x = \log\left(\frac{i_r}{i_t}\right)$$



E_0

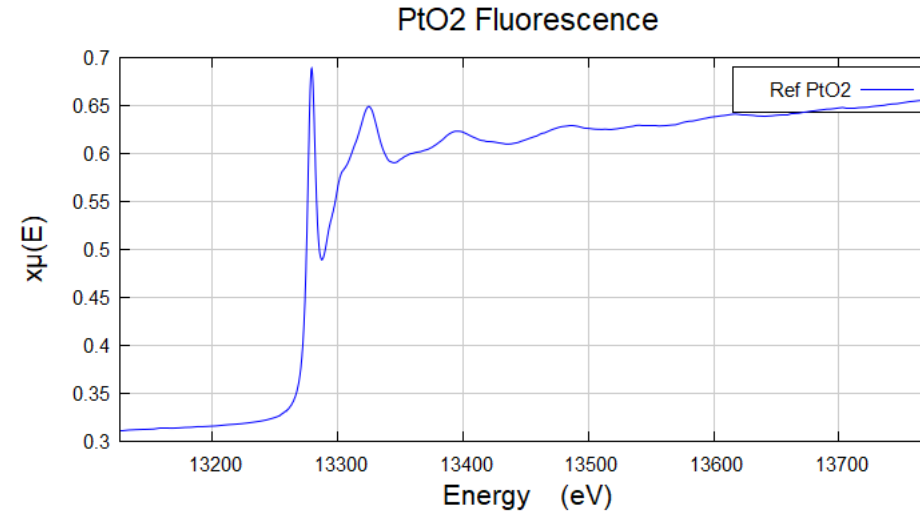
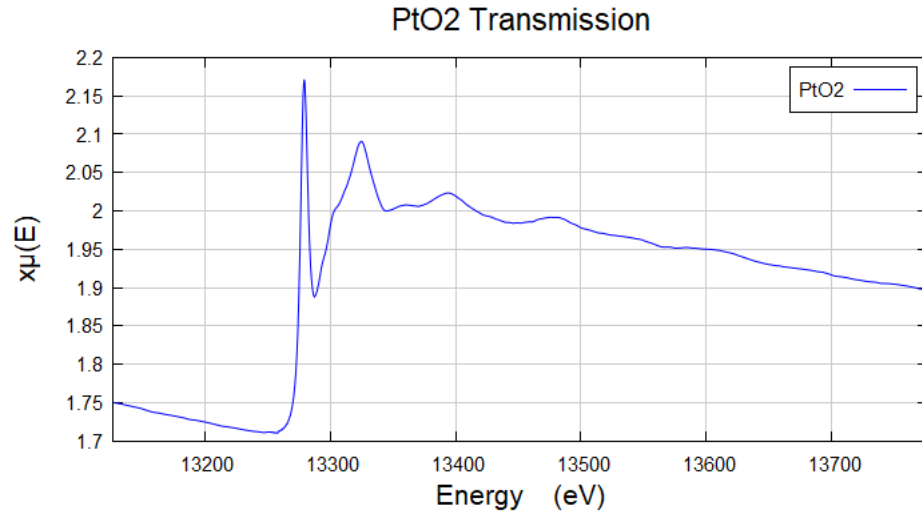


E_0 = White line

E_0 = first inflection point

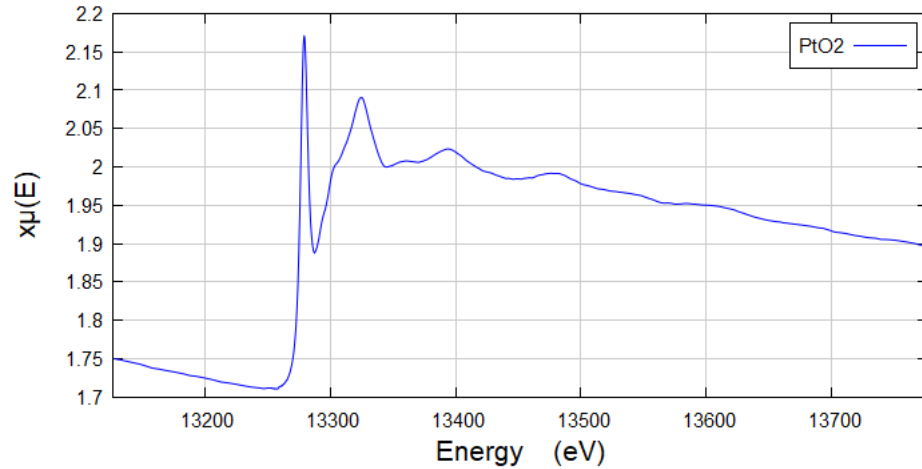
E_0 = Tabulated value

Pre-edge & Post-edge normalization

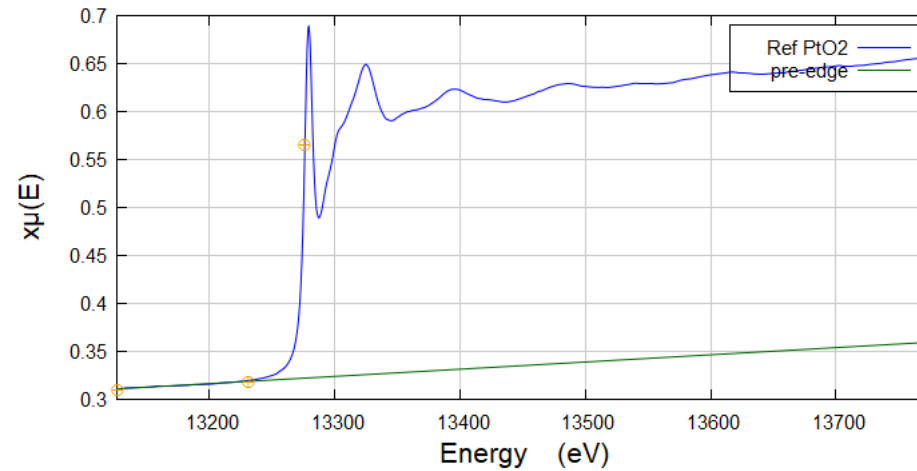
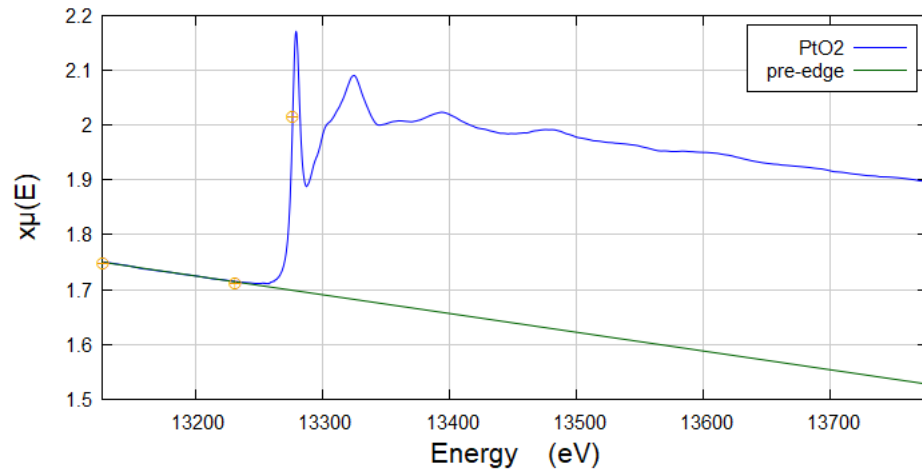
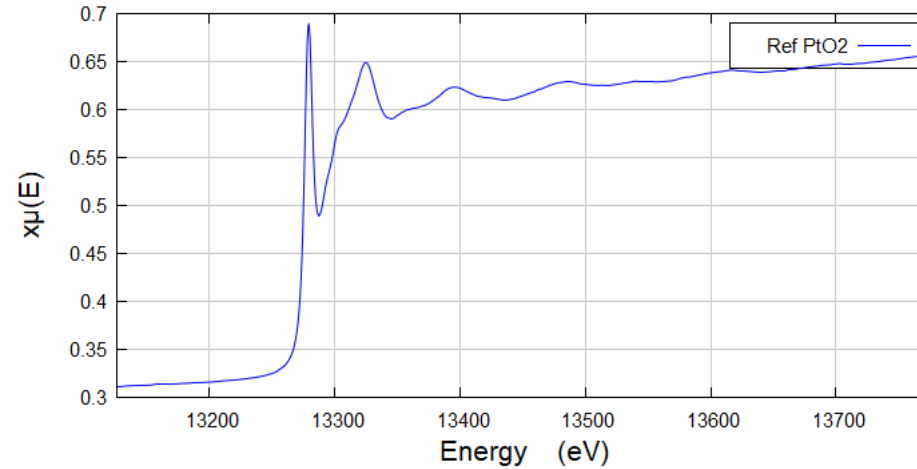


Pre-edge & Post-edge normalization

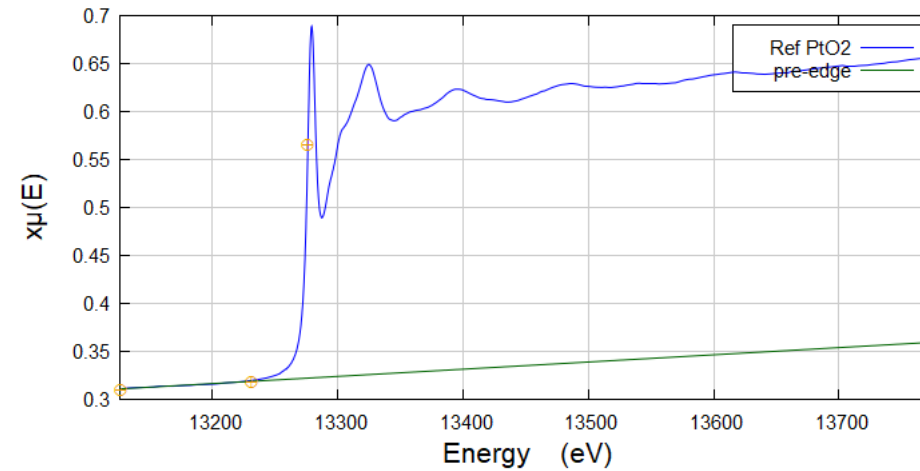
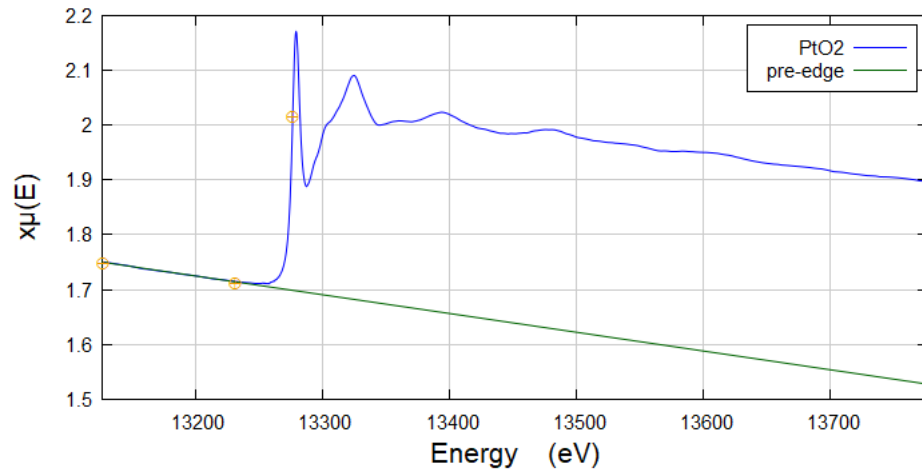
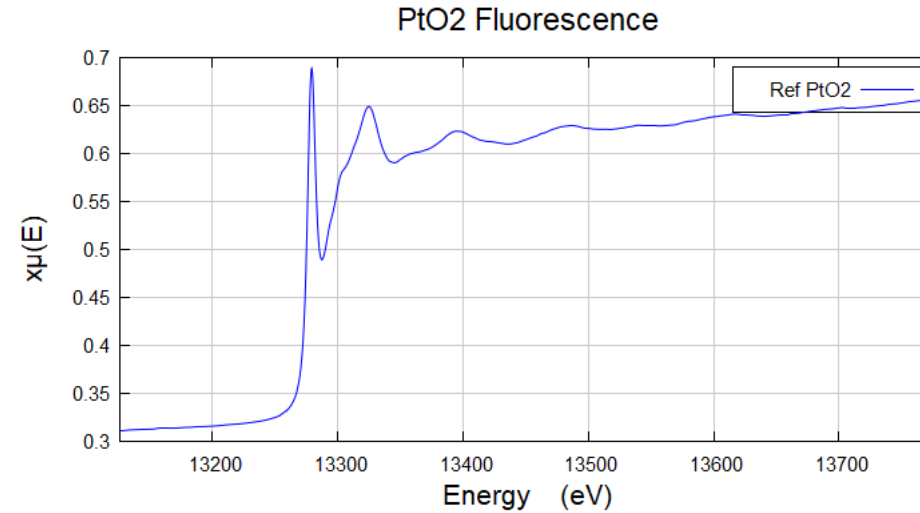
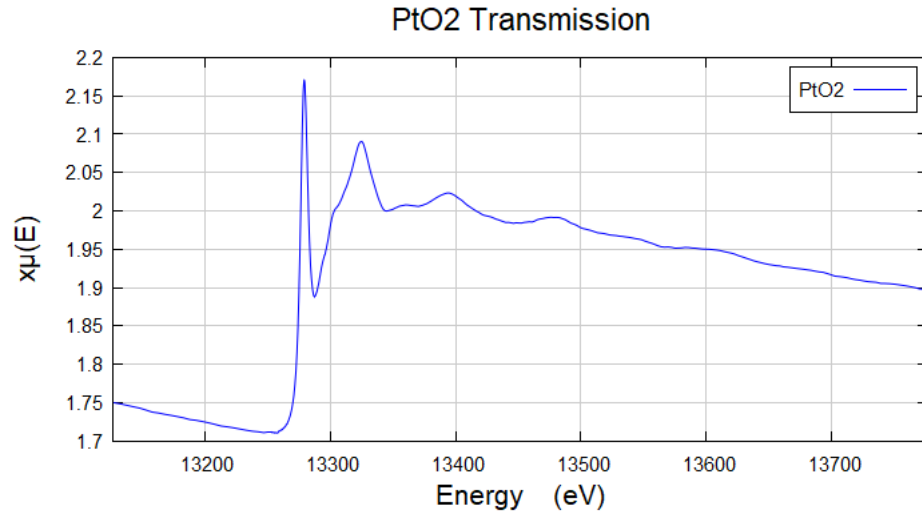
PtO2 Transmission



PtO2 Fluorescence



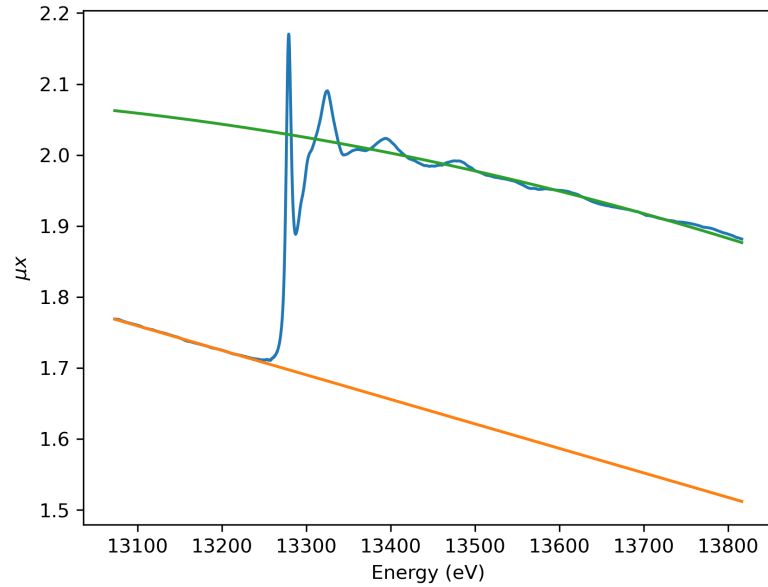
Pre-edge & Post-edge normalization



$$\mu = CE^3 - DE^4 \text{ (Victoreen Equation imperical)}$$

Pre-edge & Post-edge normalization

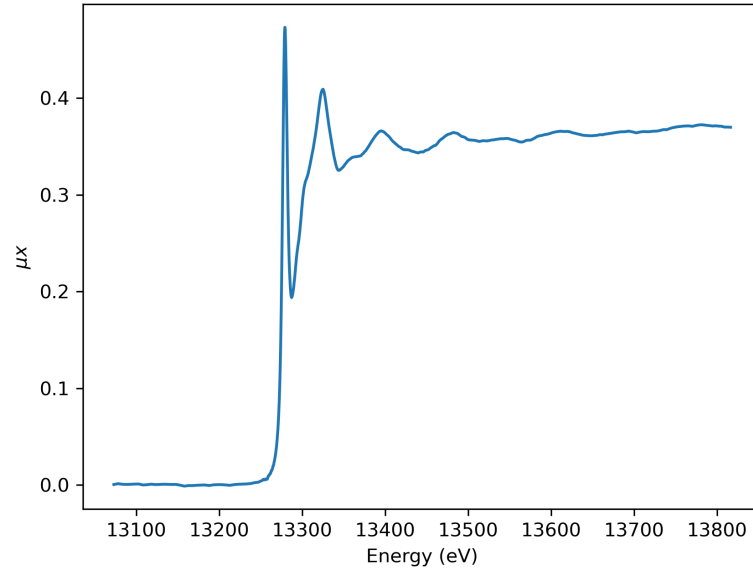
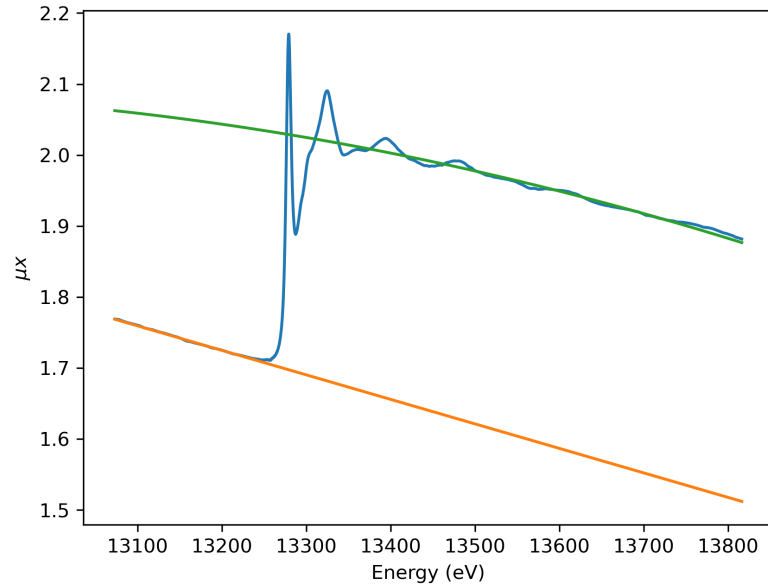
Pre-edge & Post-edge normalization



Pre-edge background

Post-edge background

Pre-edge & Post-edge normalization

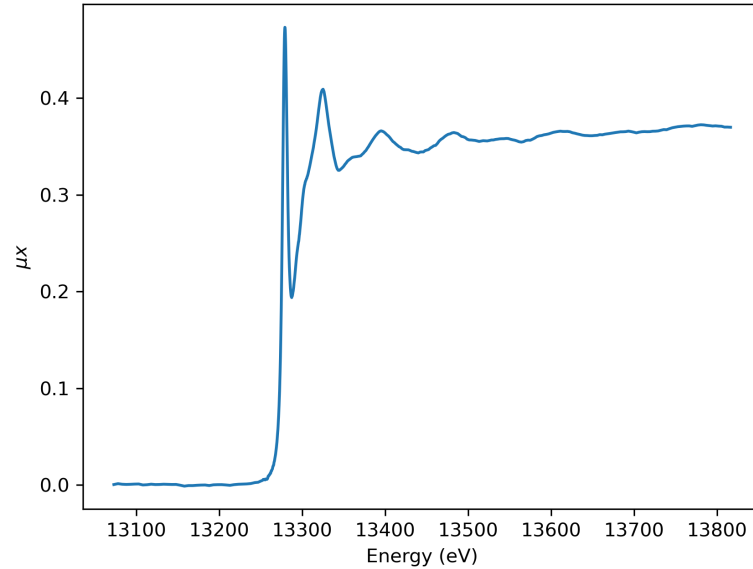
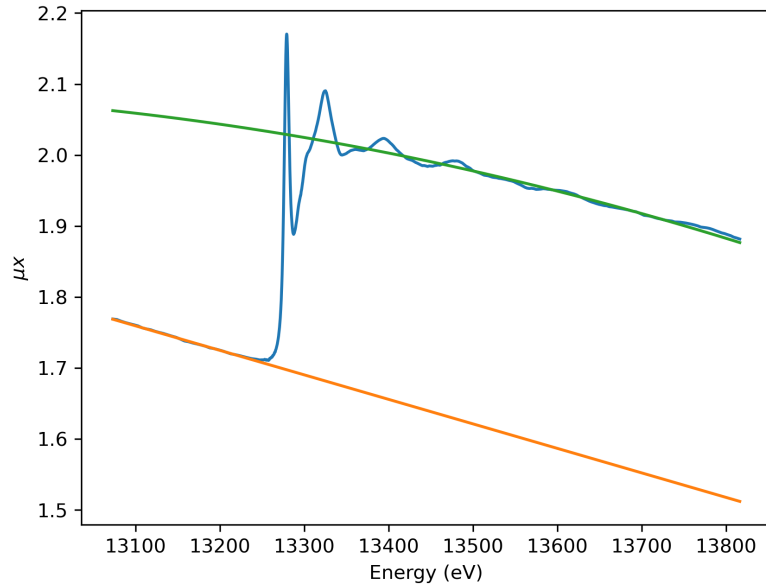


Pre-edge background

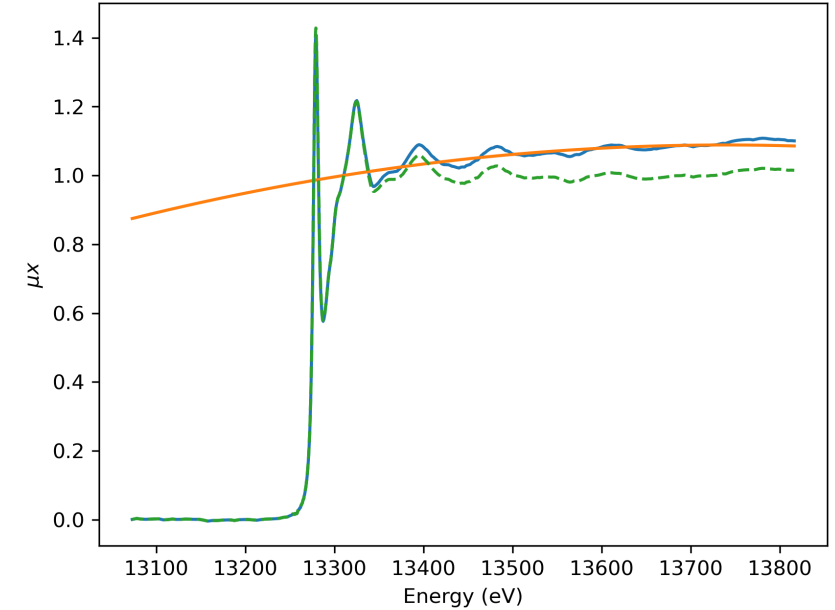
Post-edge background

Pre-edge subtracted

Pre-edge & Post-edge normalization



Pre-edge subtracted

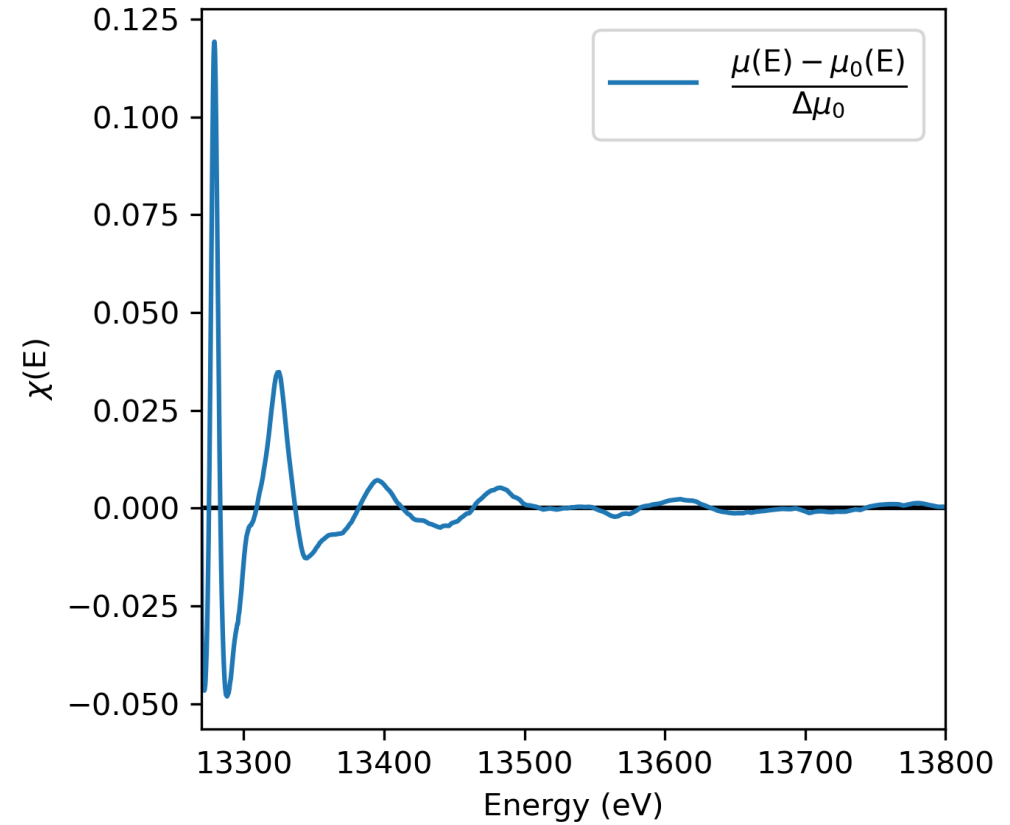
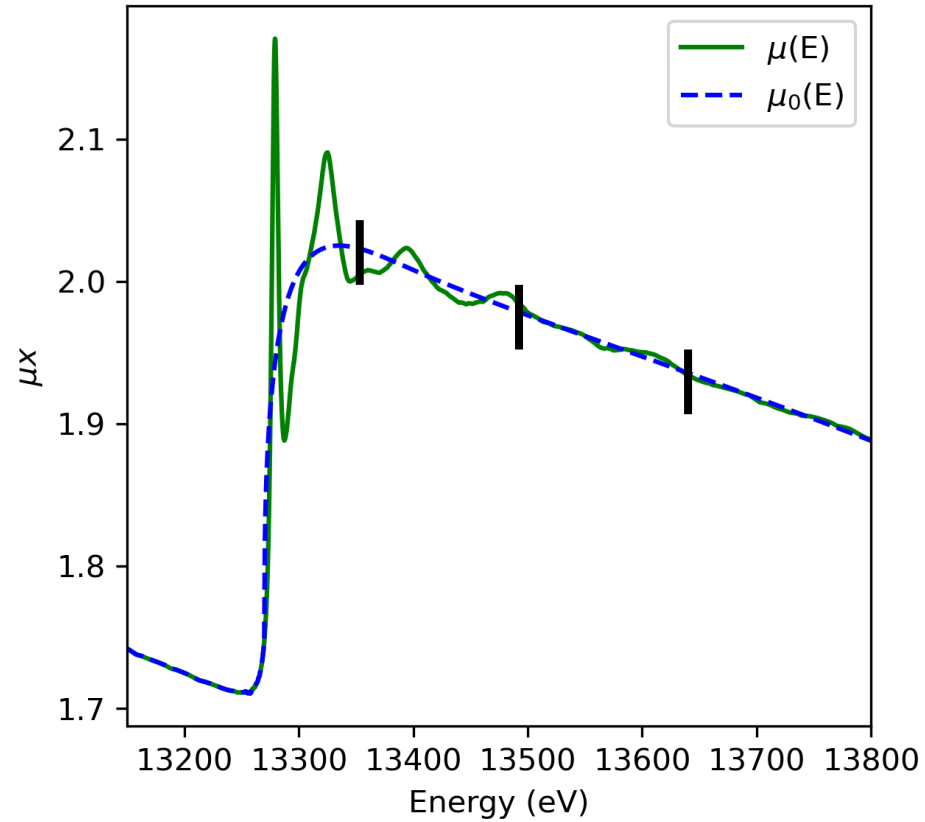


Post-edge subtracted

Pre-edge background

Post-edge background

EXAFS extraction



Conversion of E to k

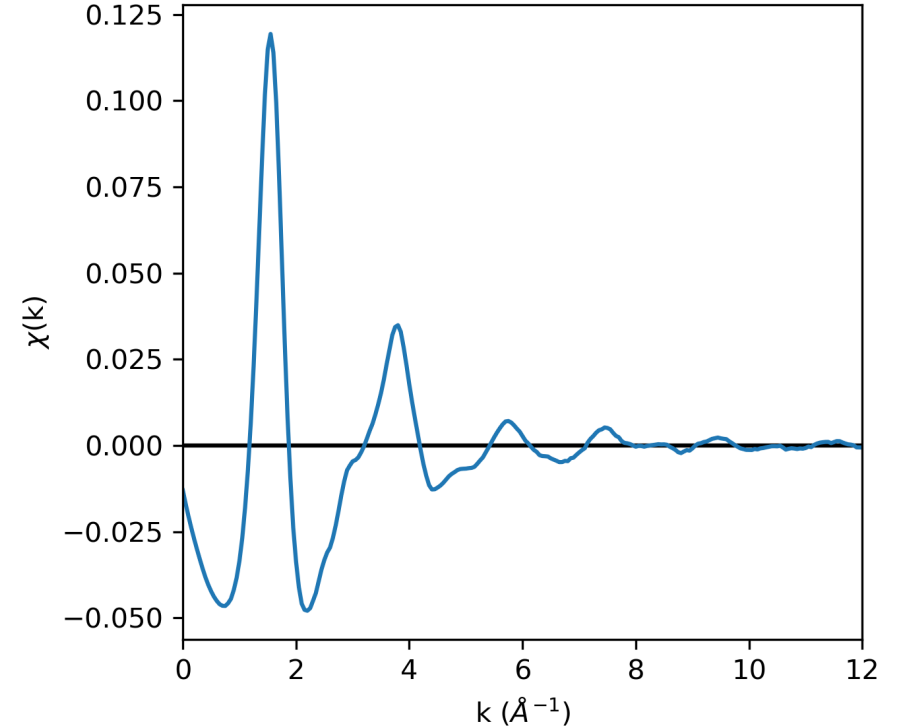
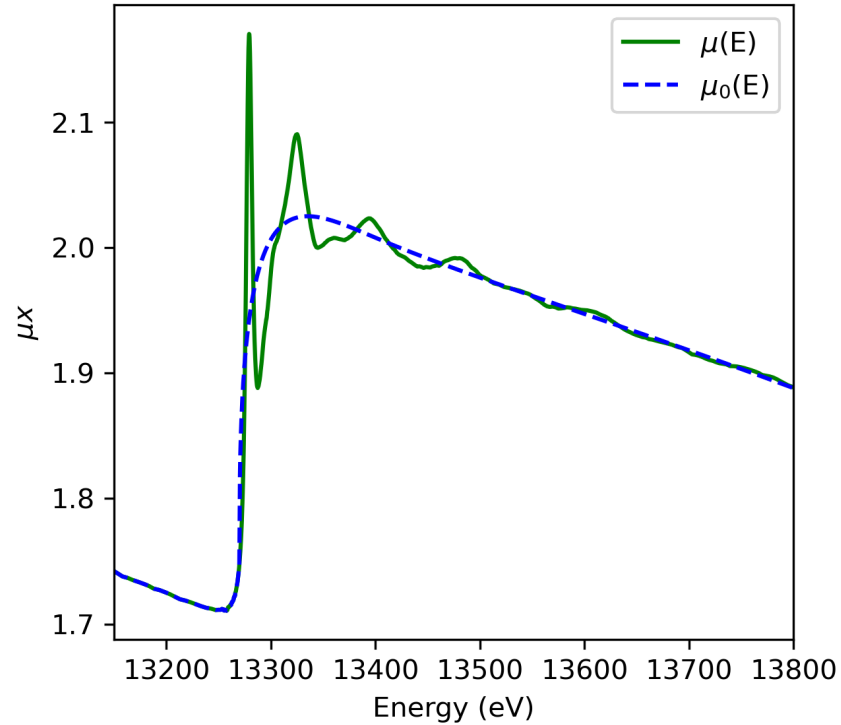
$$k = \sqrt{\frac{2m(E - E_0^{exp})}{\hbar^2}}$$

$$k = \sqrt{0.2625(E - E_0^{exp})}$$

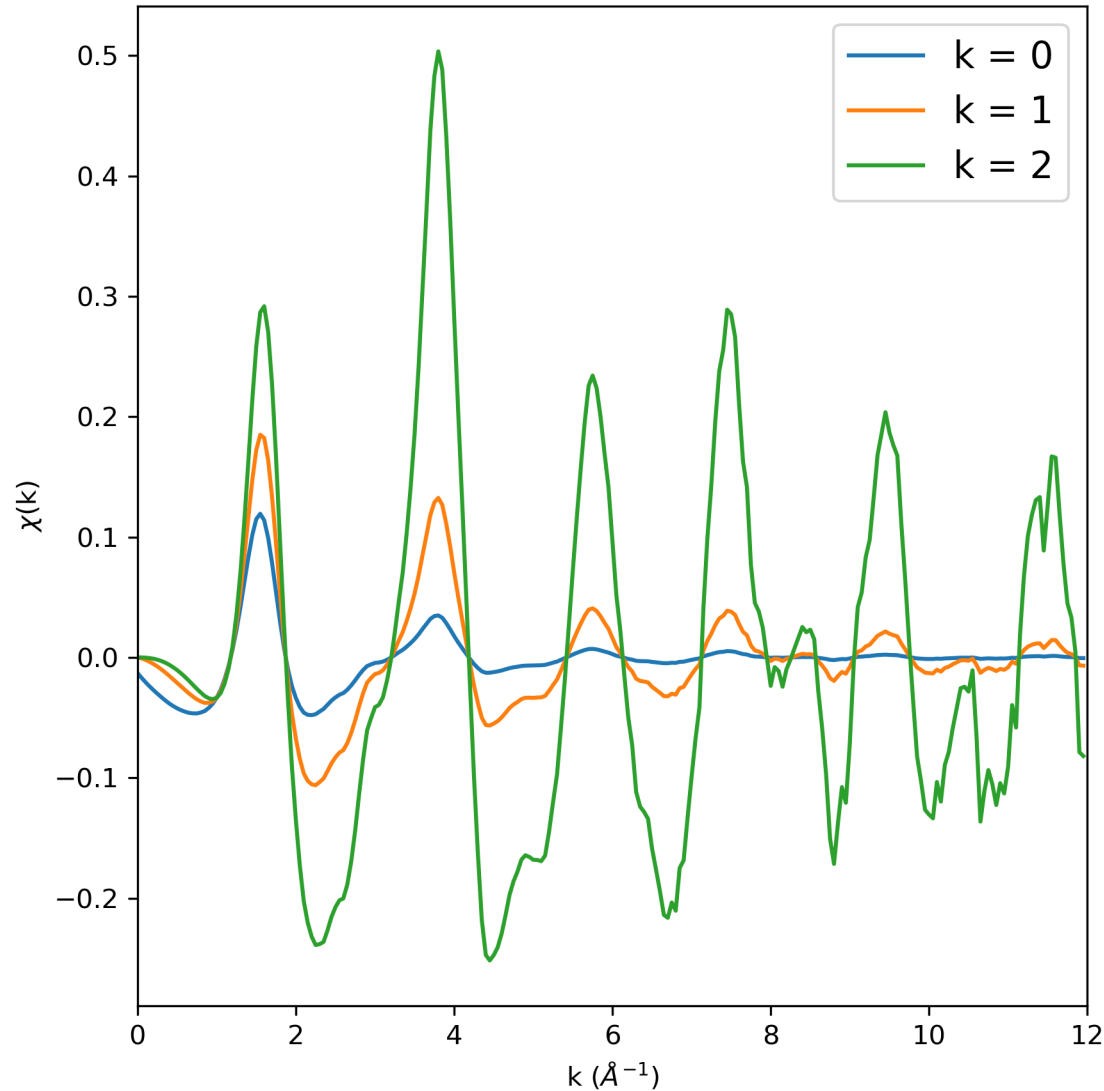
Conversion of E to k

$$k = \sqrt{\frac{2m(E - E_0^{exp})}{\hbar^2}}$$

$$k = \sqrt{0.2625(E - E_0^{exp})}$$



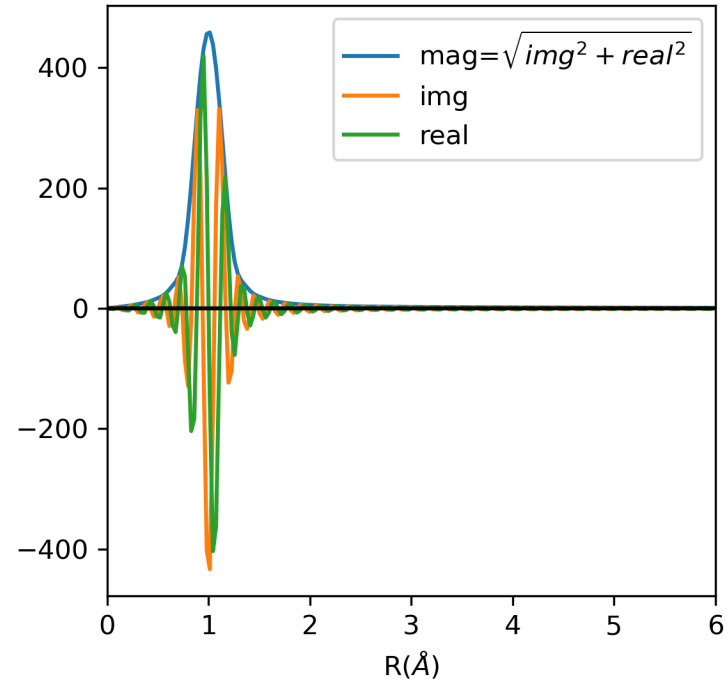
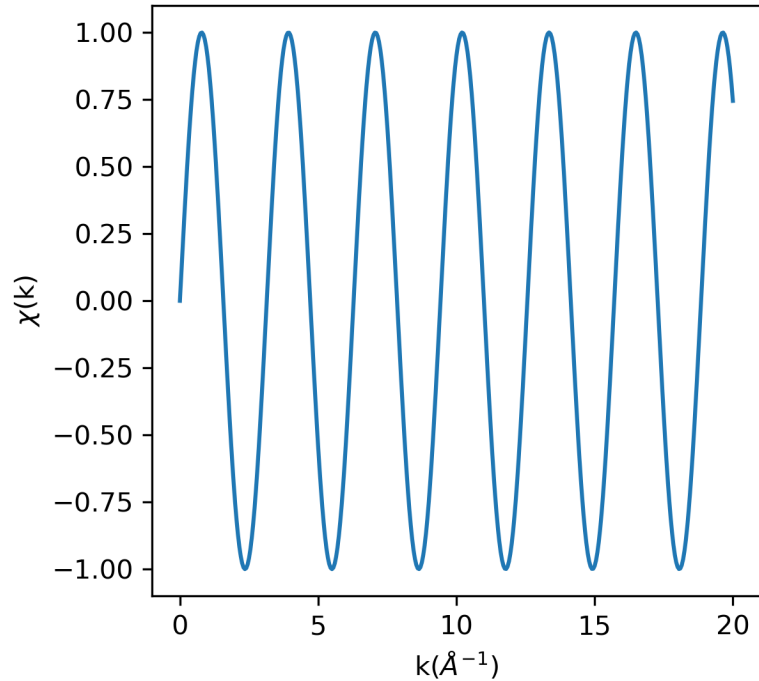
k weighting 1, 2, 3



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)

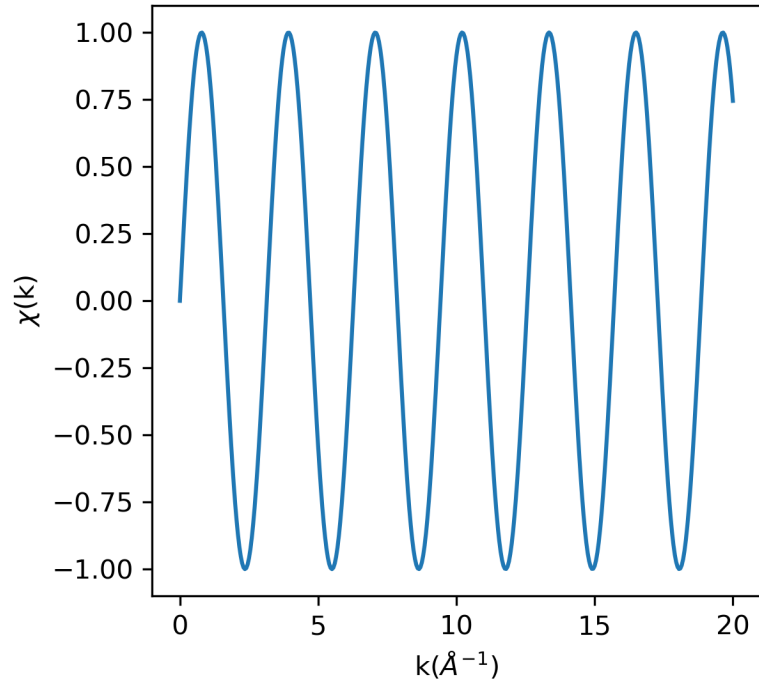
Fourier Transform



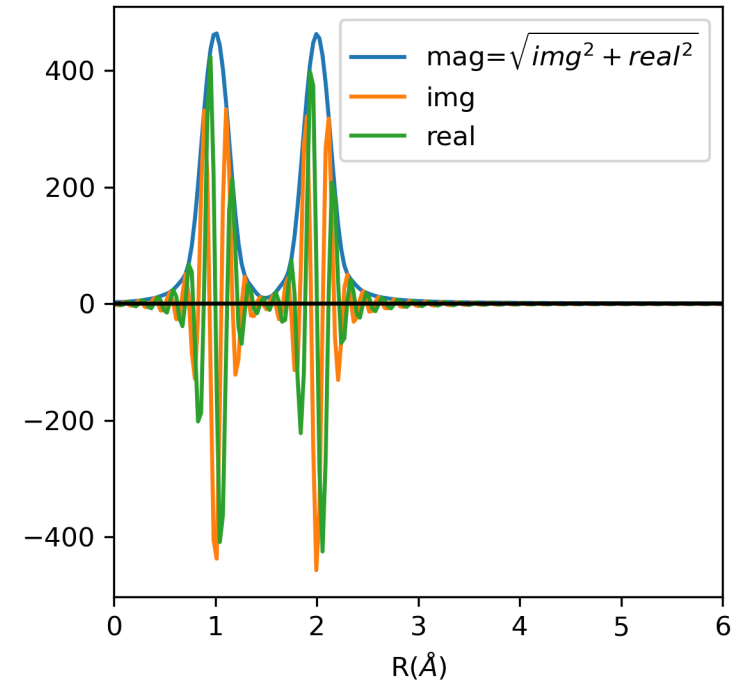
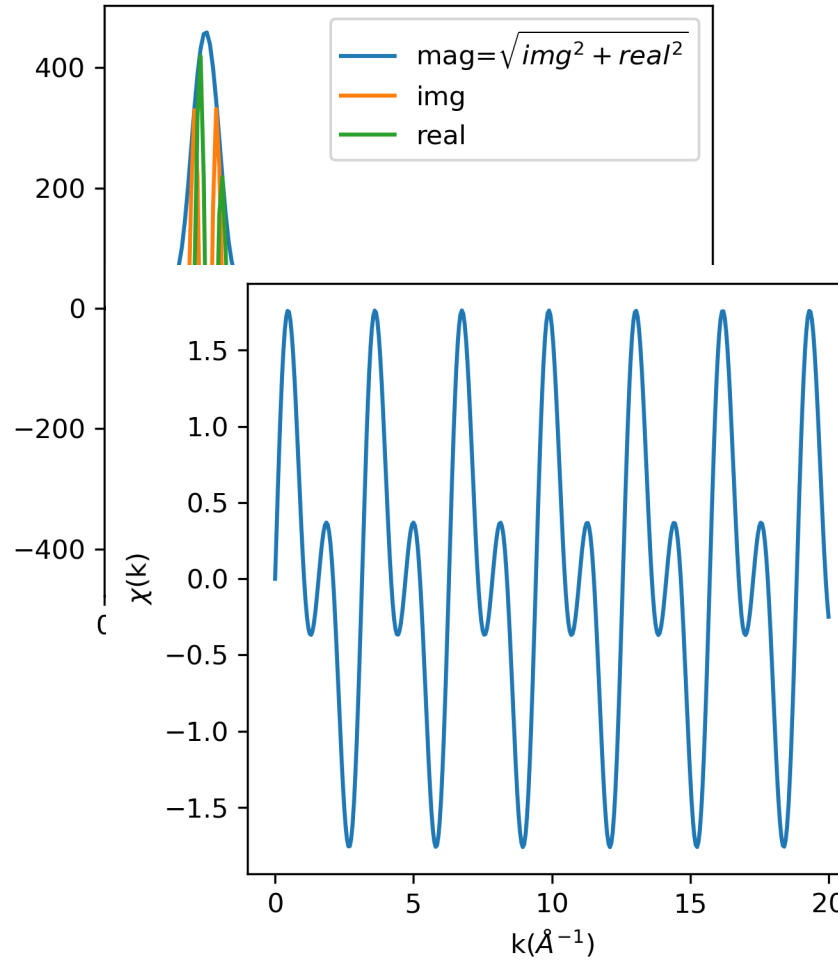
FT of a sine wave with phase $2k$

$$\chi(k) = \sin(2k)$$

Fourier Transform

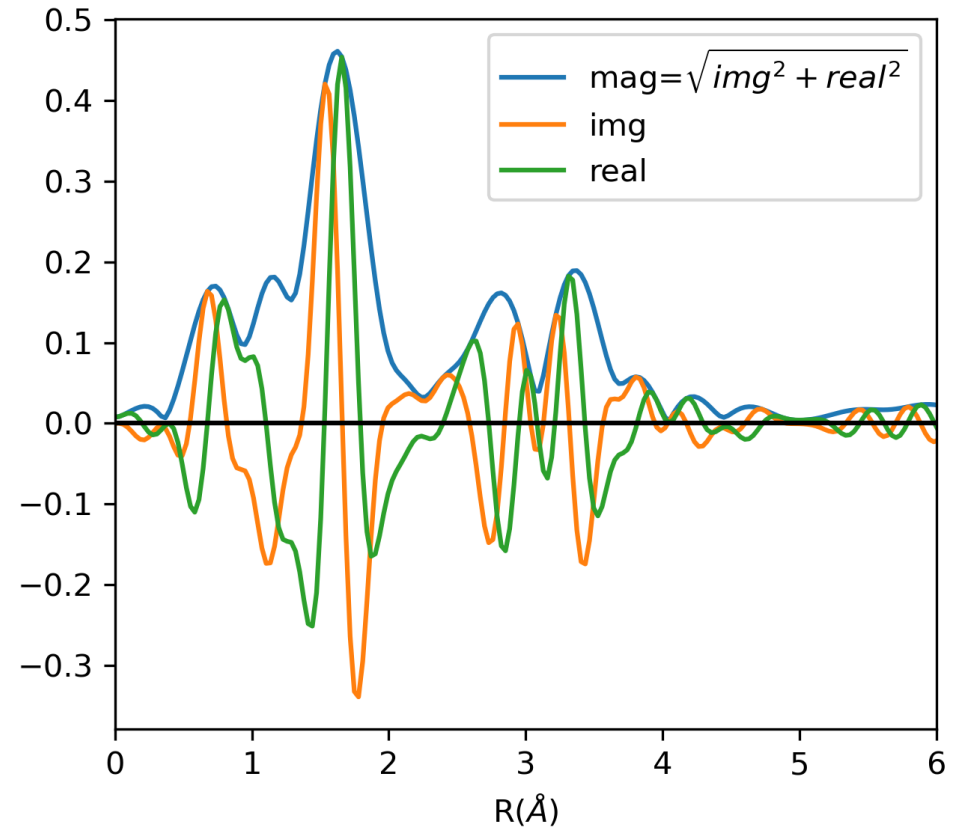
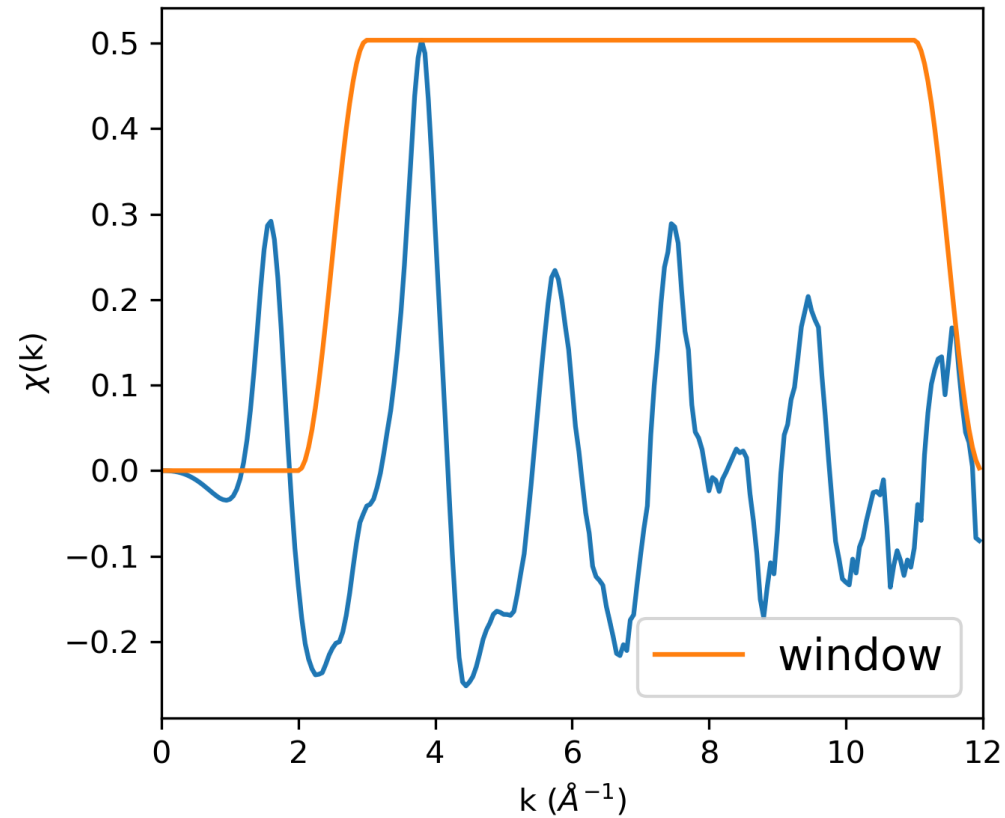


FT of a sine wave with phase $2k$
 $\chi(k) = \sin(2k)$



FT of two sine waves
 $\chi(k) = \sin(2k) + \sin(4k)$

Fourier Transform of PtO₂



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