



# Data reduction and background removal

Akhil Tayal

10-10-2023



@BrookhavenLab

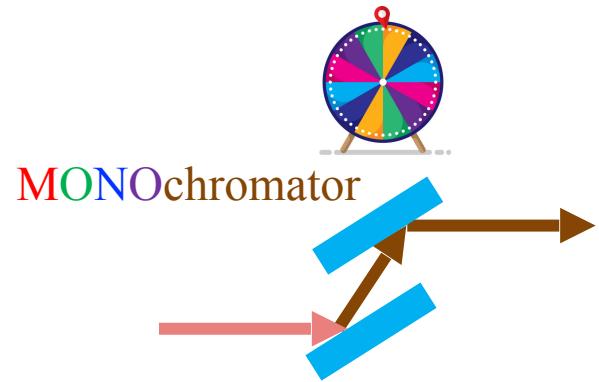
# XAFS books

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

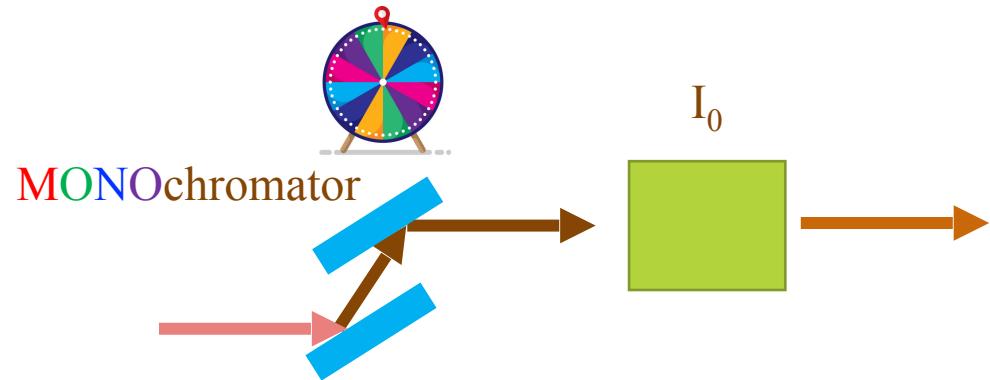
EXAFS: Basic Principles and Data Analysis  
Dr. Boon K. Teo

XAFS for Everyone  
Scott Calvin

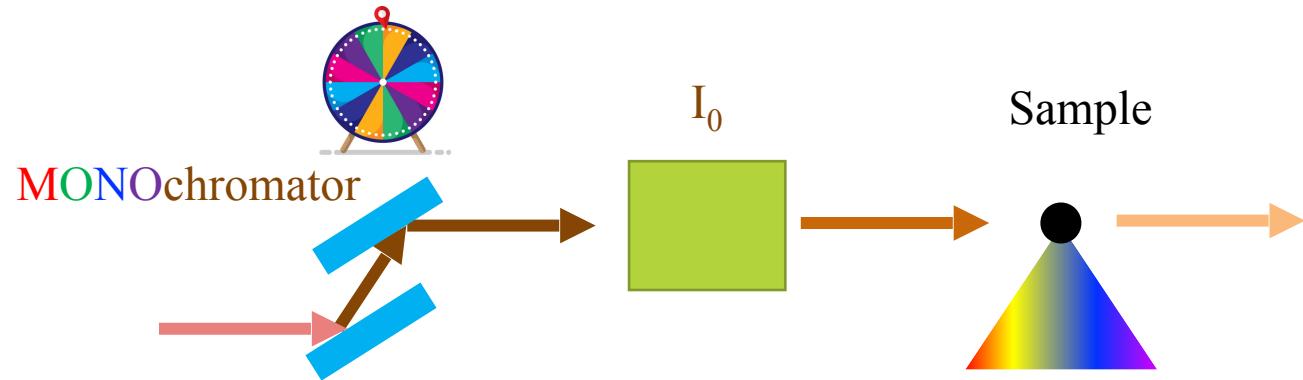
# Data collection



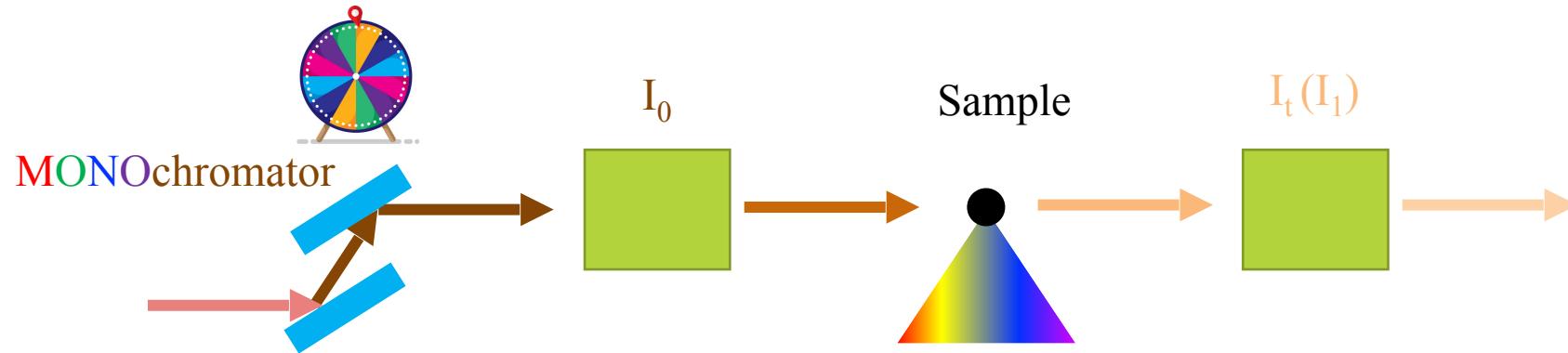
# Data collection



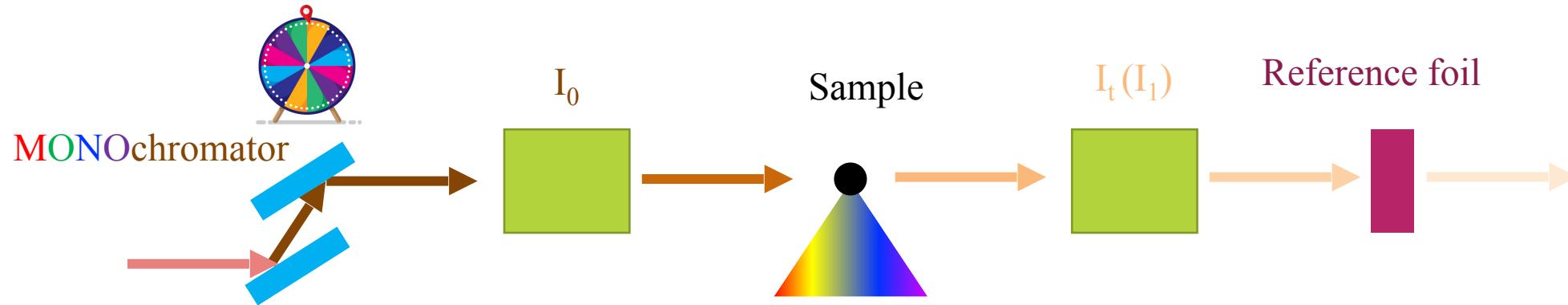
# Data collection



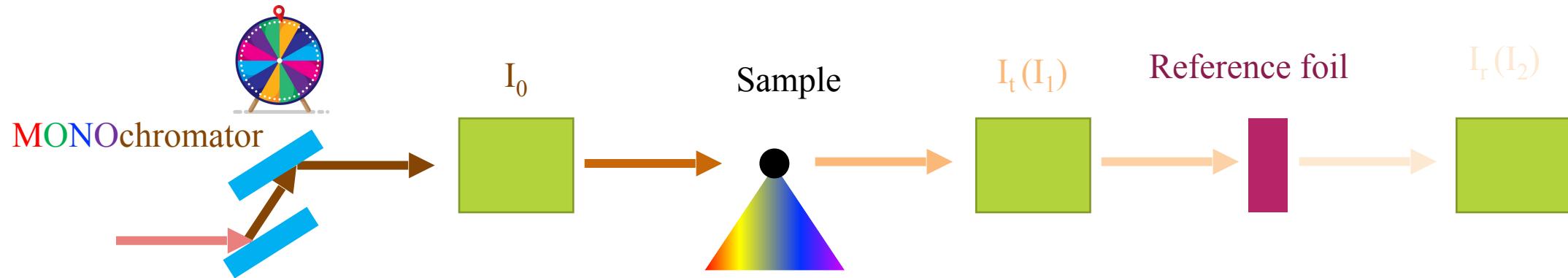
# Data collection



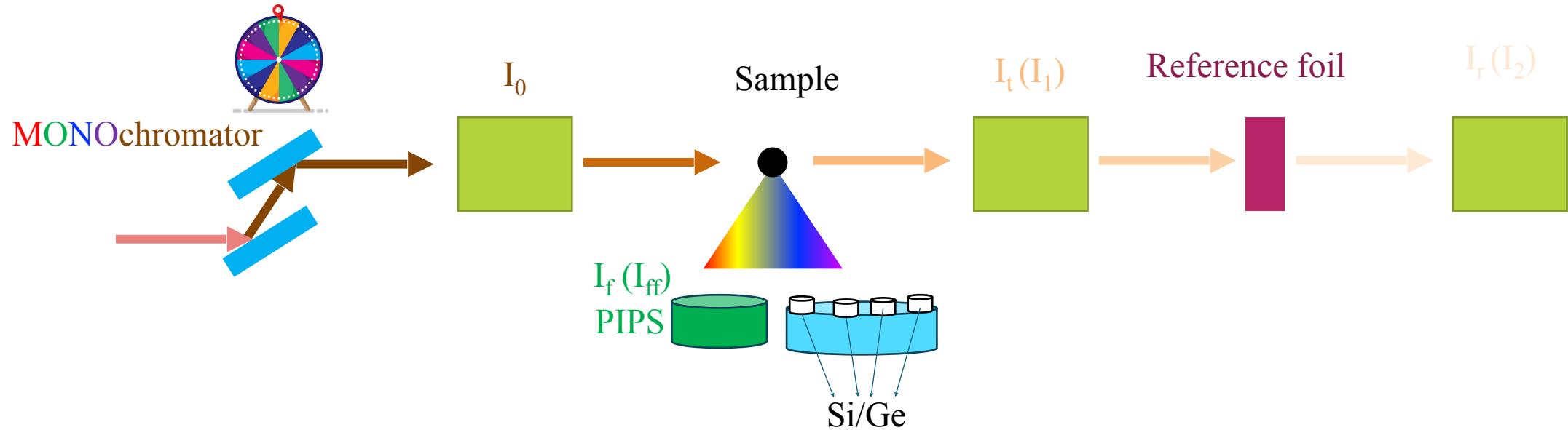
# Data collection



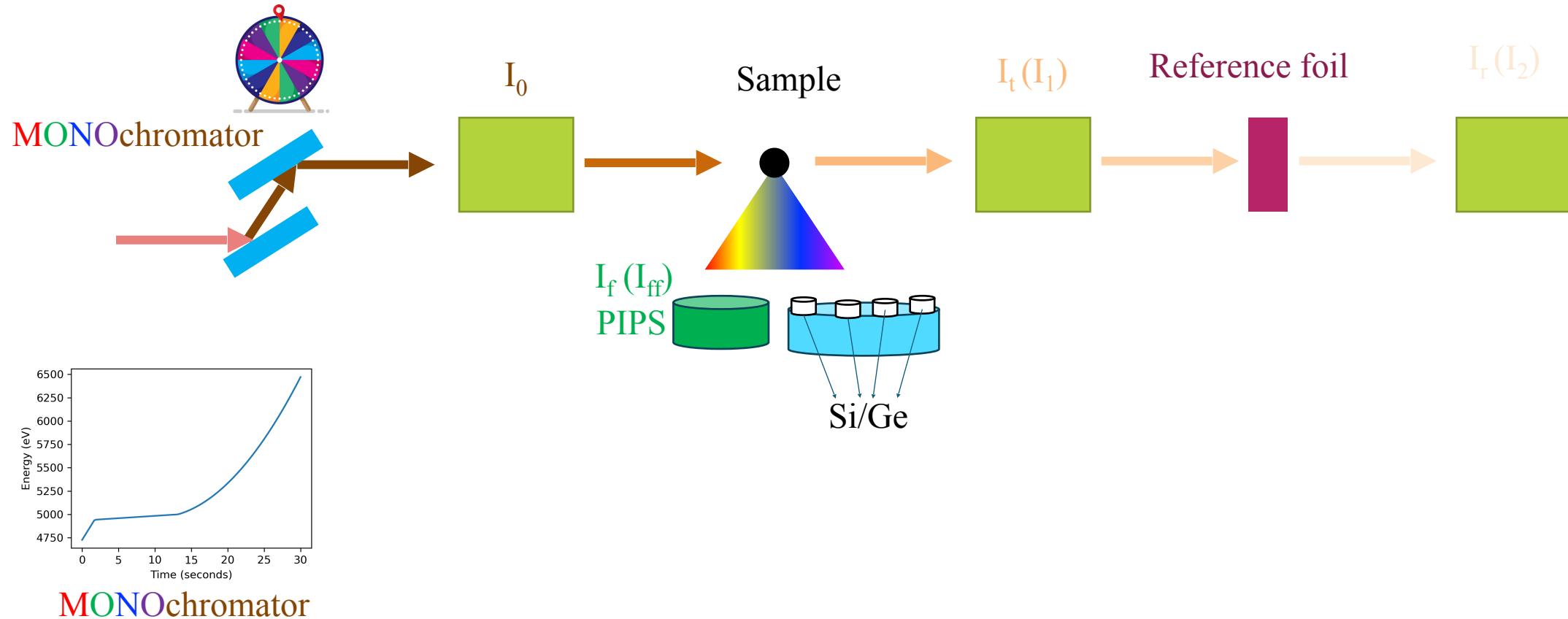
# Data collection



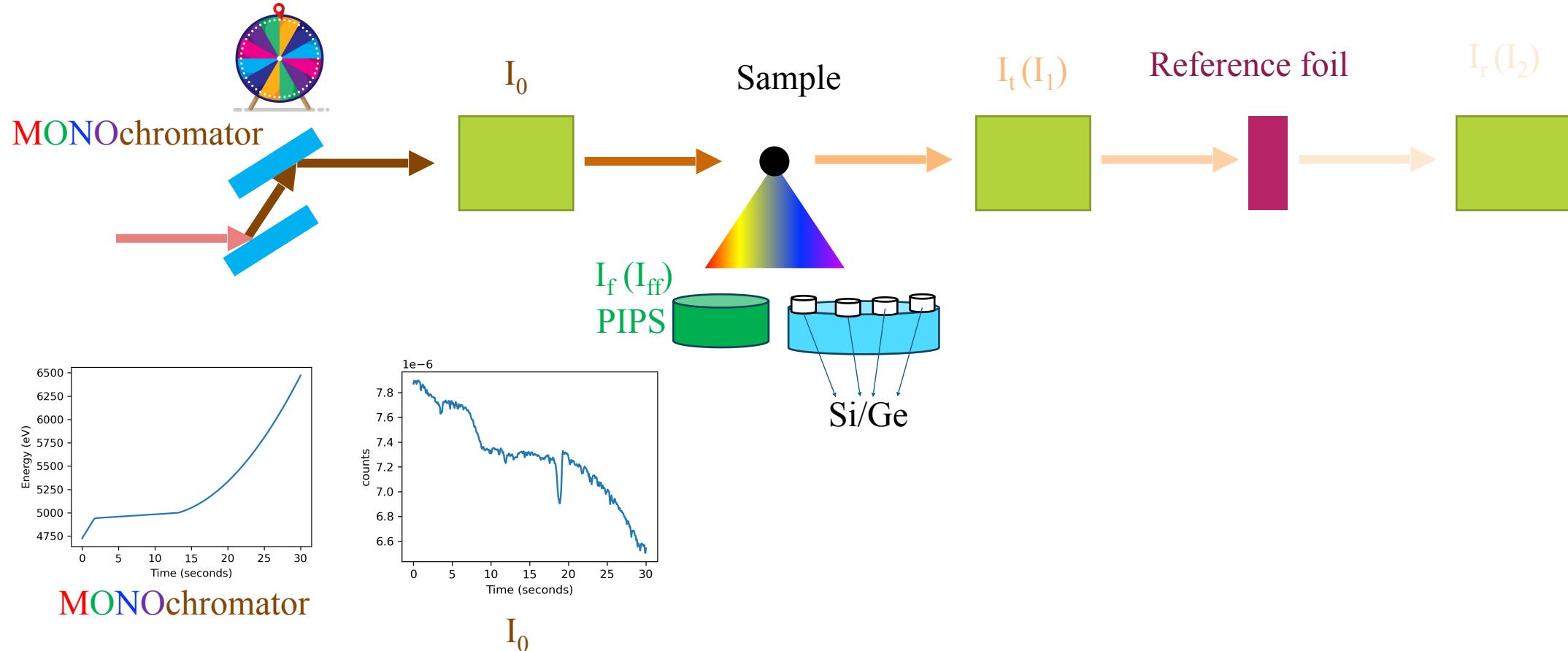
# Data collection



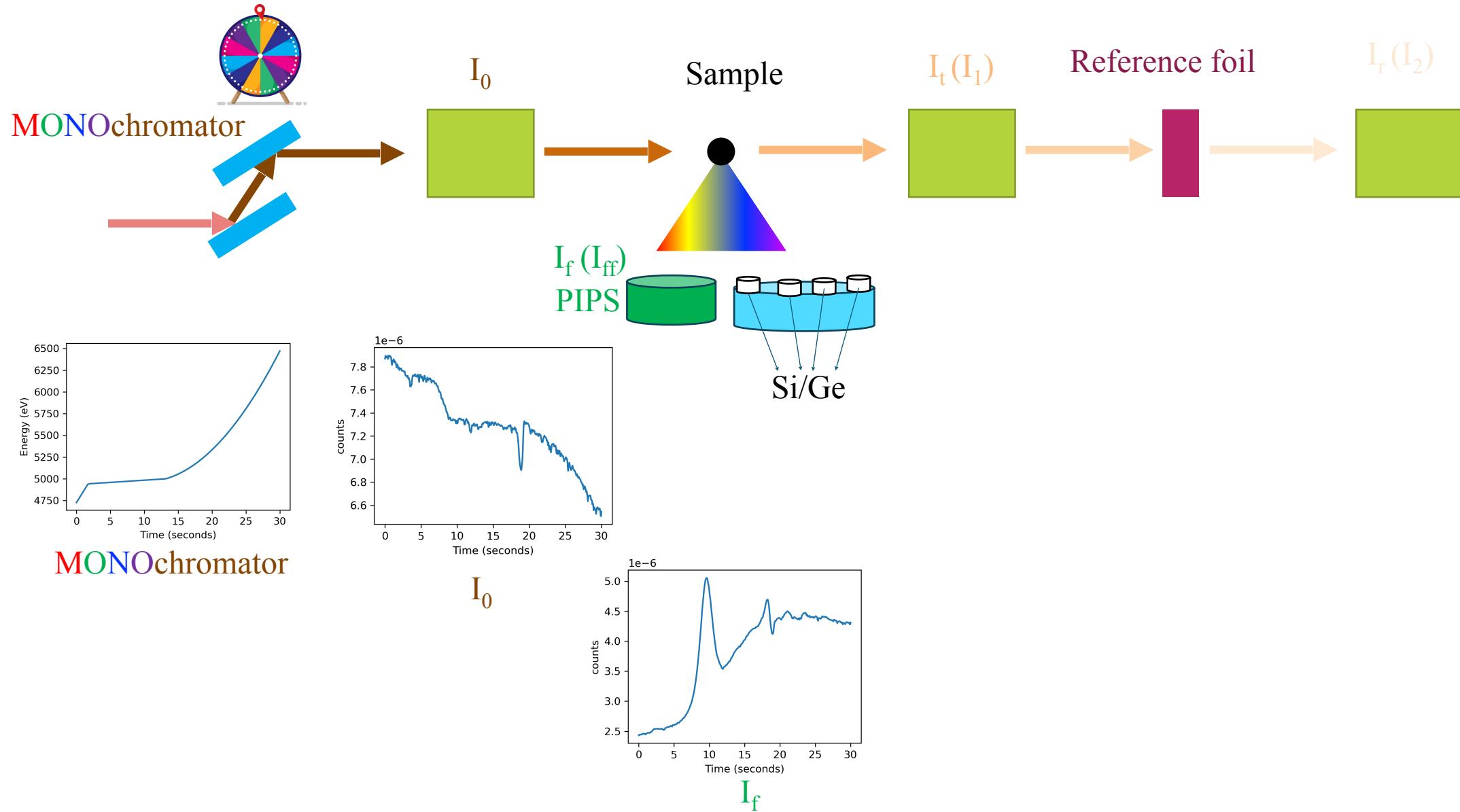
# Data collection



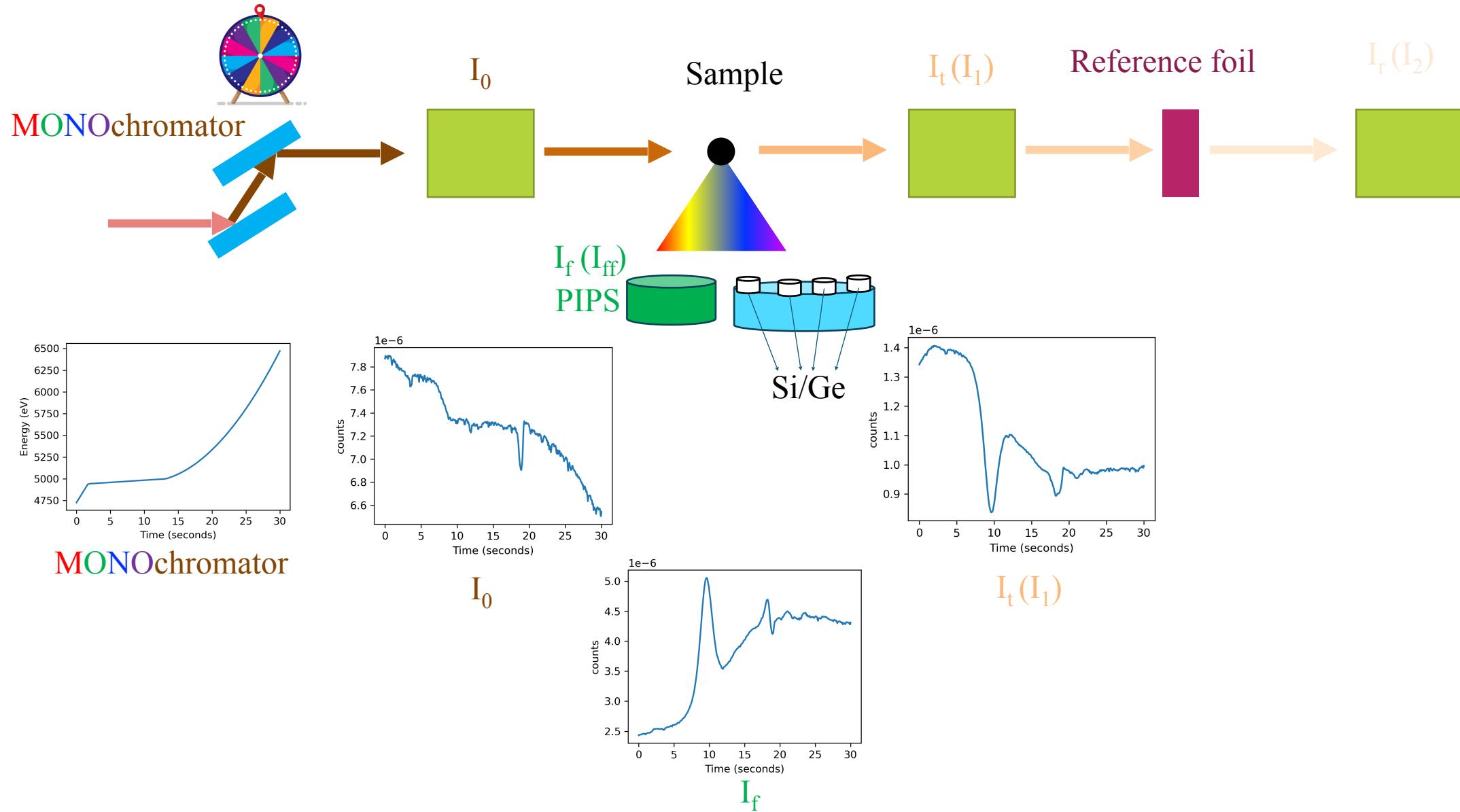
# Data collection



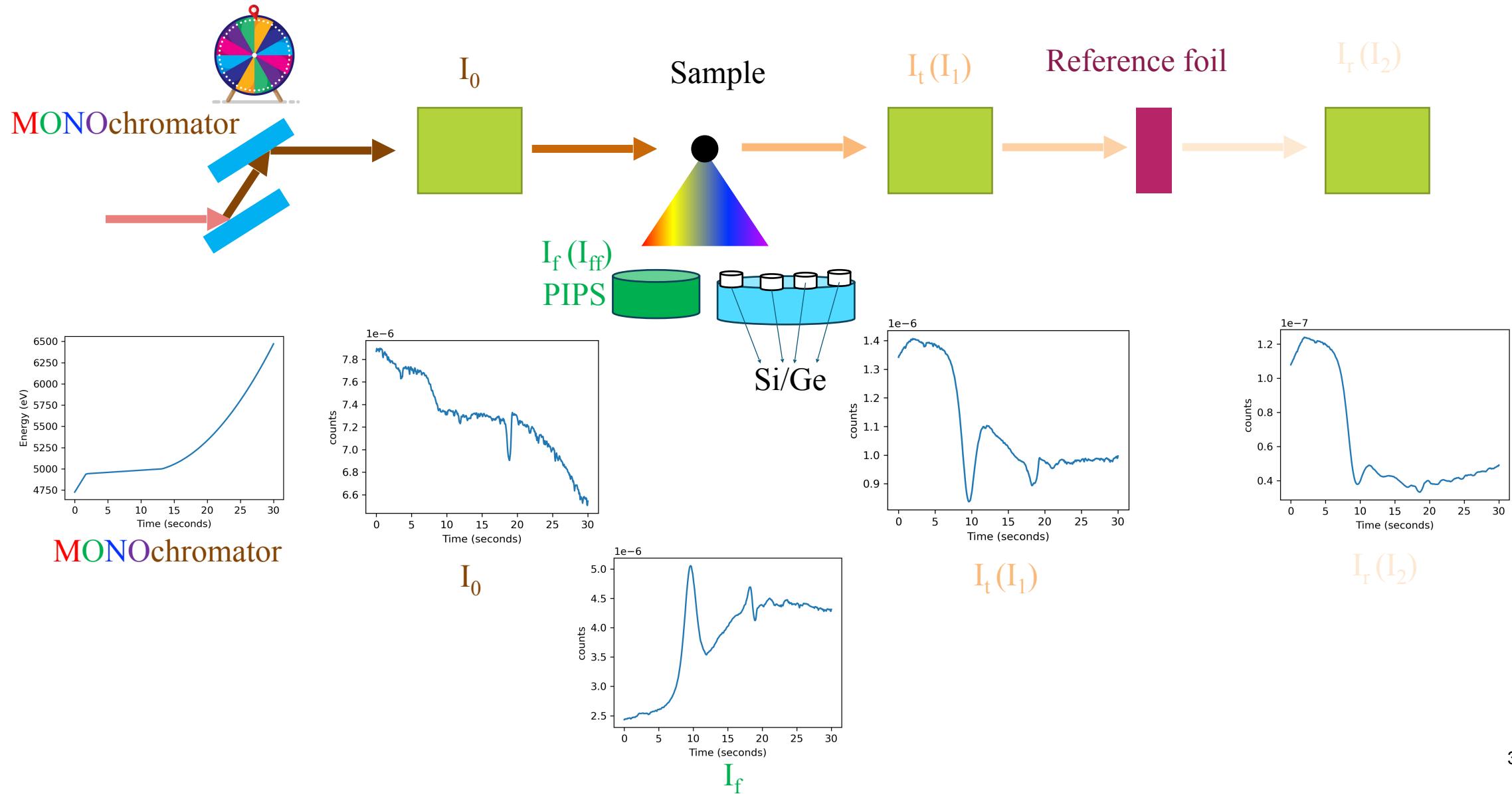
# Data collection



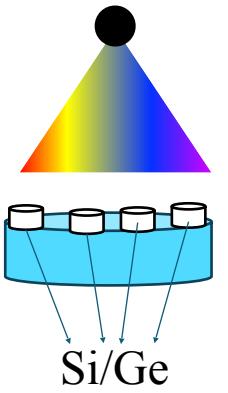
# Data collection



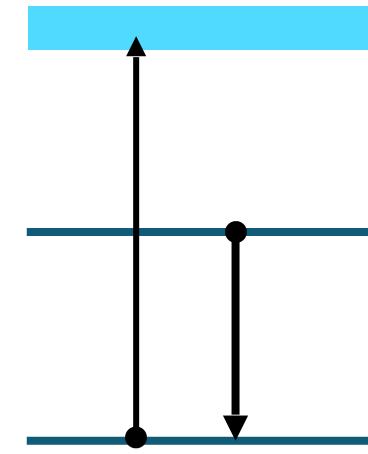
# Data collection



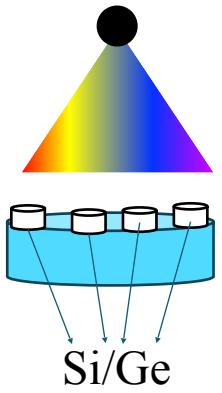
# Si/Ge detector data



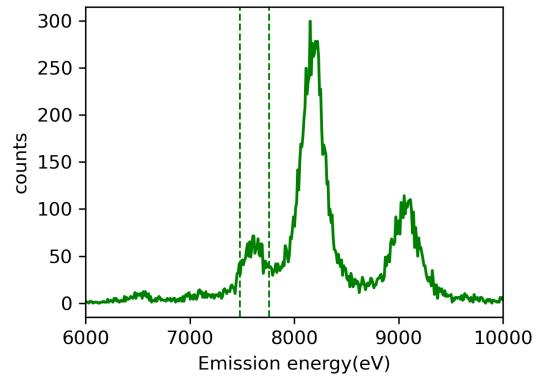
Energy Level



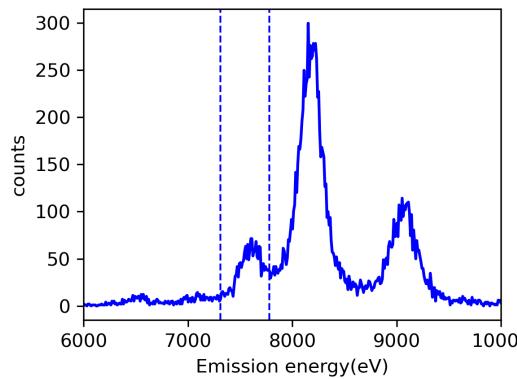
# Si/Ge detector data



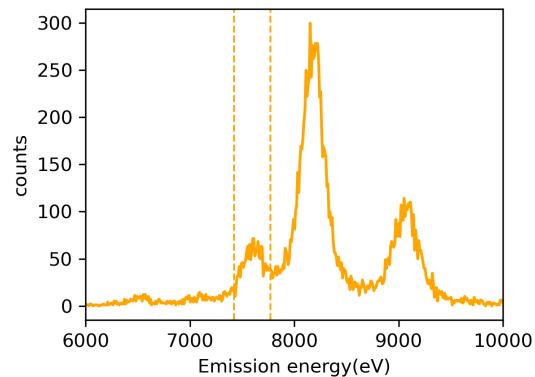
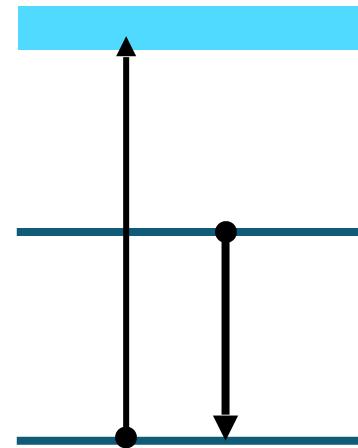
Channel 1



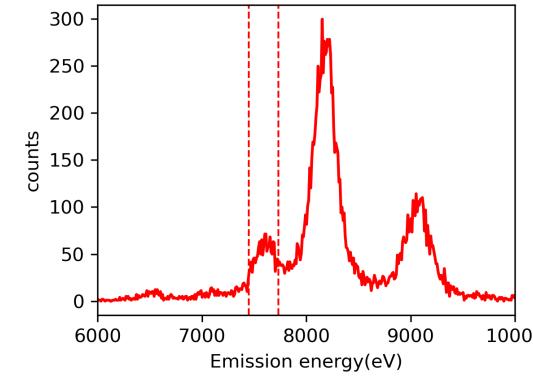
Channel 2



Energy Level

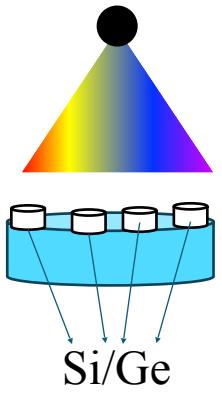


Channel 3

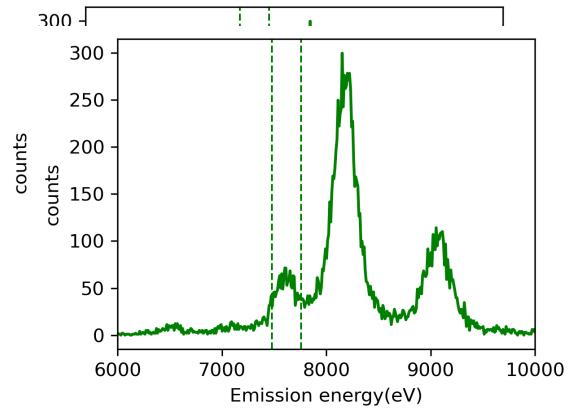


Channel 4

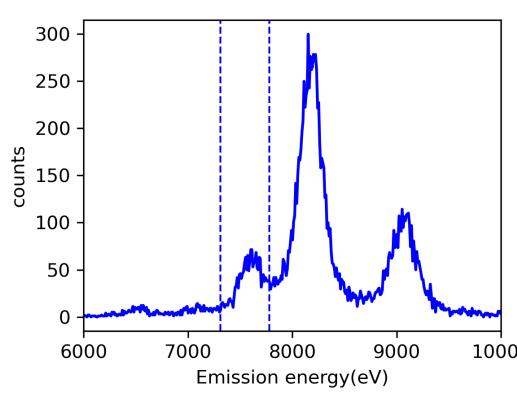
# Si/Ge detector data



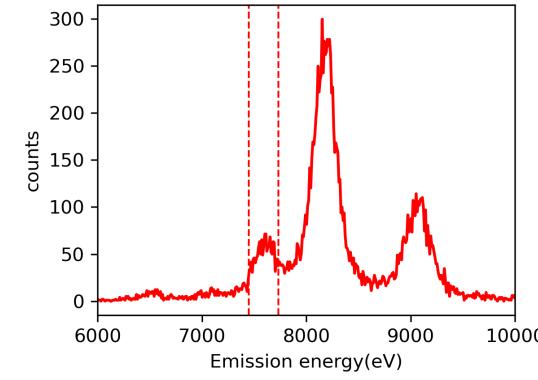
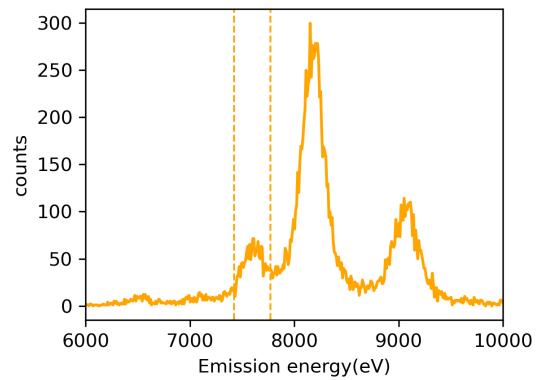
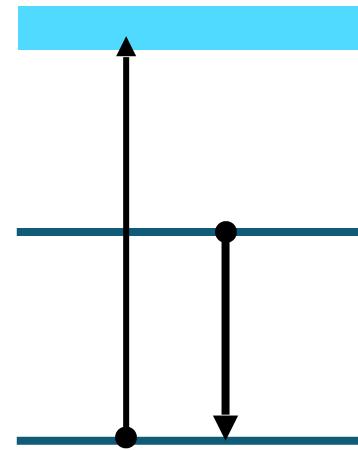
Channel 1



Channel 2



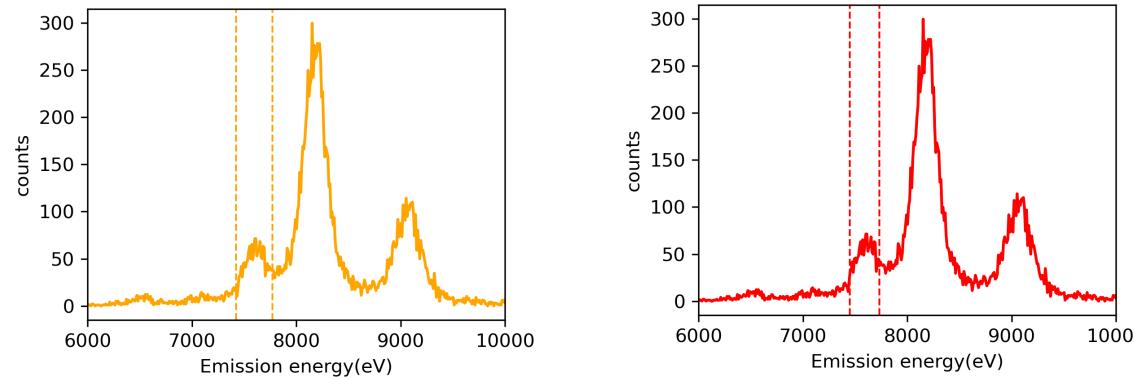
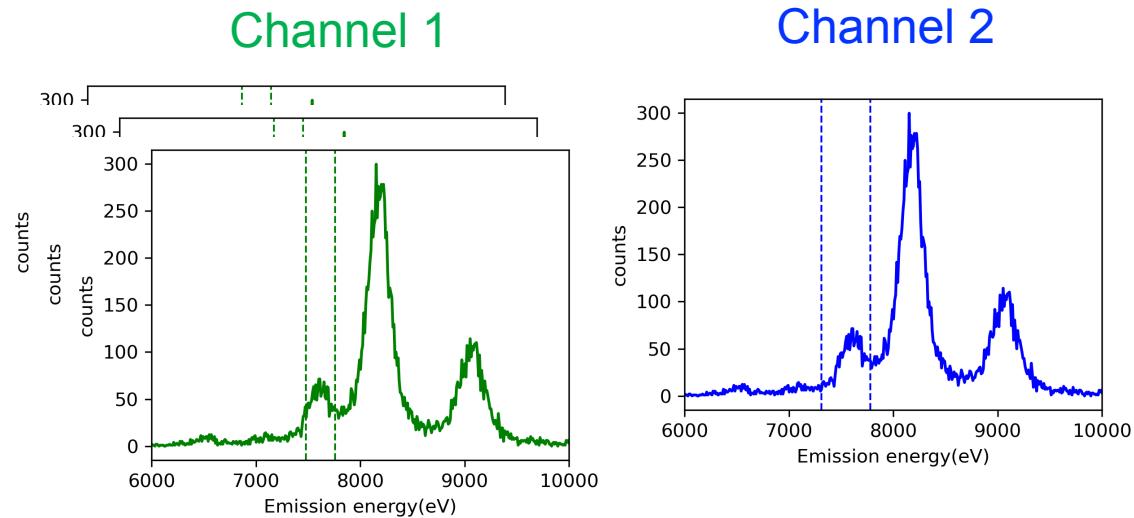
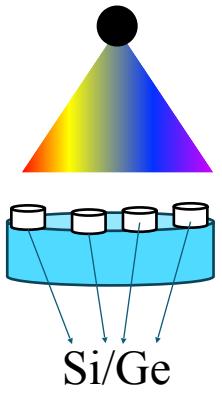
Energy Level



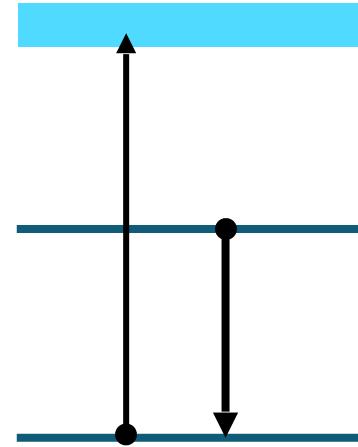
Channel 3

Channel 4

# Si/Ge detector data



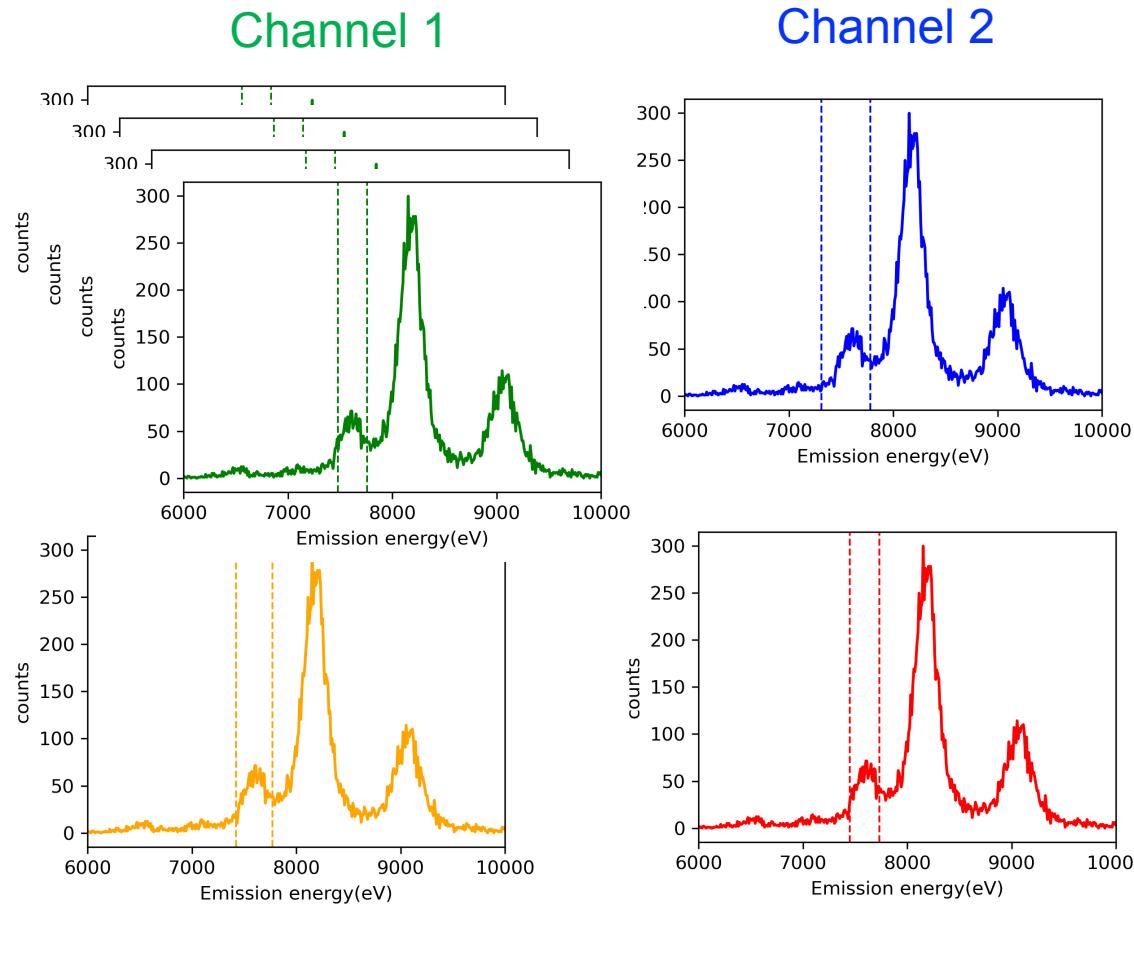
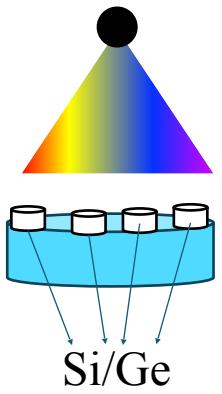
Energy Level



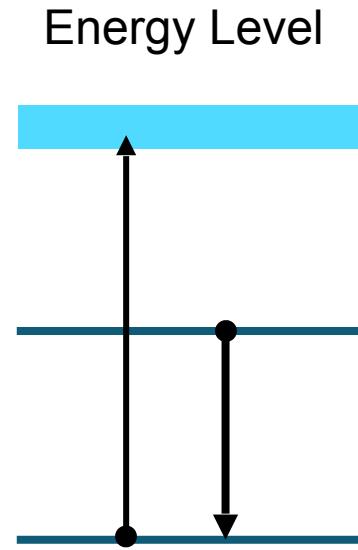
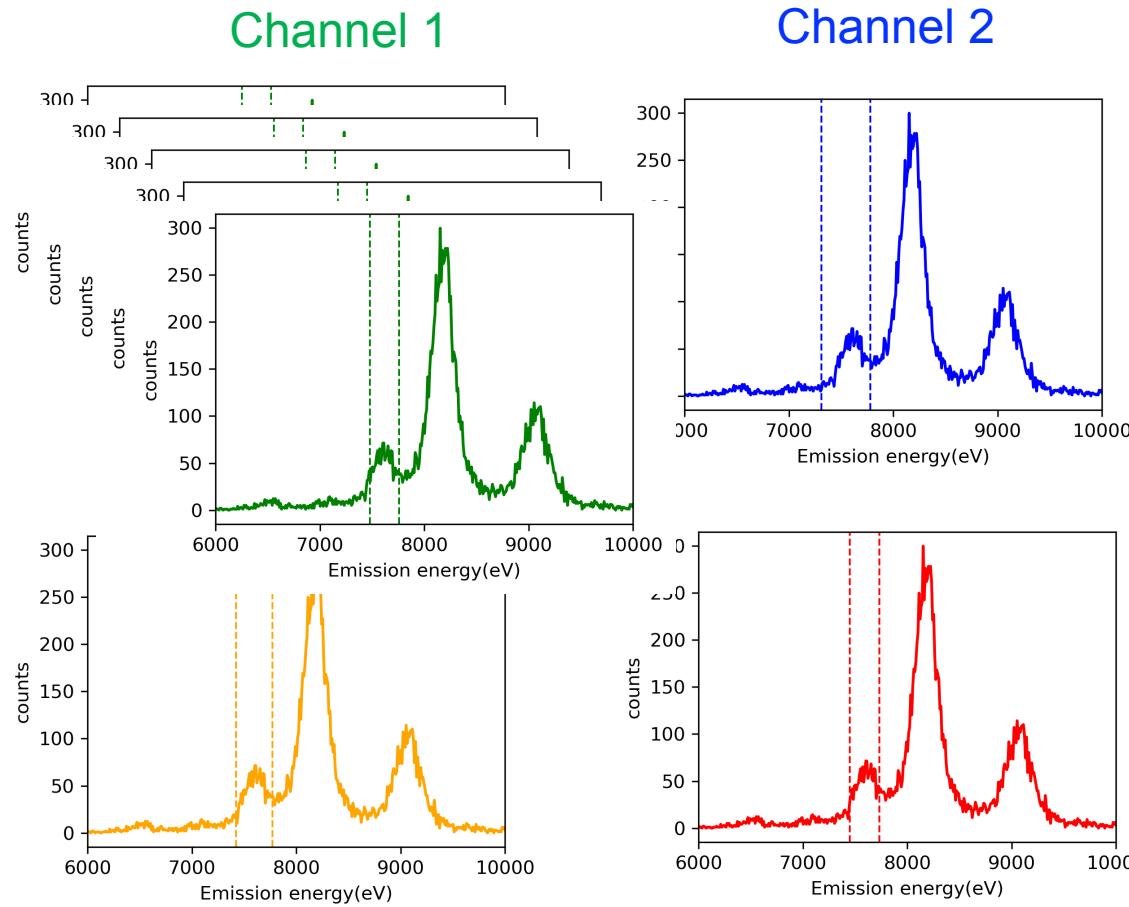
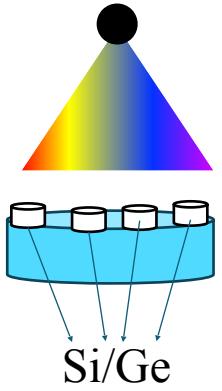
Channel 3

Channel 4

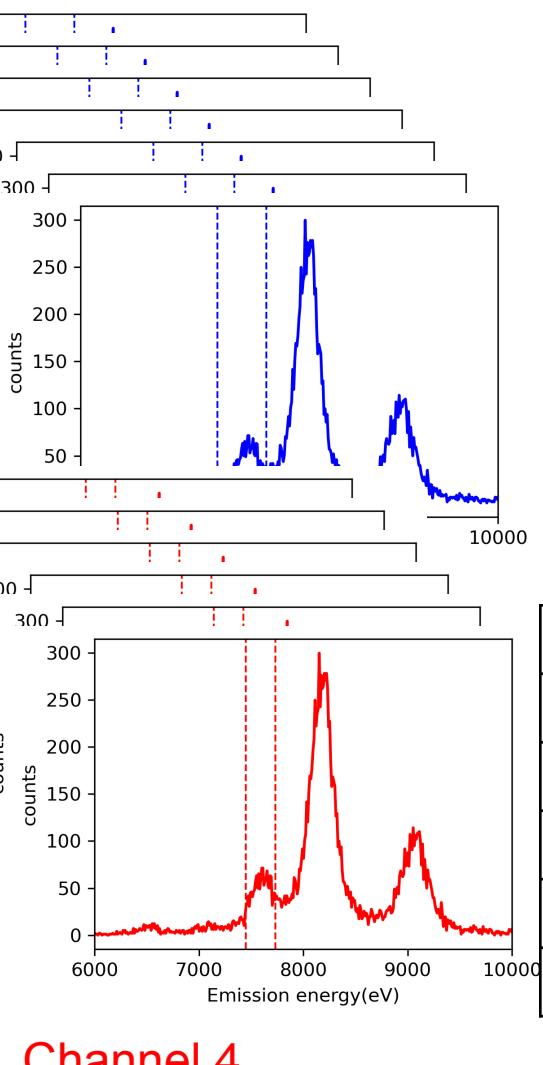
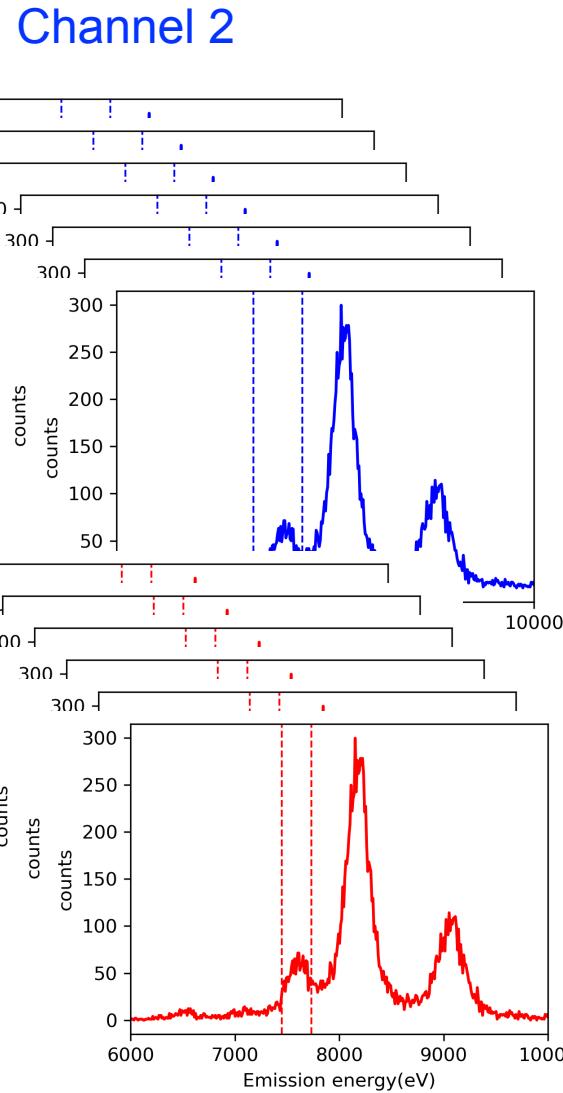
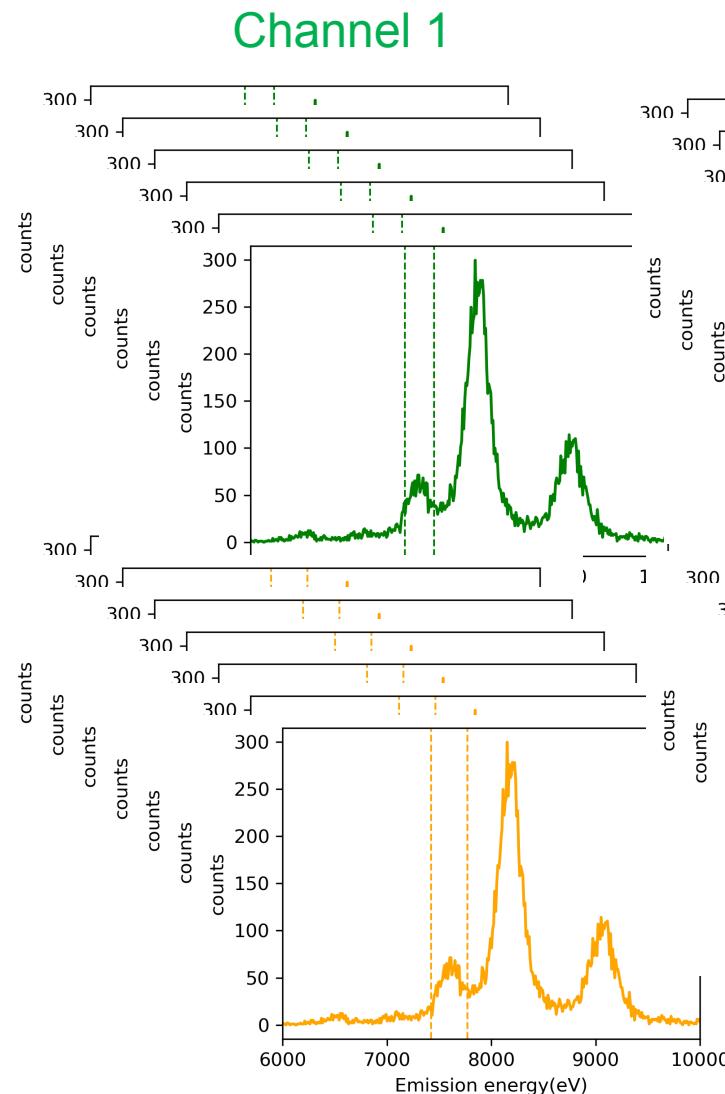
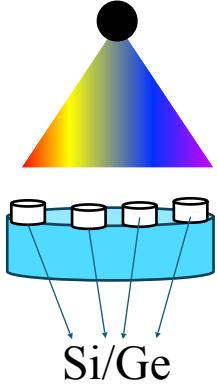
# Si/Ge detector data



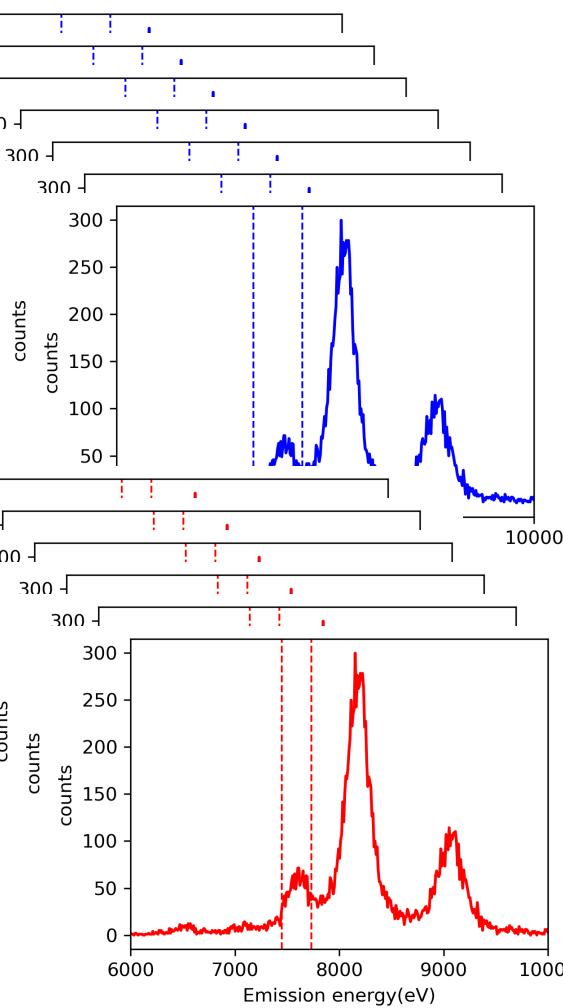
# Si/Ge detector data



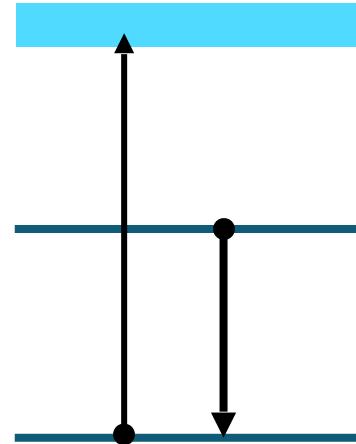
# Si/Ge detector data



**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

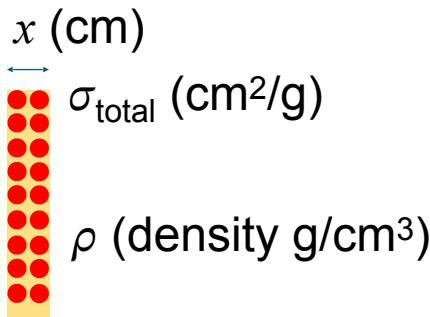
# Facility.name: NSLS-II
# Facility.mode: Beam available
# Facility.current: 399.7092291335699
# Facility.current: 3 GeV
# Facility.year: 2023
# Facility.cycle: 3
# Facility.GUP: 313873
# Facility.SAF: 312125
# Experimenter.name: Akhil Tayal
# Beamline.name: ISS (8-ID)
# Beamline.x-ray_source: damping 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: {'Xpress3': {'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.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”  $\sigma$  ( $\text{cm}^2$ )

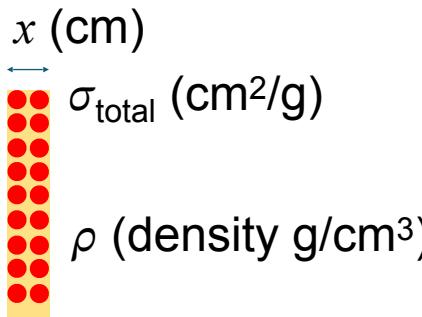
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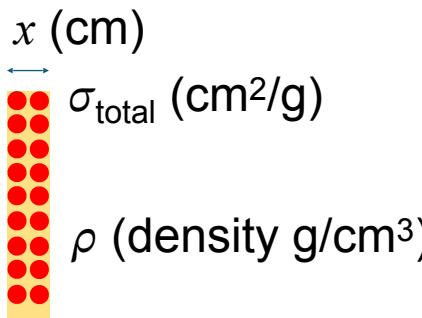
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Probability of absorption =  $x\rho\sigma_{\text{total}} = x\mu$  ( $\mu$  is linear absorption coefficient)

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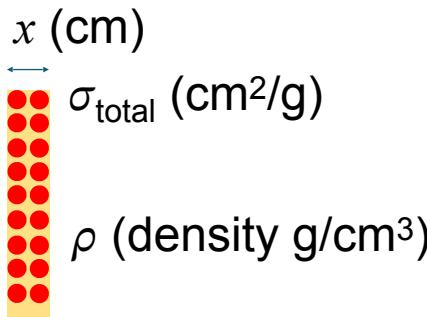
Probability of absorption =  $x\rho\sigma_{\text{total}} = x\mu$  ( $\mu$  is linear absorption coefficient)

Bouguer's Law:

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

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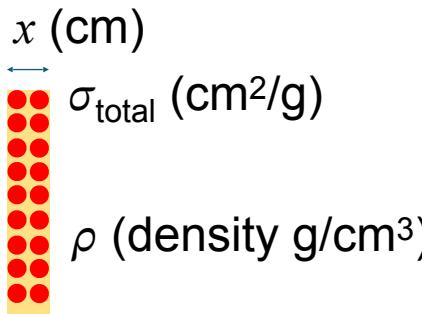
$$I_t = I_0 e^{-\mu x}$$

Absorption coefficient for transmission

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

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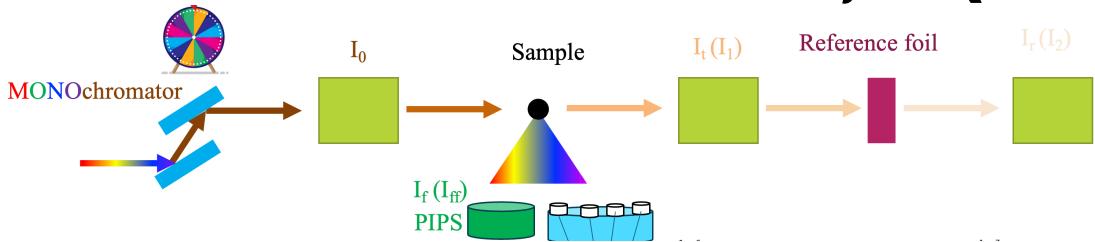
Absorption coefficient for transmission

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

Absorption coefficient for fluorescence

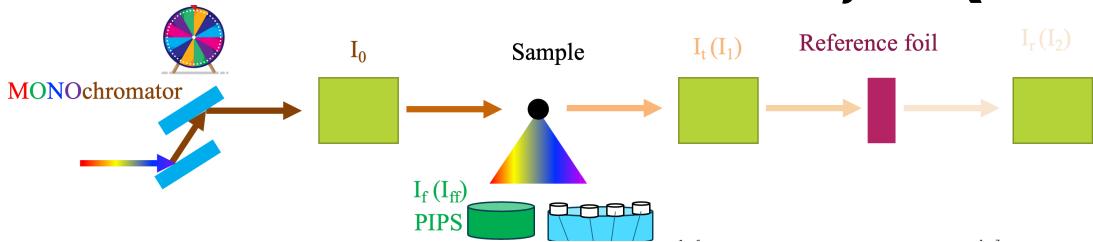
$$\mu x = \left(\frac{I_f}{I_0}\right)$$

# Calculation of $\mu$ (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 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
```

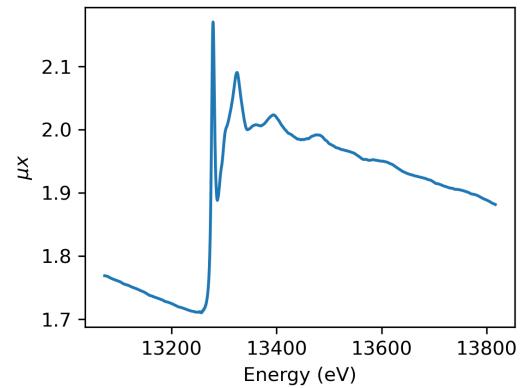
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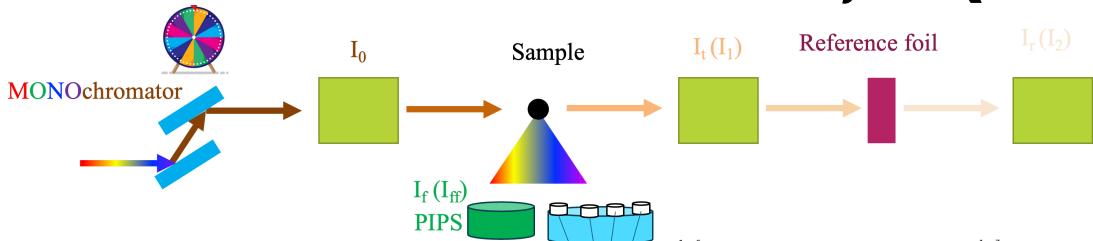
```
# energy      i0          it          ir          iff         xs_roi01    xs_ch01_roi01  xs_ch02_roi01  xs_ch03_roi01  xs_ch04_roi01
13073.000000 -3.972144e-06 -1.405205e-07 -1.108702e-08 -2.481562e-07 1.622849e-02 4.025056e-03 4.057912e-03 3.530254e-03 4.615269e-03
13078.000000 -3.987104e-06 -1.411195e-07 -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:

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



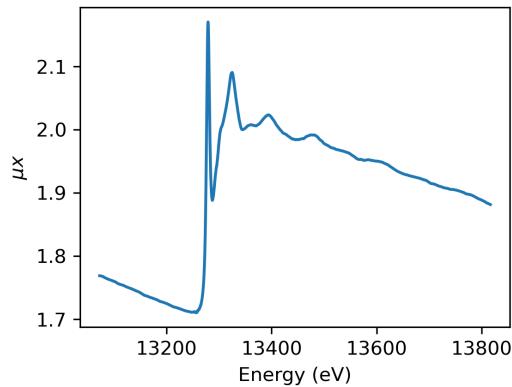
# Calculation of $\mu$ (absorption coefficient)



#	energy	$i0$	$it$	$ir$	$iff$	$xs\_roi01$	$xs\_ch01\_roi01$	$xs\_ch02\_roi01$	$xs\_ch03\_roi01$	$xs\_ch04\_roi01$
13073.00000	-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	
13078.00000	-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	
13083.00000	-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	
13088.00000	-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	
13093.00000	-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	
13098.00000	-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:

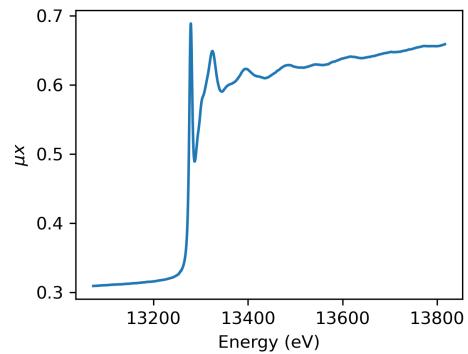
$$\mu_x = \log\left(\frac{i_0}{i_t}\right)$$



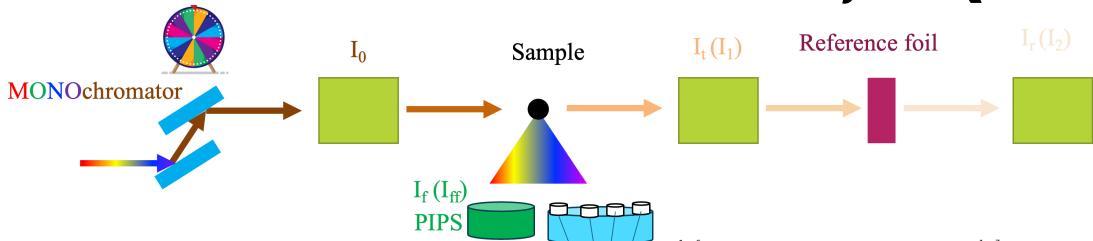
Absorption coefficient for sample fluorescence:

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

;  $\mu_x = \left( \frac{xs\_roi1}{i_0} \right)$



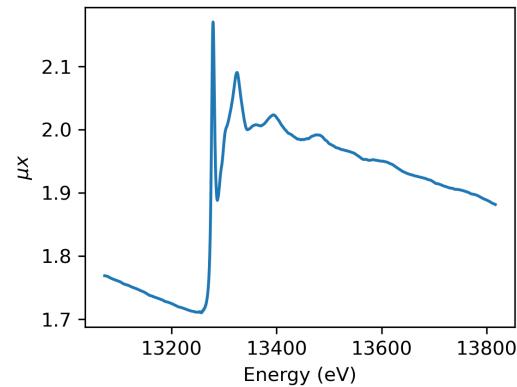
# Calculation of $\mu$ (absorption coefficient)



#	energy	$i0$	$it$	$ir$	$iff$	$xs\_roi01$	$xs\_ch01\_roi01$	$xs\_ch02\_roi01$	$xs\_ch03\_roi01$	$xs\_ch04\_roi01$
13073.	0.00000	-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.	0.00000	-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.	0.00000	-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.	0.00000	-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.	0.00000	-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.	0.00000	-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:

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

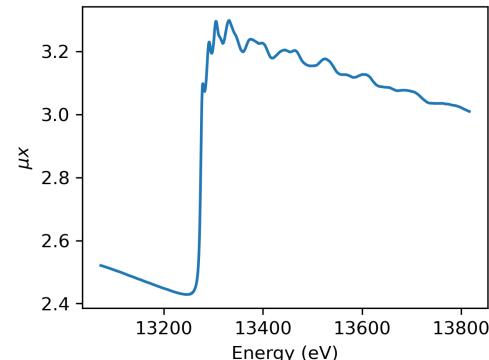


Absorption coefficient for sample fluorescence:

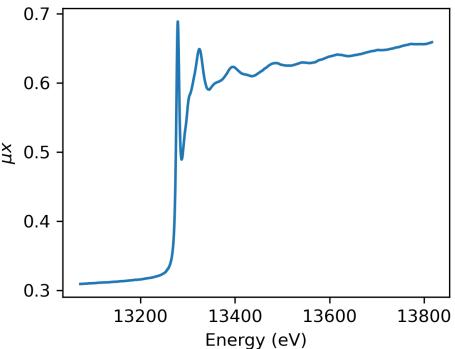
$$\mu_x = \left( \frac{i_{ff}}{i_0} \right)$$

$$; \quad \mu_x = \left( \frac{x_s\_roi1}{i_0} \right)$$

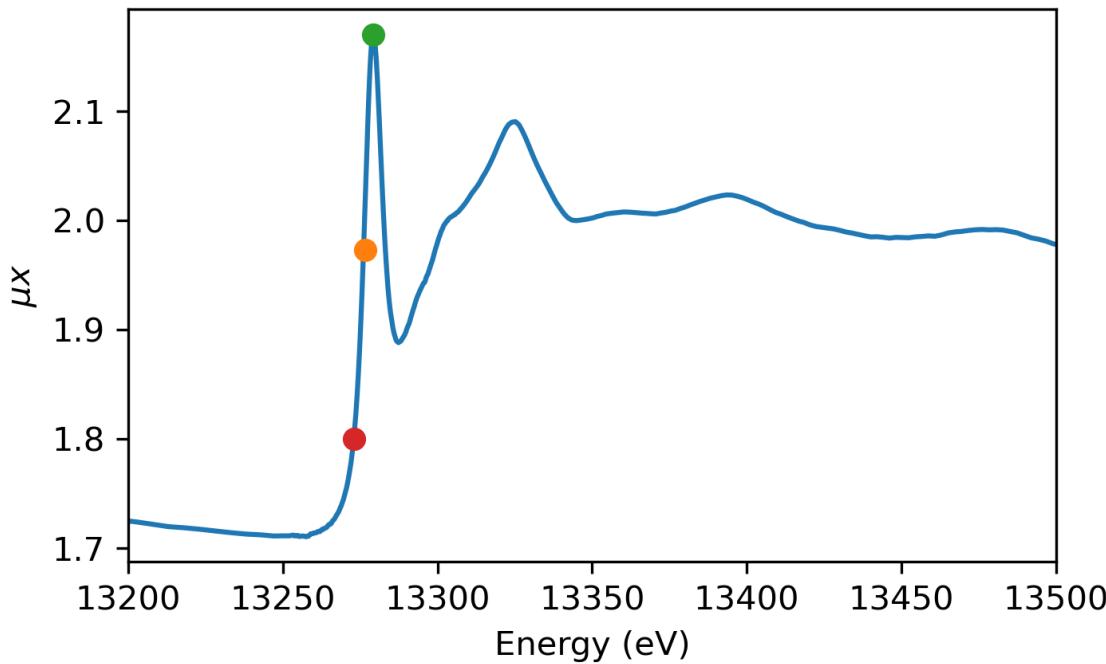
$$\mu_x = \log\left(\frac{i_r}{i_t}\right)$$



Absorption coefficient for reference transmission:



# $E_0$

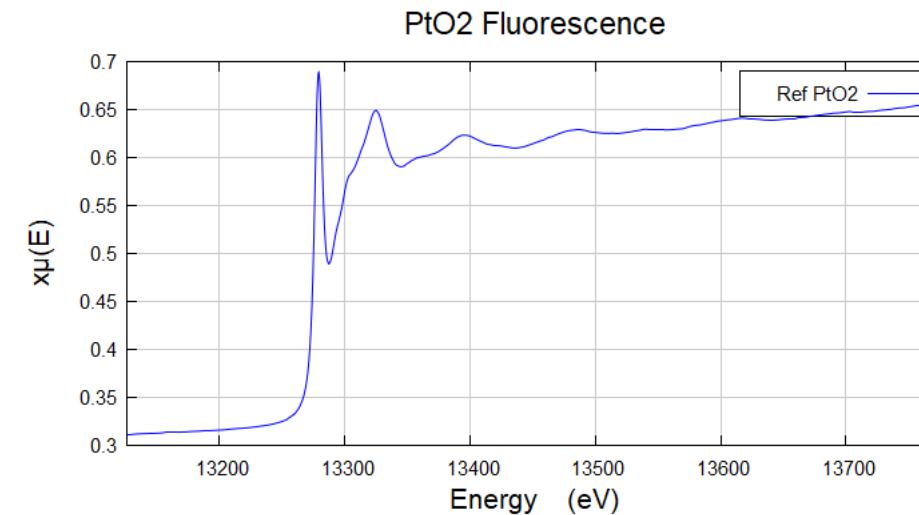
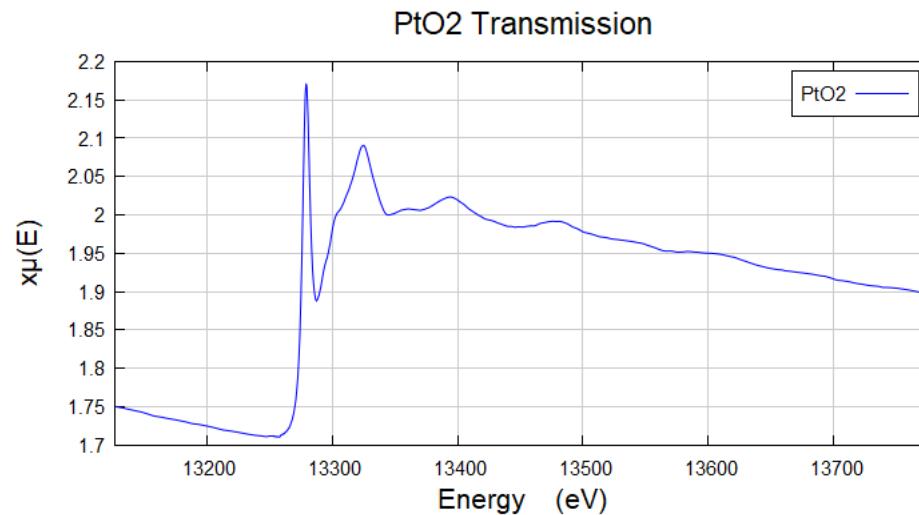


$E_0 = \text{White line}$

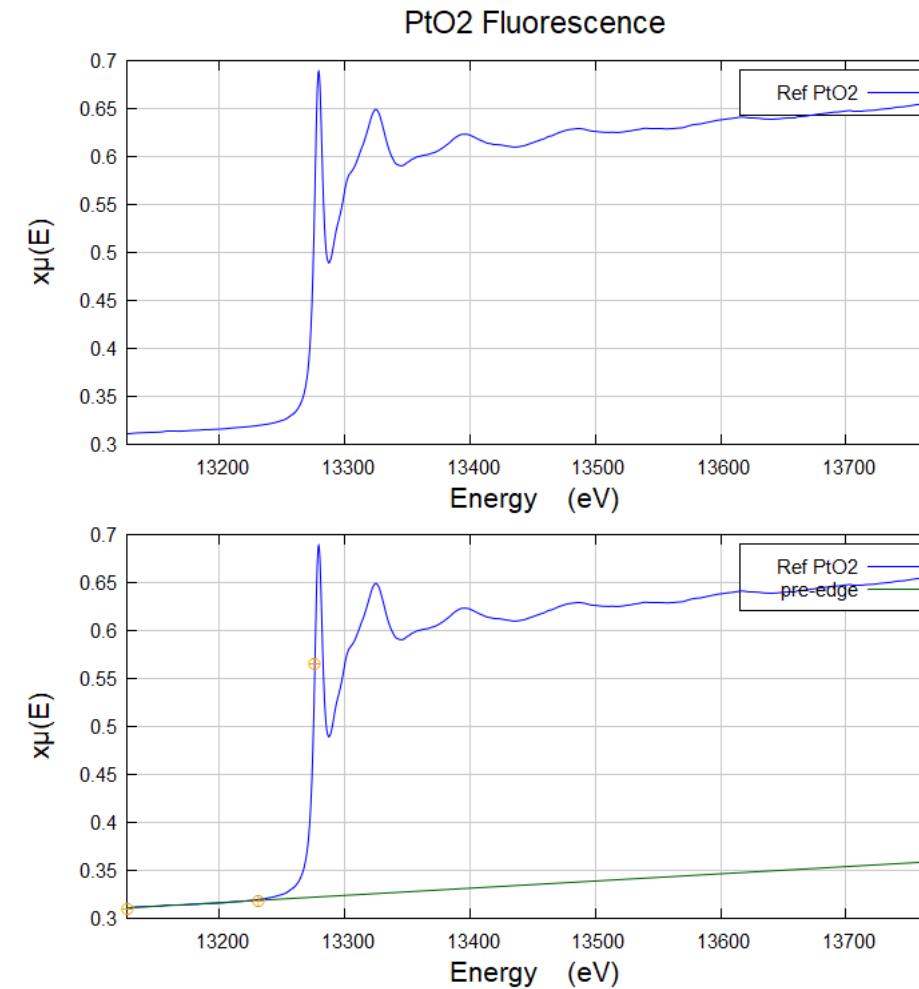
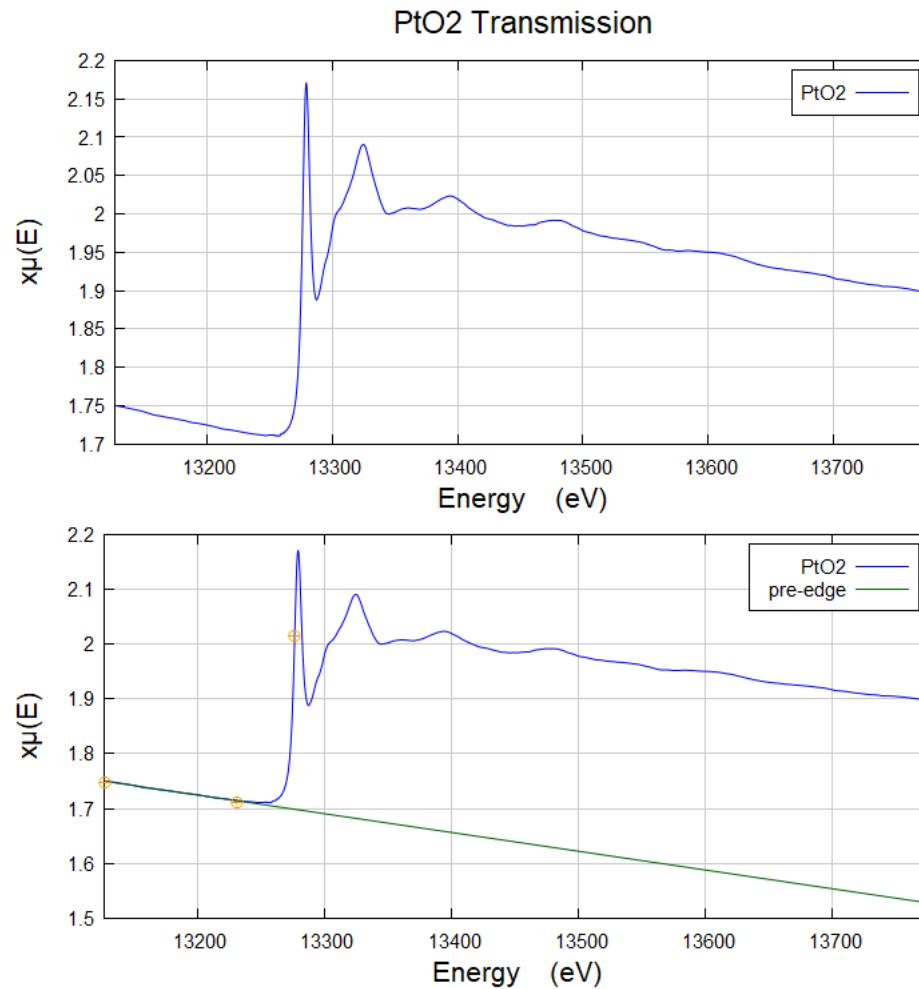
$E_0 = \text{first inflection point}$

$E_0 = \text{Tabulated value}$

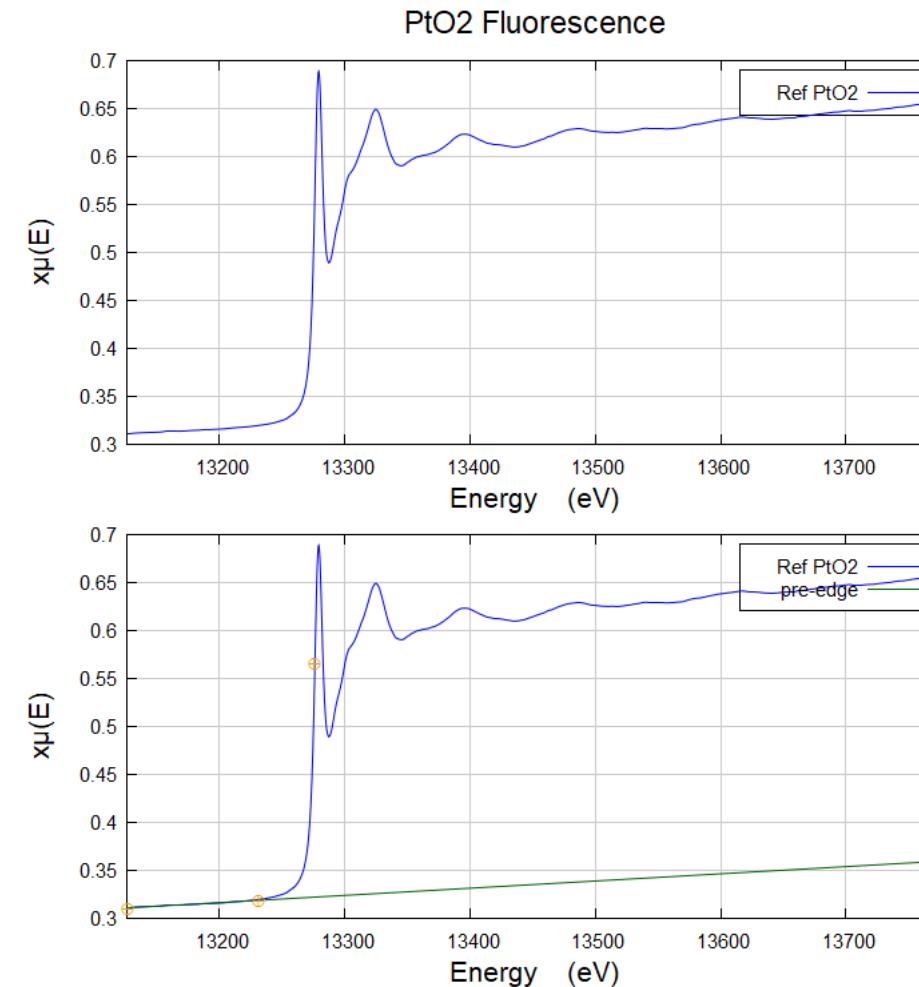
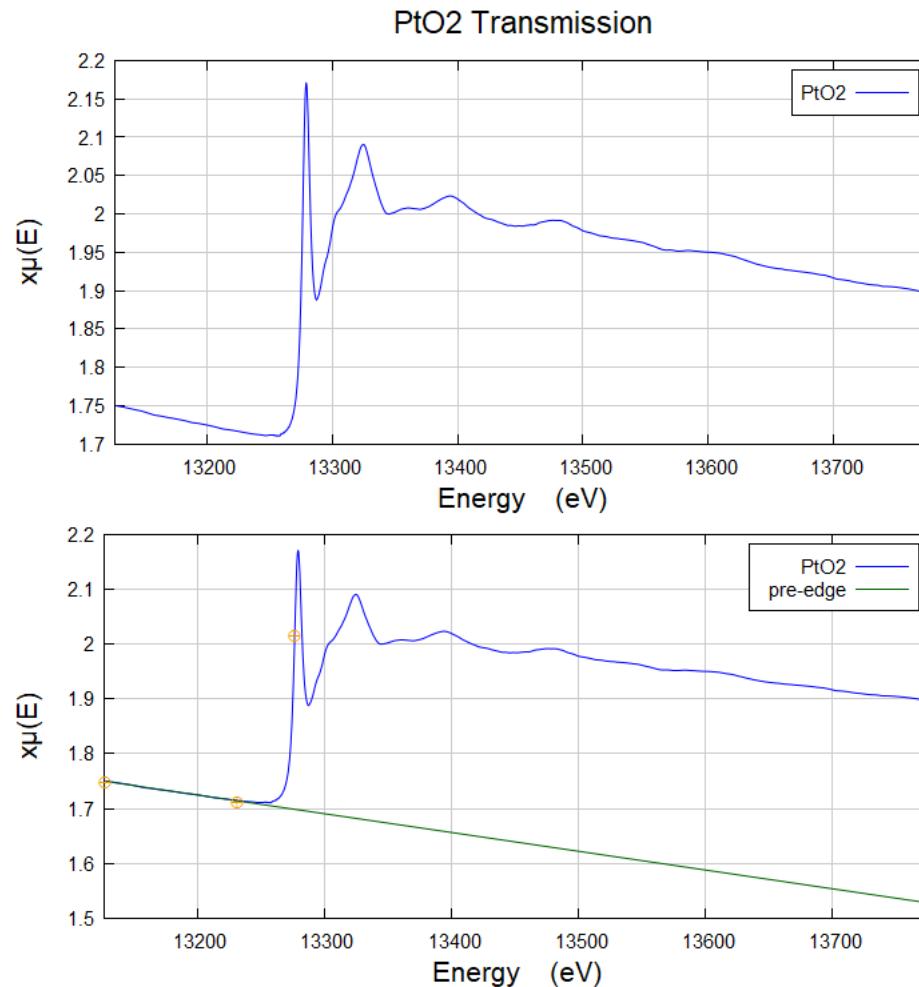
# Pre-edge & Post-edge normalization



# Pre-edge & Post-edge normalization



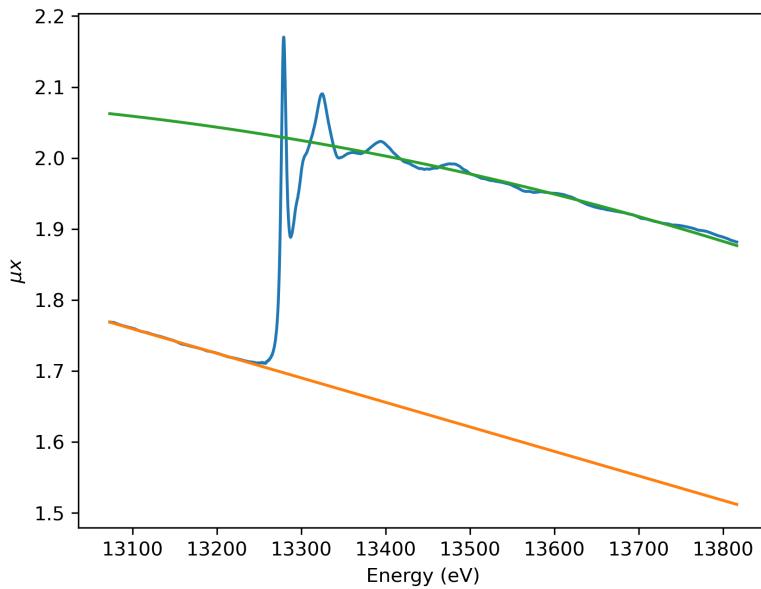
# Pre-edge & Post-edge normalization



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

# Pre-edge & Post-edge normalization

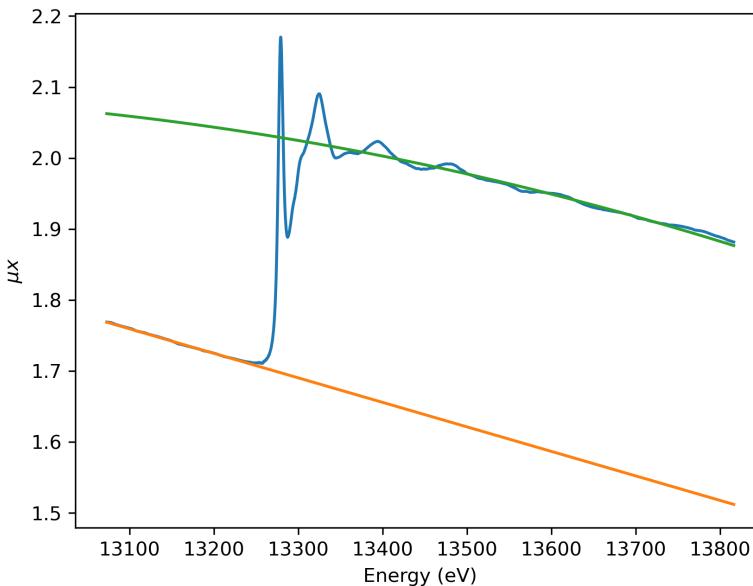
# Pre-edge & Post-edge normalization



Pre-edge background

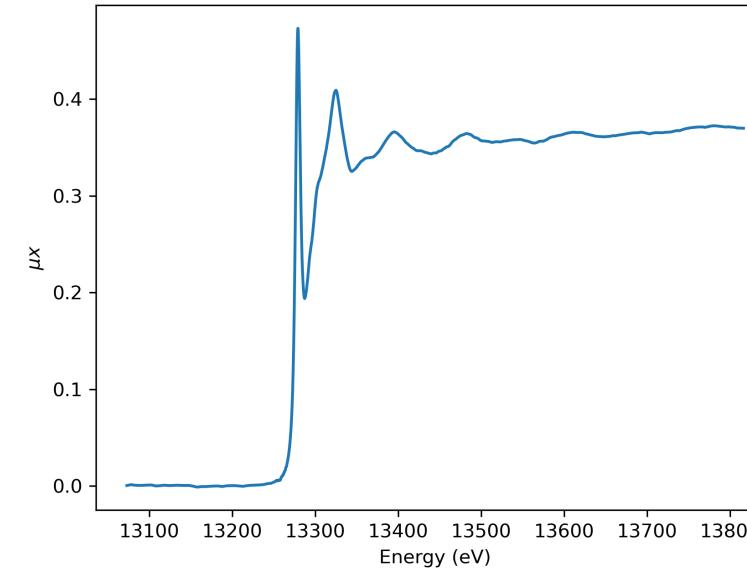
Post-edge background

# Pre-edge & Post-edge normalization



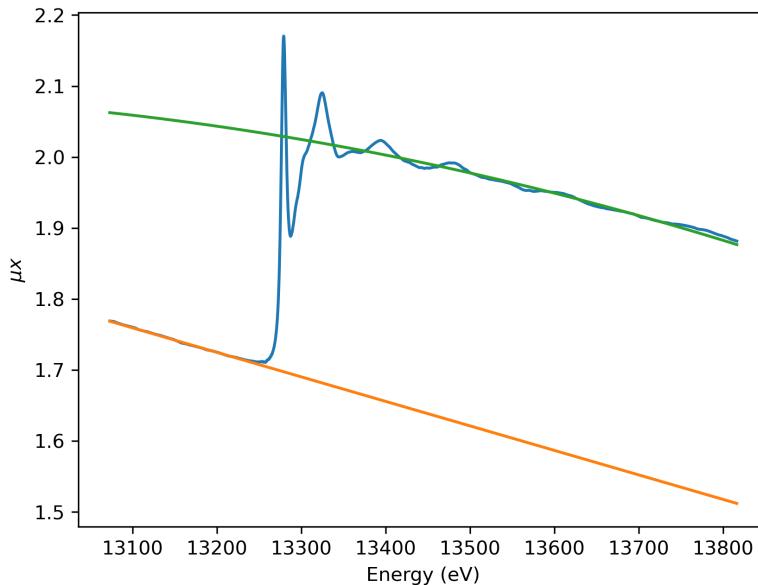
Pre-edge background

Post-edge background



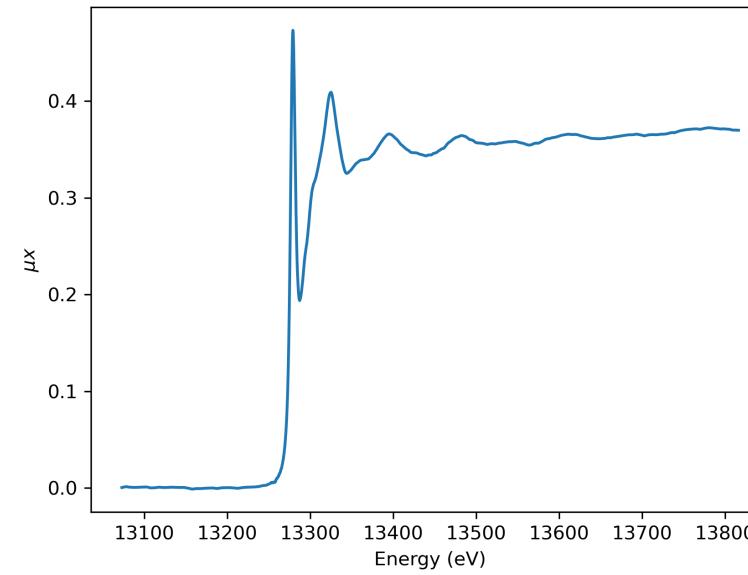
Pre-edge subtracted

# Pre-edge & Post-edge normalization

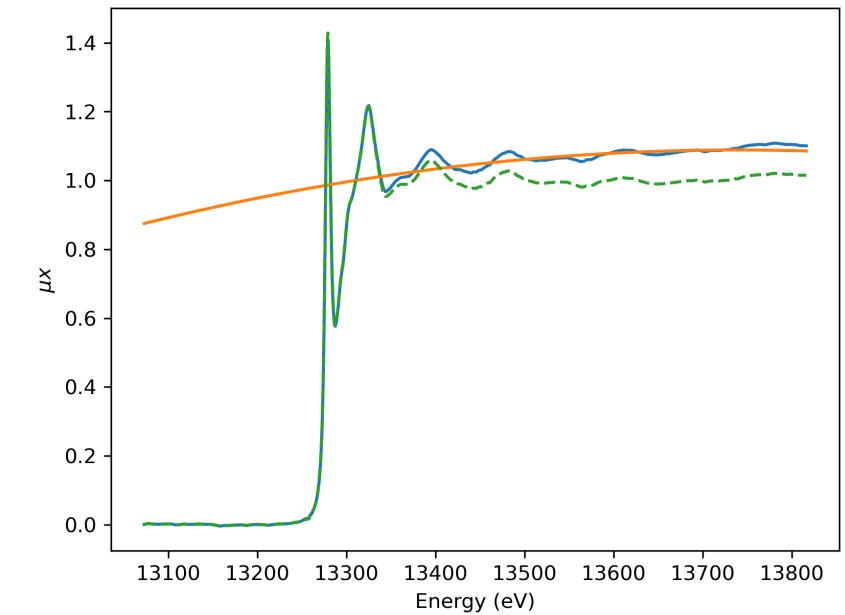


Pre-edge background

Post-edge background

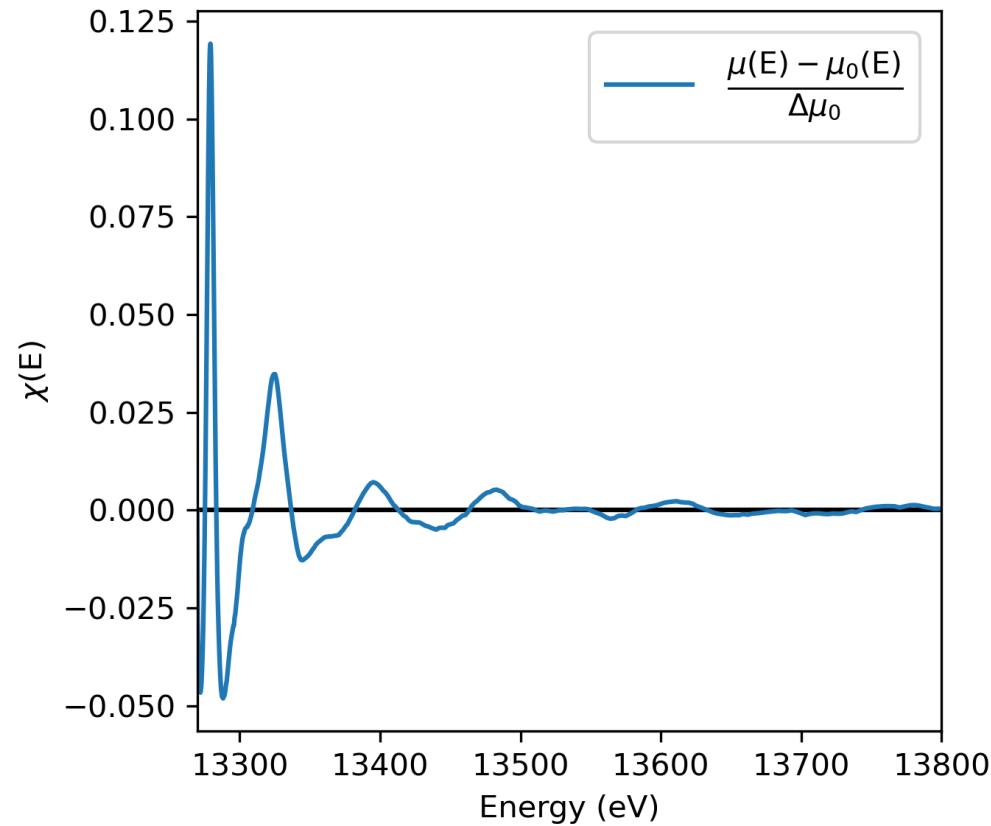
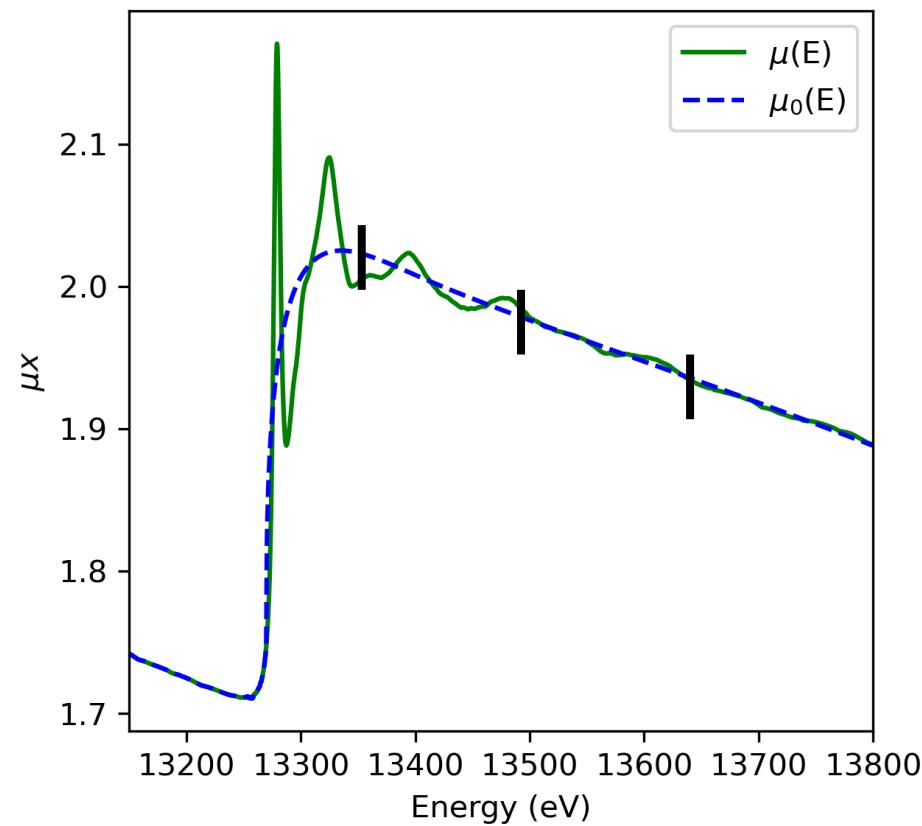


Pre-edge subtracted



Post-edge subtracted

# EXAFS extraction



# Conversion of E to k

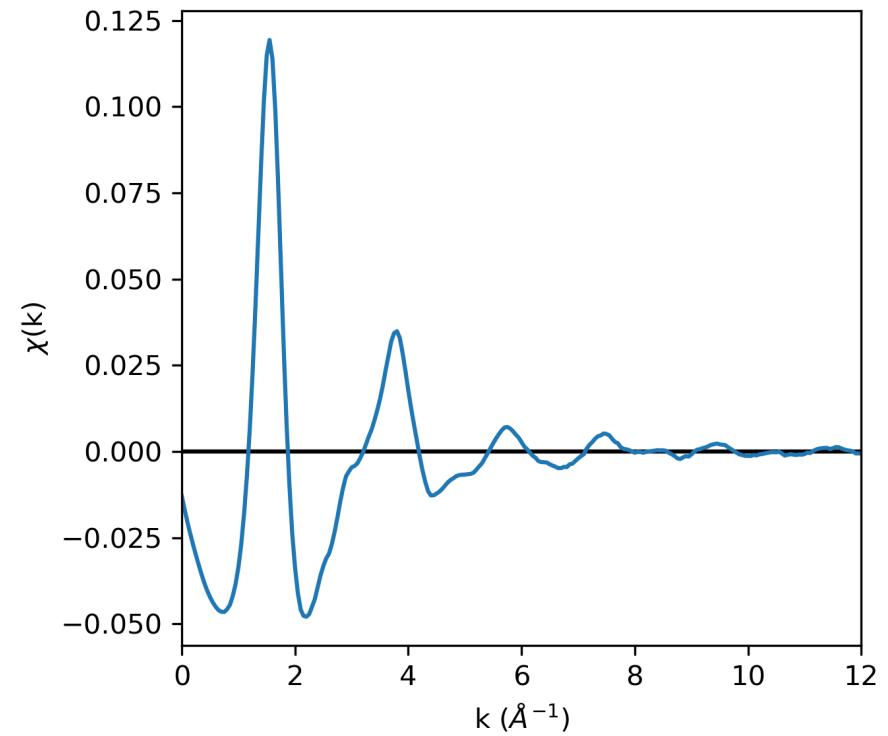
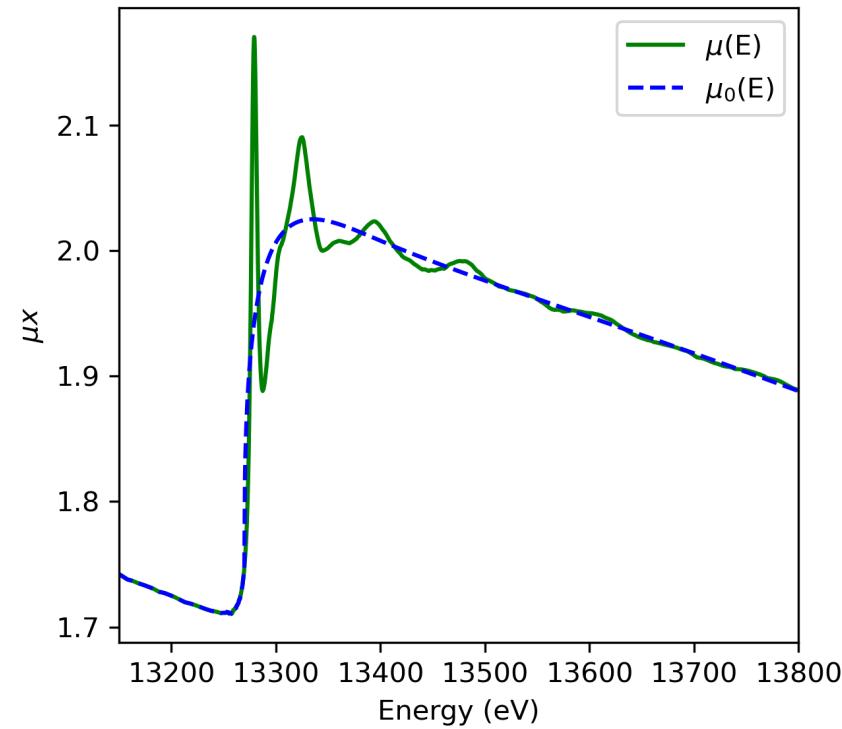
$$k = \sqrt{\frac{2m(E - E_0^{exp})}{\hbar^2}}$$

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

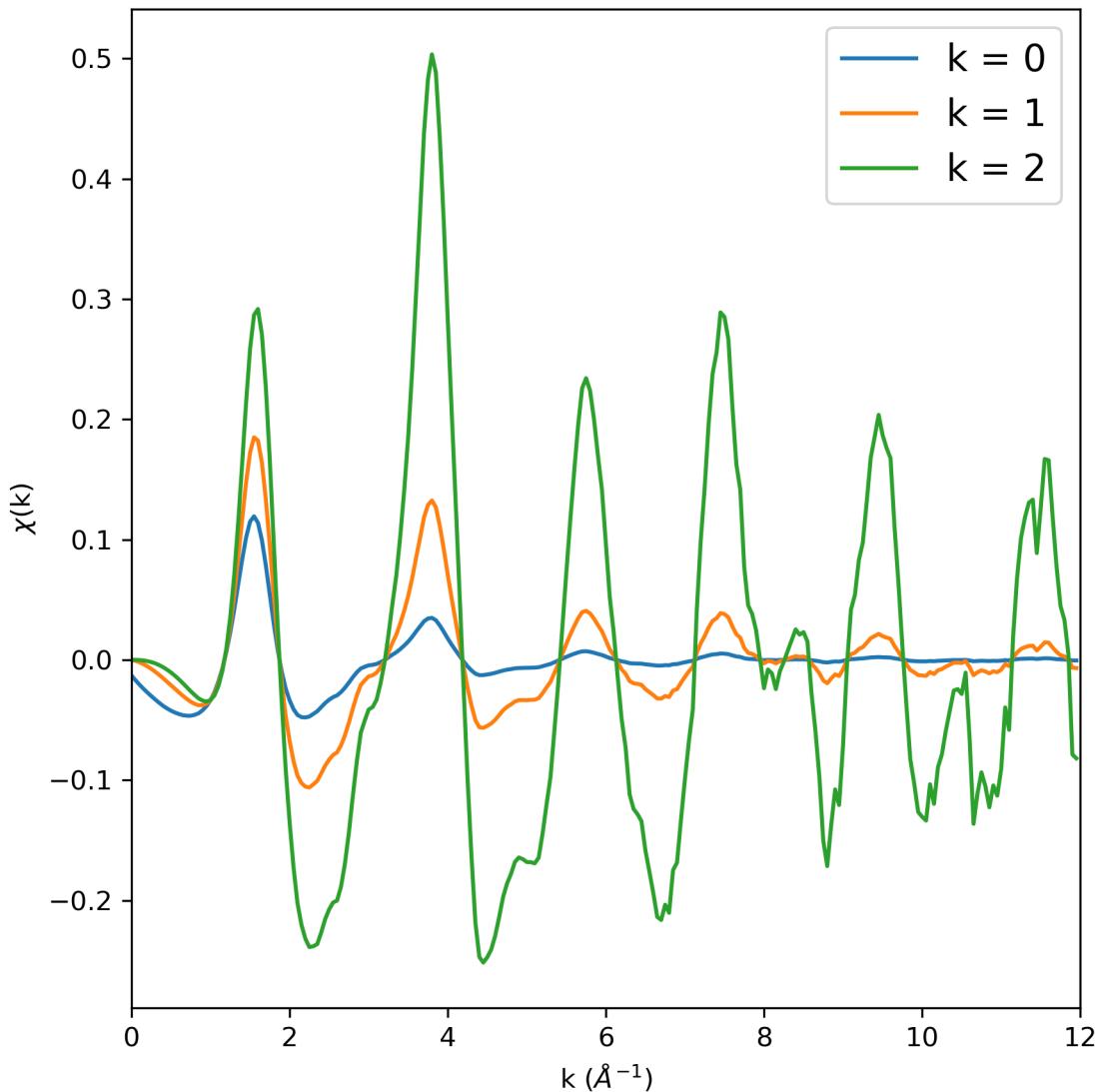
# Conversion of E to k

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

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



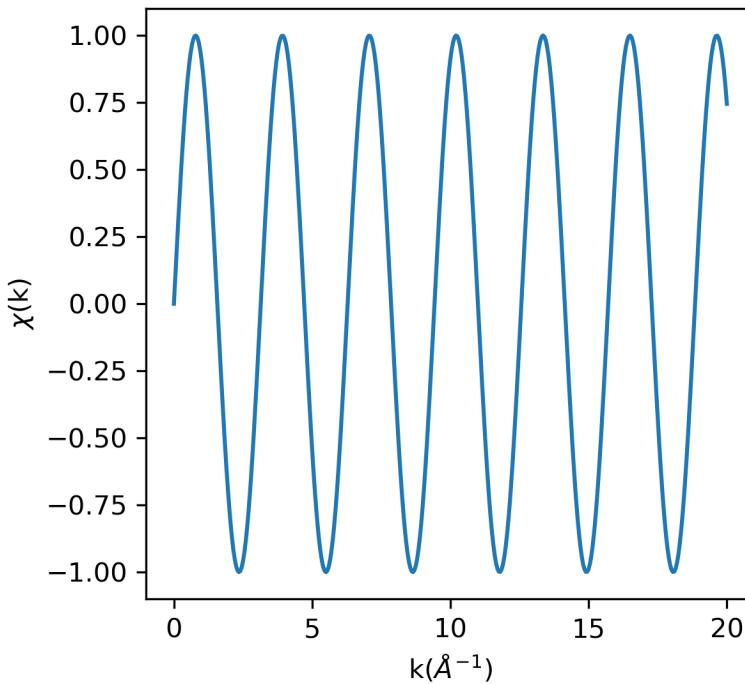
# $k$ weighting 1, 2, 3



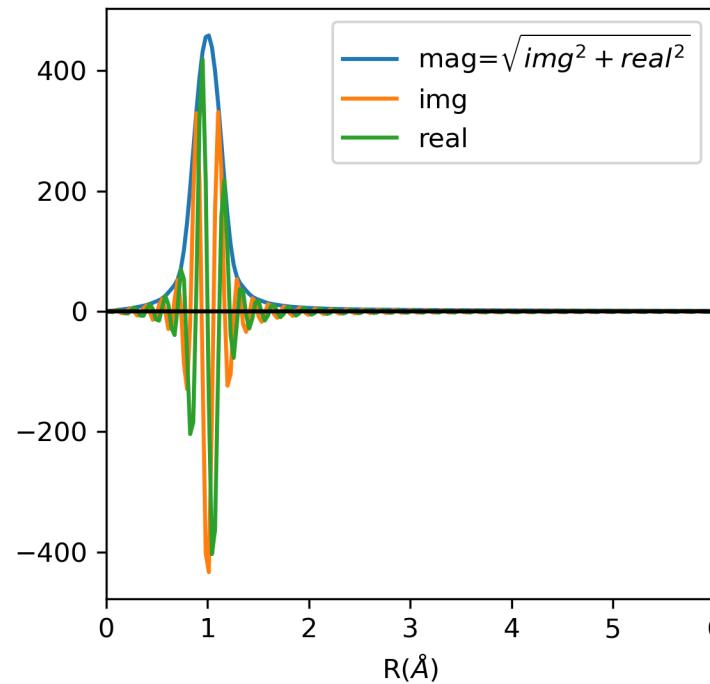
This procedure is important to prevent the larger amplitude oscillations from dominating the smaller ones in determining interatomic distances, which depends only on the frequency and not the amplitude.

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

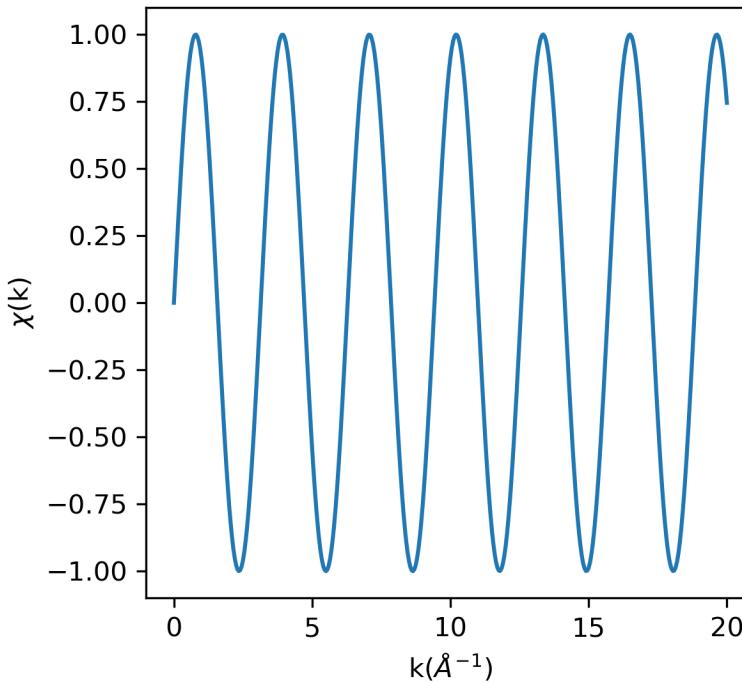
# Fourier Transform



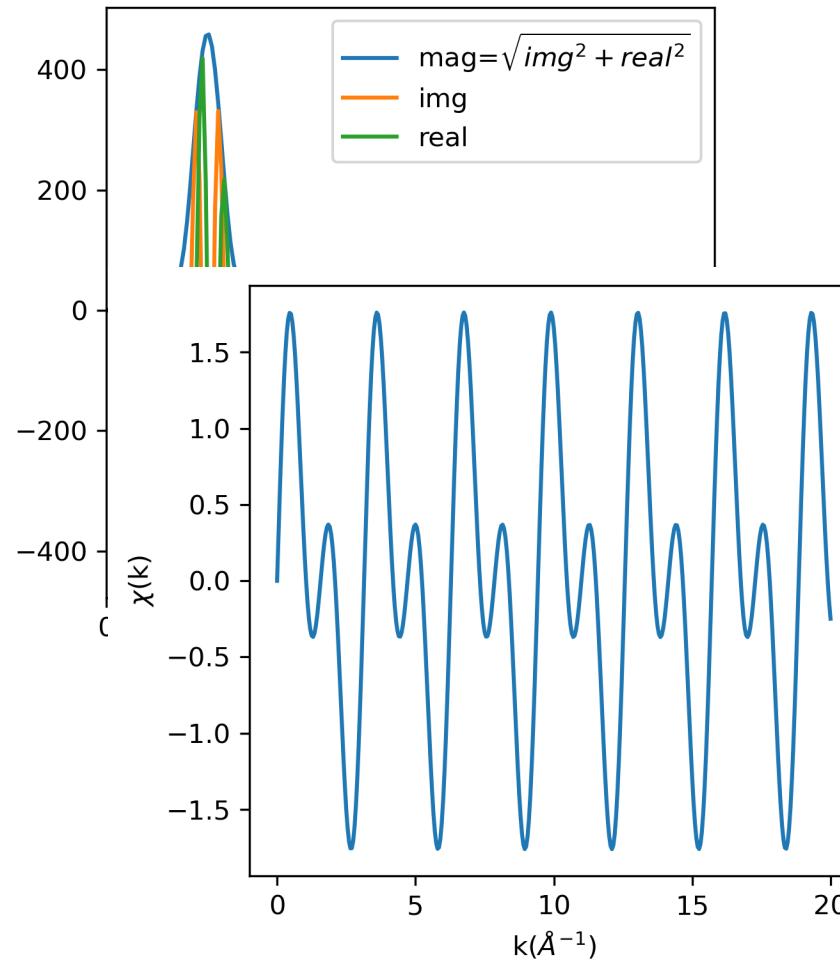
FT of a sine wave with phase  $2k$   
 $\chi(k) = \sin(2k)$



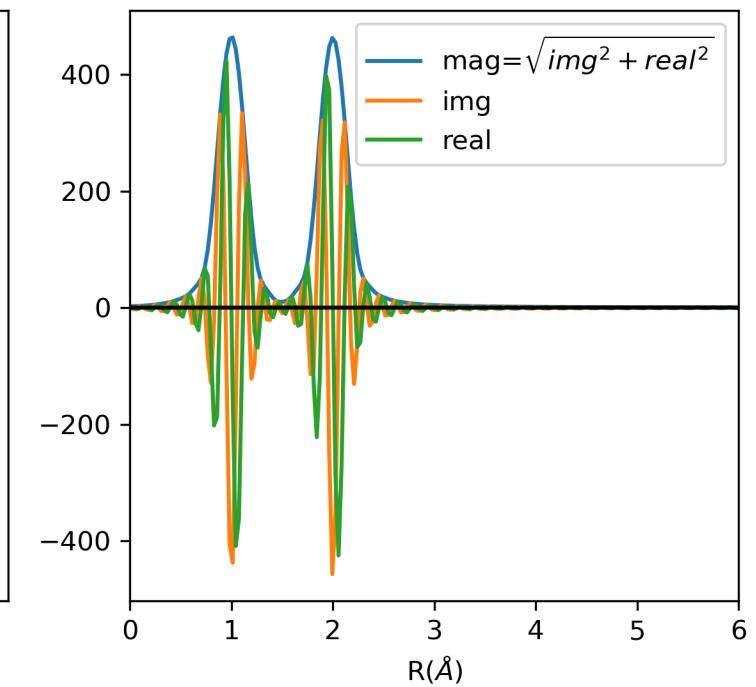
# Fourier Transform



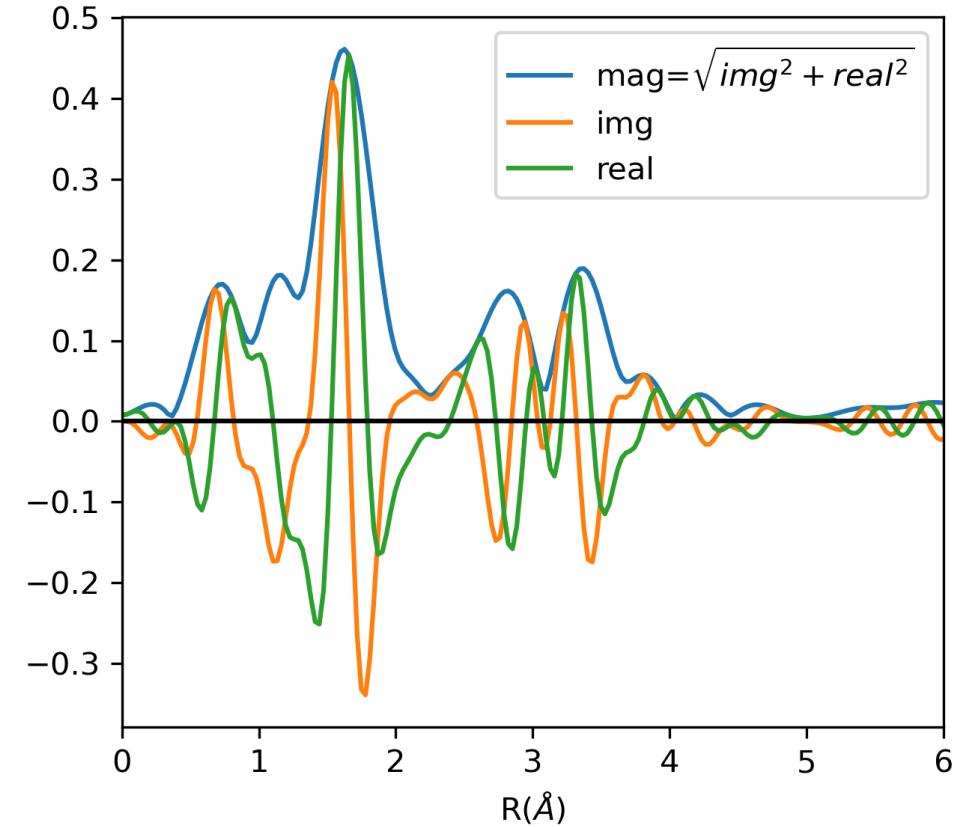
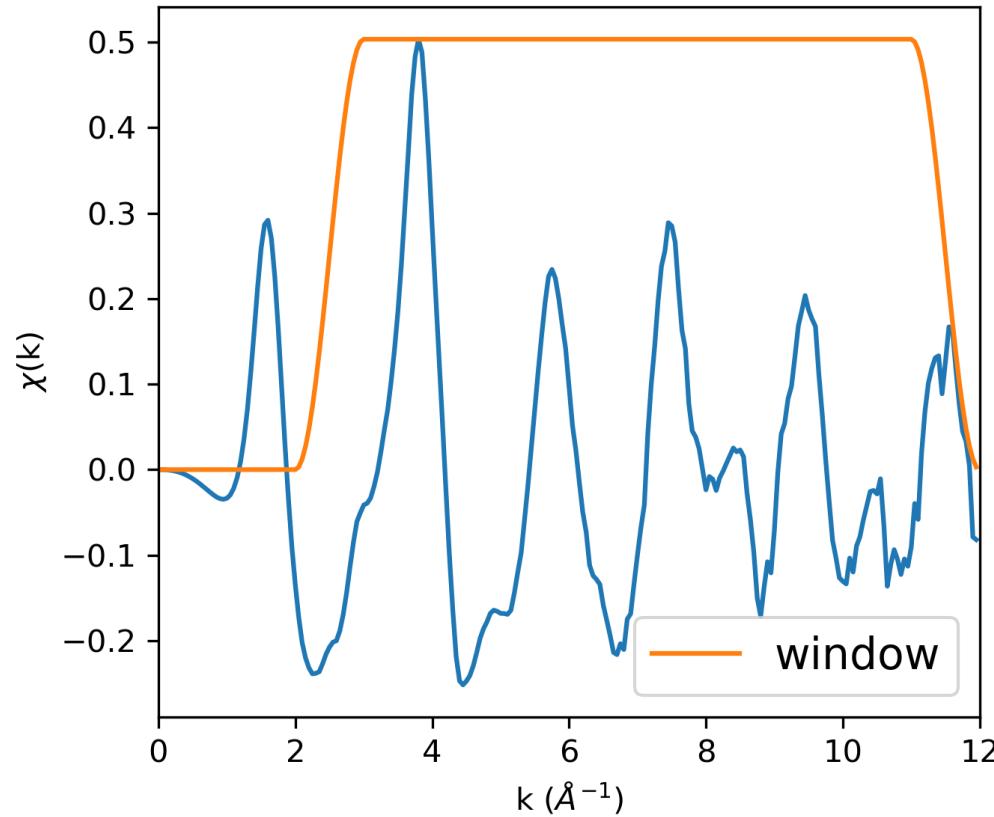
FT of a sine wave with phase  $2k$   
 $\chi(k) = \sin(2k)$



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



# Fourier Transform of PtO<sub>2</sub>



# 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