

User Manual

Version 1.2

How to install XAESA

1) Install Python from

https://www.anaconda.com/products/individual

| | Anaconda Installers | |
|---|---|--|
| Windows 🕊 | MacOS 🗉 | Linux 🔬 |
| Python 3.8 64-Bit Graphical Installer (466 MB) | Python 3.8 64-Bit Graphical Installer (462 MB) | Python 3.8 64-Bit (x86) Installer (550 MB) |
| 32-Bit Graphical Installer (397 MB) | 64-Bit Command Line Installer (454 MB) | 64-Bit (Power8 and Power9) Installer (290 MB) |

Select the version you need. For example, for Windows 10/11 select:

https://repo.anaconda.com/archive/Anaconda3-2020.07-Windows-x86_64.exe Save and install.

2) Download XAESA code from

https://gitlab.desy.de/aleksandr.kalinko/xaesa

| 🦊 😑 🔍 Search GitLab | | | ⊘ ∽ Sign in | |
|--|--|---|---------------------------------------|--|
| X xaesa | Aleksandr Kalinko > xaesa | | | |
| Project information Repository Issues Merge requests | Xaesa⊕ Project ID: 6316 ௹ ◆ 6 Commits १ 1 Branch ⊘ 0 Tags ⊟ 1.3 MiB Project 1 | Storage | ☆ Star 0 | |
| ダ CI/CD Deployments Packages and registries | improvements for herfd: (1) if no data selected select all automatically. (2) ···· Aleksandr Kalinko authored 3 weeks ago | | | |
| Monitor | main ~ xaesa | | History Find file | |
| Q Wiki | Name | Last commit | Download source code | |
| X Snippets | 🗅 feff | (1) changed color in the list for fluo signal. (2) header w | zip tar.gz tar.bz2 tar 3 weeks ago | |
| | 🗅 lib | Initial commit | 7 months ago | |
| | CHANGE.log | Initial commit | 7 months ago | |
| | 💠 alglib313_64free.dll | Initial commit | 7 months ago | |
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| | 🕒 feff.inp | Initial commit | 7 months ago | |
| | nit.py | Initial commit | 7 months ago | |
| | interpolation_k2.py | Initial commit | 7 months ago | |
| | nodified_widgets.py | Initial commit | 7 months ago | |
| | test_procedures.txt | Initial commit | 7 months ago | |
| « Collapse sidebar | net tooltiptexts.py | Initial commit | 7 months ago | |

as a ZIP archive and unzip it in any directory.

How to run XAESA

1) Open menu Start, Anaconda3 and select Spyder (Anaconda3)



2) Open xaesaGUI.py, go to the menu Run, select Configuration per file



3) Select Execute in an external system terminal and click OK



4) To run XAESA, click on

Spyder (Python 3.8)

| <u>F</u> ile <u>E</u> dit <u>S</u> ea | arch Sour <u>c</u> e <u>R</u> un <u>D</u> ebug C <u>o</u> nsoles <u>P</u> rojects <u>T</u> ools <u>V</u> iew <u>H</u> elp | |
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| D:\xaesa_v0.04 | t\xaesaGUI.py | |
| 🗖 xaesaGUI. | py × | |
| 1 2 3 4 5 6 7 | <pre># -*- coding: utf-8 -*- #""" #Created on Fri Oct 7 12:25:31 2016 # #@author: sasha #"""</pre> | |
| 8 9 10 | <pre>XAESA_VERSION = "0.04" GUI_SETTINGS_ID = "XAESA" + XAESA_VERSION incompt out</pre> | |

5) XAESA will open in the external window



XAESA keeps all data in an HDF5 format file (*.hdf5), which can be saved and opened in the menu **File**:

I XAESA - X-ray Absorption and Emission Analytics

| File | Tools Settings | | |
|------|-------------------------|--------|-----|
| | Save analysis to hdf5 | Ctrl+S | |
| | Open analysis from hdf5 | Ctrl+A | |
| | Open Nexus file | Ctrl+N | |
| | Exit | Ctrl+Q | |
| | mu | | XES |

If necessary, it can be opened and manipulated using a viewer HDFView, which can be downloaded from here

https://www.hdfgroup.org/downloads/hdfview/

The main parts of the XAESA screen

- 1) Menus to open experimental files in different formats.
- 2) Window with a list of opened files.
- 3) Menus to manipulate data.
- 4) Main graphical screen showing all data analysis.
- 5) Menus with parameters for data analysis.
- 6) EXAFS fitting using multi-component or regularization model.



Example of the analysis for the Cu K-edge in copper foil:





Definition of the main parameters for EXAFS extraction

EXAFS $\chi(E)$ is defined as

 $\chi(k)=(\mu(E)-\mu_b(E)-\mu_0(E))/\mu_0(E)$

where photoelectron wavenumber k is defined as $k=(2m_e/\hbar^2 (E-E_0))^{\frac{1}{2}}$.

There are several important points to remember:

- 1) $\mu_0(E)$ can be corrected using the zero-line correction (zlc) parameter.
- 2) Normalization of EXAFS $\chi(k)$ can be done at specified energy.
- 3) EXAFS $\chi(k)$ can be multiplied by k^n (n=0,1,2,3).
- 4) Glitches can be removed, if present.

The Fourier transform (FT) of EXAFS $\chi(k)k^n$ is calculated from K_{min} to K_{max} with a step dK using the 10% Gaussian window. The FT range is defined by R_{min} and R_{max} with a step dR.

The inverse FT (back-FT) is calculated from BFT R_{min} to BFT R_{max} using the Hanning window with a BFT window parameter.

How to load data

There are several possibilities for how experimental or theoretical spectra can be loaded into XAESA using the button Open File(s) ...

1) X-ray absorption coefficient $\mu(E)$ stored in a multi-column ASCII file can be loaded by, first, specifying the columns for the energy E and the absorption coefficient $\mu(E)$, and, next, by pressing the button mu

| Open File(s |) | | Remov | e File(s) |
|----------------------|----------|-----|-------|-----------|
| mu | | XES | | EXAFS |
| Skip lines 0 | Energy 0 | | mu 1 | mu ref _1 |
| Calculate absorption | | | | |

If necessary, one can skip several lines from the beginning of the file. N.B. All lines starting with "#" will be skipped automatically.

2) When experimental data are stored as signals from ionisation chambers, one needs to select

| Calculate absorption, the experimental mode (| Transmission | or | Fluorescence |) and |
|---|--------------|----|--------------|-------|
| specify the columns for IO and I1: | | | | , |

| Open File(s |) | Ren | nove File(s) |
|----------------------|----------|--------------|--------------|
| mu | | XES | EXAFS |
| Skip lines 0 | Energy 0 | mu <u>1</u> | mu ref -1 |
| Calculate absorption | | Transmission | Fluorescence |
| I0 1 | I1 2 | | I2 -1 |

X-ray absorption coefficient will be automatically calculated as $\mu(E)=\ln(IO(E)/I1(E))$ for transmission or $\mu(E)=I1(E)/I0(E)$ for fluorescence.

| 3) X-ray emission spectrum (XES) can be loaded by selecting | | XES . |
|---|---------------------|-------|
| Open File(s) | Remove File(s) | |
| mu | ES EXAFS | _ |
| Skip lines 0 Energy 0 | Emission 1 | |
| 4) EXAFS spectrum $\chi(k)$ can be | loaded by selecting | EXAFS |
| Open File(s) | Remove File(s) | |
| mu | ES EXAFS | |
| Skip lines 0 k 0 | EXAFS 1 | |

How to export data

Absorption coefficient $\mu(E)$, XANES $\mu(E)$, EXAFS $\chi(k)k^n$, FT(R), and BFT $\chi(k)k^n$ spectra can be Save ... exported in an ASCII format by pressing the button

| Save | · • |
|--|---------------|
| Save mu Save XANES Save EXAFS Save FT Save BFT | s to selected |

How to average/merge data

To average or merge several spectra, press the button choose what to do:

Ŧ Average / merge and

| | Average / mer | rge 🔹 |
|---|-------------------|---------------|
| | Average mu direct | Linear com |
| | Average mu spline | |
| | Average EXAFS | PCA and |
| D | Merge mu | -6104 seconds |

How to rebin data

alveie

Often original experimental spectra contain too many points, especially, at large energies. In this case, one can reduce the total number of points using the rebinning procedure.

| То | do this, press the button | Rebin | and choose what to do: |
|----|---------------------------|-------|------------------------|
| | Rebin | • | |
| 1 | Rebin mu | | |
| | Return to original mu | | |

How to compare data sets

To compare several data sets, first select them in the window with a list of opened files:

| Cu_foil_RT_Cu_K(rebin) |
|--------------------------|
| Cu_foil_011K_Cu_K(rebin) |
| Cu_foil_050K_Cu_K(rebin) |
| Cu_foil_100K_Cu_K(rebin) |
| Cu_foil_150K_Cu_K(rebin) |
| Cu_foil_175K_Cu_K(rebin) |
| Cu_foil_200K_Cu_K(rebin) |
| Cu_foil_225K_Cu_K(rebin) |
| Cu_foil_250K_Cu_K(rebin) |
| Cu_foil_275K_Cu_K(rebin) |
| Cu_foil_293K_Cu_K(rebin) |
| |

This can be done by pressing CTRL + Mouse click.

Compare i0 Compare i1 Compare i2

Compare i fluorescence Compare mu ref Compare amplitude Compare phase

Compare mu rebin vs original

Compare ...

| Nex | t, press the button | Compare | and choose what data to compare from |
|-----|---------------------|---------|--|
| the | list. | | |
| | Compare mu | | |
| | Compare XANES | | |
| | Compare EXAFS | | |
| | Compare FT | | |
| | Compare BFT | | |

How to apply the parameters to another set(s) of data

-

The parameters of the analysis for a data set can be copied to Clipboard and applied to another data set(s). This is very convenient when many spectra should be analysed using the same set of parameters.

To do this, select a data set in the window with a list of opened files:

| Cu_foil_RT_Cu_K(rebin) | |
|--------------------------|--|
| Cu_foil_011K_Cu_K(rebin) | |
| Cu_foil_050K_Cu_K(rebin) | |
| Cu_foil_100K_Cu_K(rebin) | |
| Cu_foil_150K_Cu_K(rebin) | |
| Cu_foil_175K_Cu_K(rebin) | |
| Cu_foil_200K_Cu_K(rebin) | |
| Cu_foil_225K_Cu_K(rebin) | |
| Cu_foil_250K_Cu_K(rebin) | |
| Cu_foil_275K_Cu_K(rebin) | |
| Cu_foil_293K_Cu_K(rebin) | |
| | |

Press the button

Next, select one or more data sets in the window with a list of opened files by pressing CTRL + Mouse click:

| Cu_foil_RT_Cu_K(rebin) | |
|--------------------------|--------------------------|
| Cu_foil_011K_Cu_K(rebin) | |
| Cu_foil_050K_Cu_K(rebin) | |
| Cu_foil_100K_Cu_K(rebin) | |
| Cu_foil_150K_Cu_K(rebin) | |
| Cu_foil_175K_Cu_K(rebin) | |
| Cu_foil_200K_Cu_K(rebin) | |
| Cu_foil_225K_Cu_K(rebin) | |
| Cu_foil_250K_Cu_K(rebin) | |
| Cu_foil_275K_Cu_K(rebin) | |
| Cu_foil_293K_Cu_K(rebin) | |
| | |
| | |
| Press the hutton | Apply params to selected |
| | |

How to perform a multi-shell fit

A multi-shell fit is based on an EXAFS equation:

$$\chi(k) = S_0^2 \sum_{i=1}^M \frac{N_i}{kR_i^2} f_l(\pi, k, R_i) \exp(-2\sigma_i^2 k^2 + \frac{2}{3}C_{4i}k^4 - \frac{4}{45}C_{6i}k^6) \exp\left(-\frac{2R_i}{\lambda(k)}\right) \\ \times \sin\left(2kR_i - \frac{4}{3}C_{3i}k^3 + \frac{4}{15}C_{5i}k^5 + \phi_l(\pi, k, R_i) + 2\delta_c^l(k) - l\pi\right)$$

where

- M the number of coordination shells,
- N_i the coordination number of the *i*-shell,
- R_i the radius of the *i*-shell (the interatomic distance),

 σ_i^2 - the mean square radial displacement (MSRD) (or the Debye-Waller factor) between the absorber and back-scatterer atoms located in the *i*-shell,

- C_{ji} the cumulants of the distribution, which account for anharmonic effects and non-Gaussian disorder,
- S_0^2 the scale factor, which accounts for the multielectron effects,

 $\lambda(k)$ - the mean free path of the photoelectron,

 $f_i(\pi, k, R_i)$ - the backscattering amplitude of the atoms in the *i*-shell,

 $\phi_i(\pi, k, R_i)$ - the backscattering phase of the atoms in the *i*-shell,

 $\delta_c^{\prime}(k)$ the absorbing atom phase shift,

l - the angular momentum of the photoelectron (l = 1 for K, L₁-edges and l = 2 or 0 for L_{2,3}-edges).

Note that $f_l(\pi, k, R_i)$, $\phi_l(\pi, k, R_i)$, $\delta_c^l(k)$, and $\lambda(k)$ functions must be calculated in advance using, for example, a FEFF code. As a result of such calculation, a set of feff*****.dat files should be obtained for all required shells.

To perform a multi-shell fit, press the button the new window will open:



Multi-shell fit ...

and

The window shows the experimental EXAFS spectrum by blue lines and the best-fitted EXAFS spectrum by orange and red lines in *k*- and *R*-space, respectively.

In this window, the parameters of the fit should be specified.

First, choose the required number of shells using two buttons:

| Add shell | Remove shell | |
|-----------|--------------|--|
|-----------|--------------|--|

Next, for each shell:

choose the feff*****.dat file with the information on the neighbouring atoms located in that shell using the button
 Open feff file(s) ...
 and select the required amplitude and phase shift functions from the dropdown lists:

| E:/_EDA_/XAESA/FEFF_Cu/feff0001.dat.amp | • |
|---|---|
| | |
| | |
| | E:/_EDA_/XAESA/FEFF_Cu/feff0001.dat.amp |

set the initial, minimum and maximum allowed values for each structural parameter (N, R, σ² (≡ Sigma), Cj (j=3,4, 5,6) in the shell:

| Shell 1 | | | | | | |
|---------|-----------|---------------------|------|------------|-----|--|
| N | 10.02009 | Min. limit | 0 | Max. limit | 16 | |
| R | 2.50687 | Min. limit | 0 | Max. limit | 4 | |
| Sigma | 0.00254 | Min. limit | 0 | Max. limit | 1 | |
| C3 | -2.04E-04 | Min . l imit | -0.1 | Max. limit | 0.1 | |
| C4 | 0 | Min. limit | -0.1 | Max. limit | 0.1 | |
| C5 | 0 | Min. limit | -0.1 | Max. limit | 0.1 | |
| C6 | 0 | Min. limit | -0.1 | Max. limit | 0.1 | |

Use checkboxes at the right to fix (unchecked) or vary (checked) the required parameter.

Finally, the range of the fit in *k*-space should be set:

| | K min | 3.5 | K max | 19.0 | dK | 0.050 | |
|--|------------------|-----|-------|-------|----|----------------|--|
| | | | | | | | |
| To start fitting, | press the button | Fit | | | | | |
| The results of the fit can be saved by pressing the button | | | | ton (| Sa | ve Fit results | |

How to reconstruct a radial distribution function (RDF)

This method allows one to reconstruct a radial distribution function (RDF) using the regularization-like method.

The EXAFS model is defined by the equation

$$\chi(k) = S_0^2 \int_{R_{\rm min}}^{R_{\rm max}} \frac{G(R)}{kR^2} F(\pi,k,R) \sin(2kR + \Phi(\pi,k,R)) \mathrm{d}R$$

where the coordination number is defined as

$$N = \int_{R_{\min}}^{R_{\max}} G(R) \mathrm{d}R$$

The method can be only used to fit the first coordination shell contribution containing atoms of one type. This method is useful when the first shell is distorted so that there is a distribution of close distances which cannot be resolved within the multi-shell model.

To perform a multi-shell fit, press the button Reconstruct RDF ... and the new window will open:



The window shows the experimental EXAFS spectrum by blue lines and the best-fitted EXAFS spectrum by green lines in *k*- and *R*-space, respectively. In addition, the true RDF is shown in the right panel by filled circles.

In this window, the parameters of the fit should be specified.

First, choose the feff*****.dat file with the information on the neighbouring atoms located in

that shell using the button Open feff file(s) ... and select the required amplitude and phase shift functions from the dropdown lists

| Ampl | E:/_EDA_/XAESA/FEFF_Cu/feff0001.dat.amp | • |
|-------|---|---|
| | | |
| Phase | E:/_EDA_/XAESA/FEFF_Cu/feff0001.dat.pha | |

Next, set the range of the fit in k-space, the range of the RDF g(R) in R-space and the maximum number of iterations:

| K min | 0.5 | K max | 15 | dK | 0.05 |
|-----------------------|-------|-------|-----|----|------|
| Rmin | 0.5 | Rmax | 3.0 | dR | 0.02 |
| Max. number of iterat | tions | | 20 | | |

| To start fitting, press the button | Fit |). | |
|-------------------------------------|--------------------------|----------|--|
| The results of the fit can be saved | l by pressing the button | Save RDF | |