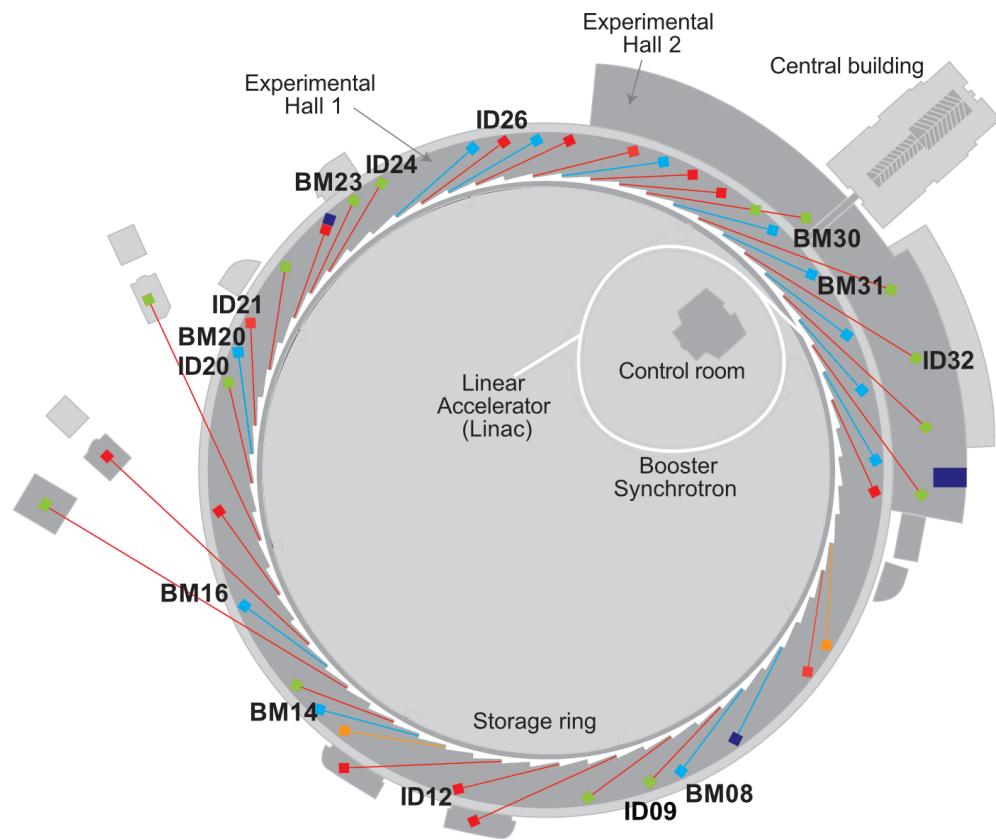


The background image shows a wide-angle aerial view of the CERN facility at night. The iconic Large Hadron Collider (LHC) ring is visible, a massive circular structure with a dark interior and a metallic outer wall. The ring is illuminated from within, creating a bright glow against the dark sky. The surrounding area is filled with numerous smaller buildings, roads, and parking lots, all of which are brightly lit with yellow and white lights. In the distance, the silhouette of the Swiss Alps is visible against a clear blue sky.

Overview of data analysis tools and computational software

Marius Retegan
Algorithms & Scientific Data Analysis Group
Experiments Division

SPECTROSCOPY BEAMLINES AT ESRF



	XAS	XMCD	XES	RIXS
ID09				✓
ID12	✓	✓		
ID20	✓	✓	✓	✓
ID21	✓			
ID24	✓		✓	
ID26	✓	✓	✓	✓
ID32	✓	✓		✓
BM08	✓			
BM14	✓			
BM16	✓		✓	✓
BM20	✓		✓	✓
BM23	✓			
BM30	✓			
BM31	✓			

XAS – X-ray Absorption, **XMCD** – X-ray Magnetic Circular Dichroism
XES – X-ray Emission, **RIXS** – Resonant Inelastic X-ray Scattering

1. Getting from raw data to publishable plot

- spectra averaging, rebinning, etc.
- background subtraction
- outliers removal
- plotting

2. Interpreting and understanding the experimental data

- assignment of spectral features
- extraction of structural and electronic properties: oxidation state, bond lengths, crystal field parameters, etc.



BeamLine Instrumentation Support Software

The BLISS control system provides a global approach to running synchrotron experiments requiring synchronously controlled motors, detectors, and various acquisition devices thanks to hardware integration, Python sequences, and an advanced scanning engine.



HDF5 is file format to organize large amounts of data.



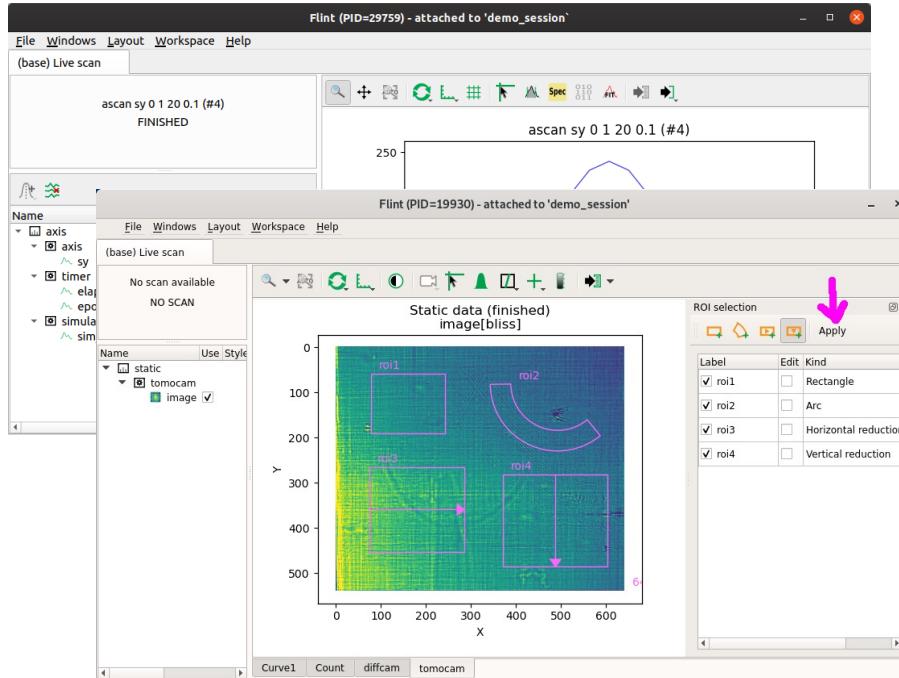
Adds additional rules and structure to help people and software understand how to read a HDF5 file.

<https://manual.nexusformat.org/impatient>



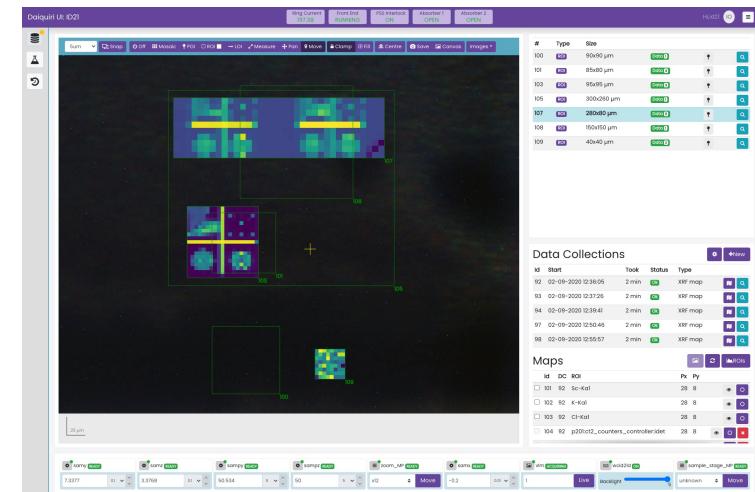
TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

Flint is the GUI companion for BLISS that provides a live display for current scans.



Daiquiri is a Python-based framework for beamline control and data acquisition.

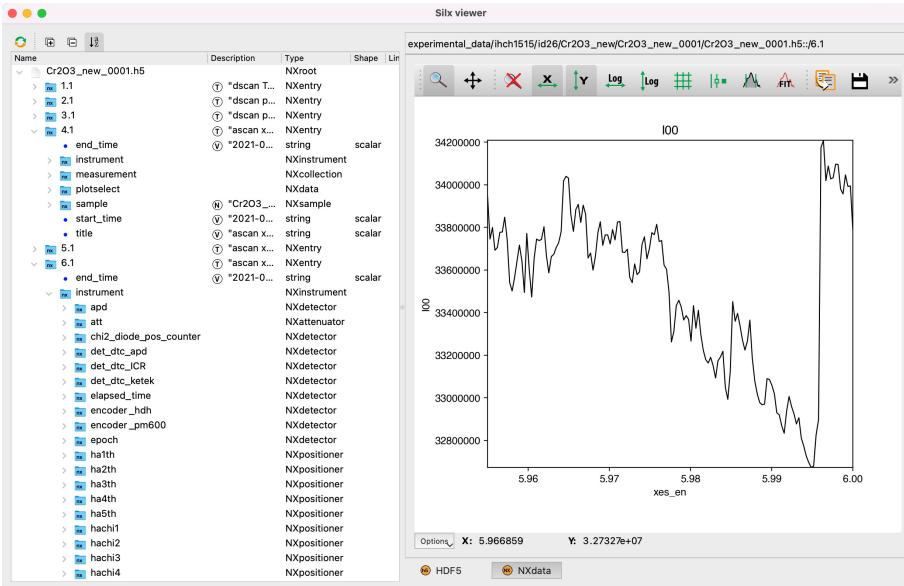
Daiquiri UI is the web-based JavaScript User Interface for Daiquiri.



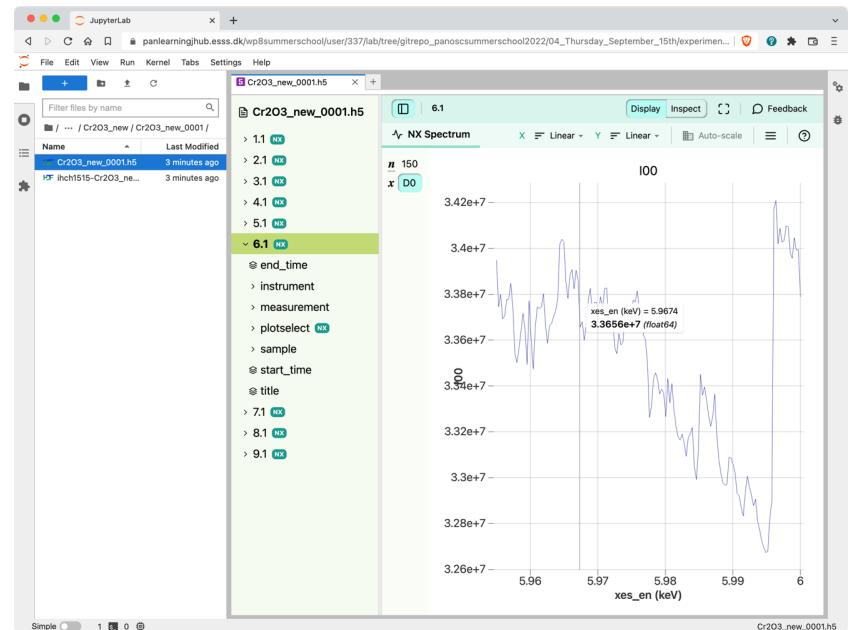
<https://bliss.gitlab-pages.esrf.fr>

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

silx view a unified viewer for HDF5, SPEC, and image file formats



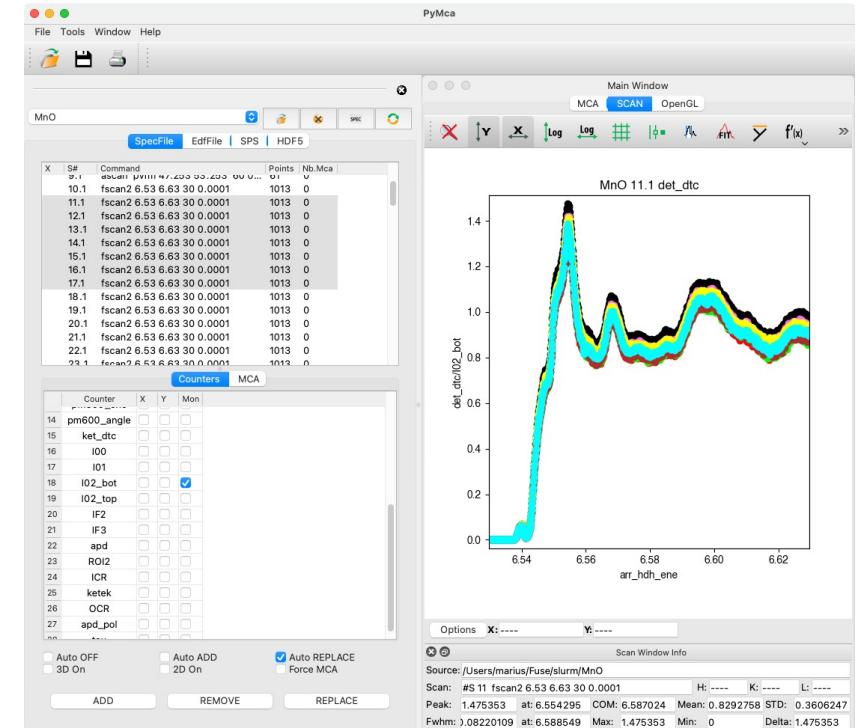
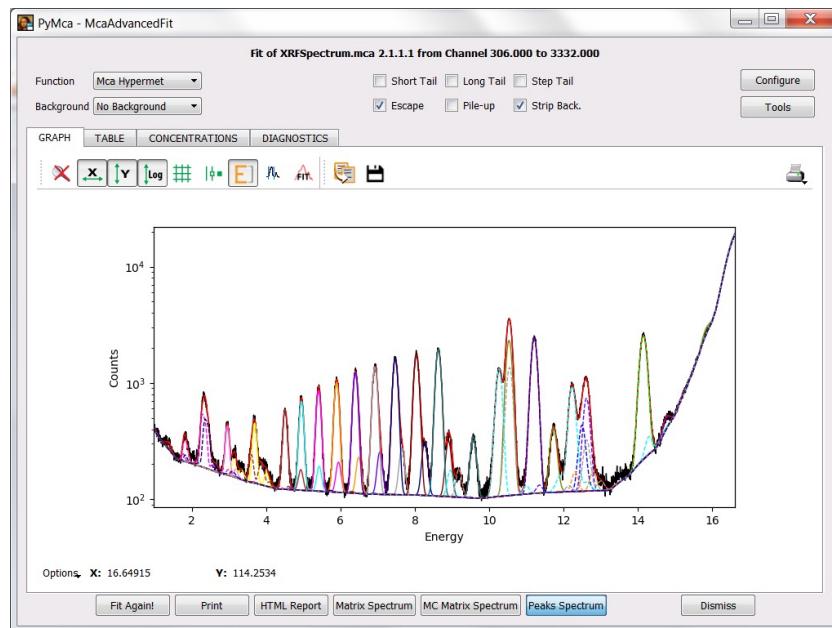
h5web a collection of components to visualize and explore data



<http://www.silx.org>

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

PyMCA is a ready to use, and in many aspects state-of-the-art, set of applications implementing most of the needs of X-ray fluorescence (XRF) data analysis.



<http://www.silx.org>

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

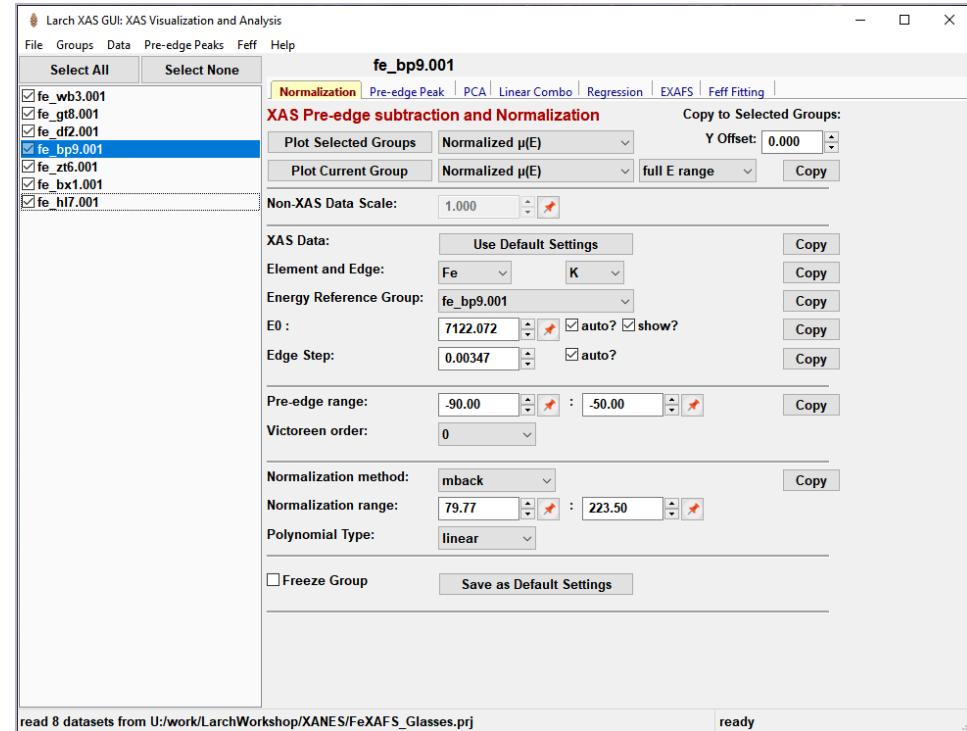
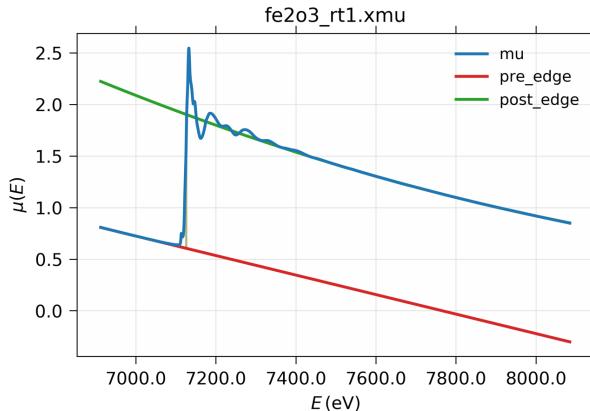
Larch is an open-source library and set of applications for processing and analyzing X-ray fluorescence (XRF) and X-ray absorption spectroscopy (XAS).

```
from larch.io import read_ascii
from larch.xafs import pre_edge
from wxmplot.interactive import plot

fname = 'fe2o3_rt1.xmu'
dat = read_ascii(fname, labels='energy mu i0')

pre_edge(dat, group=dat)

plot(dat.energy, dat.mu, label='mu', xlabel='Energy (eV)',
     title=fname, show_legend=True)
plot(dat.energy, dat.pre_edge, label='pre-edge line')
plot(dat.energy, dat.post_edge, label='post-edge curve')
```



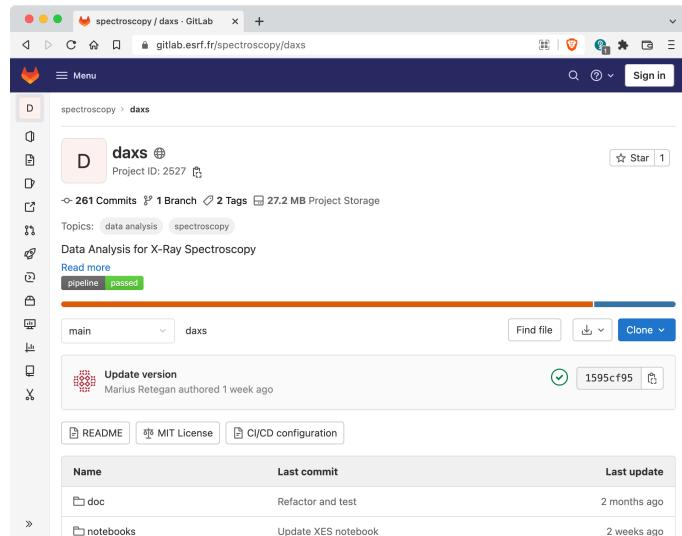
<https://millenia.cars.aps.anl.gov/xraylarch>

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

Visualization

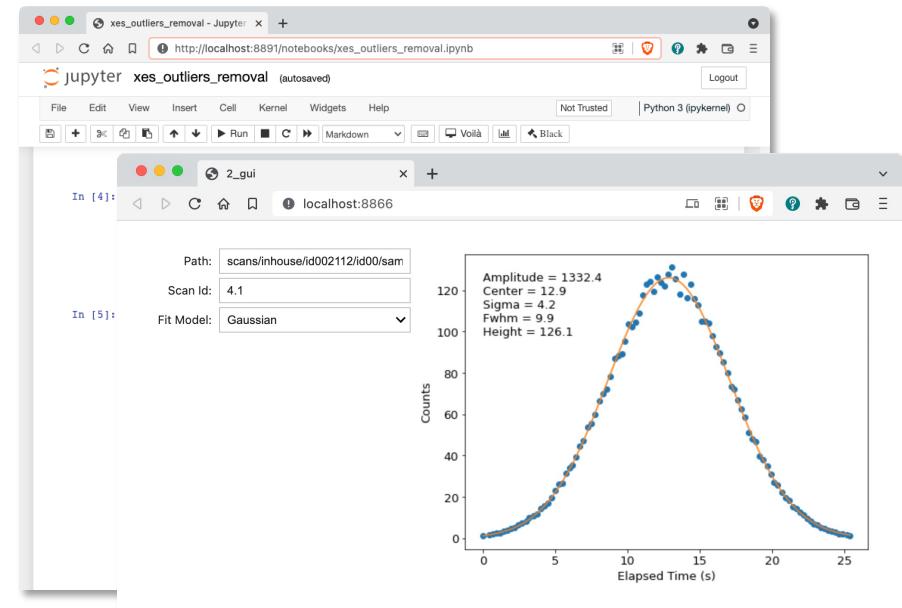
Several tools can be used to look at the acquired data during an experiment:
Flint, Daiquiri, silx view, h5web

The analysis tools are focused on XAS, and there are no tools to treat XES or RIXS measurements.



Analysis

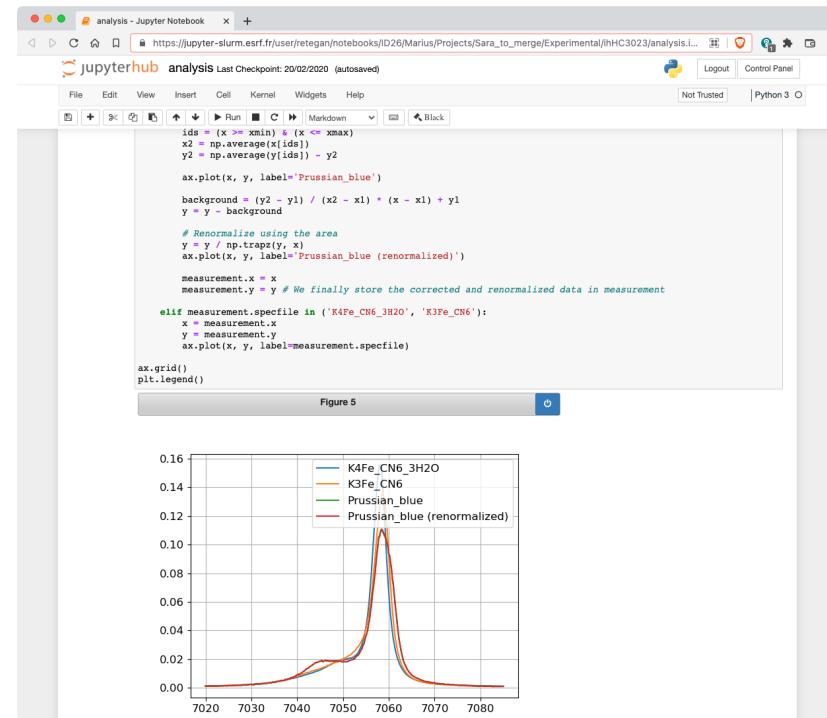
There are a plethora of tools to analyze XANES/EXAFS data: **PyMCA, Larch, GNXAS, PyFitlt**



<https://gitlab.esrf.fr/spectroscopy/d axs>

JUPYTERHUB AT ESRF

The JupyterHub installation can be used to access computing resources and measured data.



<https://jupyter-slurm.esrf.fr>

THE ESRF DATA CATALOGUE

The screenshot displays the ESRF Data Catalogue interface across three main sections:

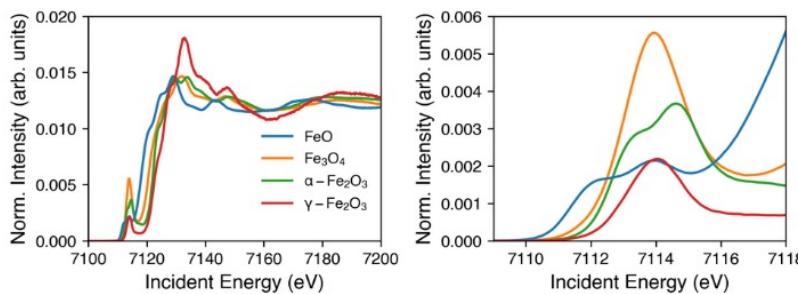
- Search Results:** On the left, a table lists various proposals and beamlines. Key columns include "Proposal", "Beamline", "Start", and "Title". Some entries have small icons next to them.
- File Preview:** In the center, a table shows two files with columns "Preview", "Location", and "Size".

Preview	Location	Size
	/NiO_diluted_Ka1_rixs_cc_0002.h5	78.3 MB
	/lhch1527-NiO_diluted-Ka1_rixs_cc_0002.h5	17.1 KB
- Data Visualization:** On the right, a plot titled "NX Spectrum" shows "det_dtc_apd" versus "elapsed_time". The y-axis ranges from 0 to 4e+5, and the x-axis ranges from 0 to 60. A blue curve starts at zero and rises sharply after 20 units of elapsed time. The plot includes a legend with "n 102" and "x D0".

<https://data.esrf.fr>

X-RAY SPECTROSCOPY: EXPERIMENT AND COMPUTATION

Experimental X-ray spectroscopy data are often evaluated by comparison to reference compounds.



Computational X-ray spectroscopy provides a deeper insight by **maximizing** the amount of information that can be extracted from the experimental data.

Specialized *ab initio* codes:

FEFF, FDMNES, OCEAN, ...

Generic *ab initio* codes:

ORCA, MOLCAS, ADF, Wien2k, VASP, Quantum ESPRESSO, ...

Semi-empirical multiplets codes:

Cowan's Codes (RCN), Quanty, Xclaim, XTLS, Hilbert++, ...

SEMI-EMPIRICAL MULTIPLETS: THE EARLY DAYS



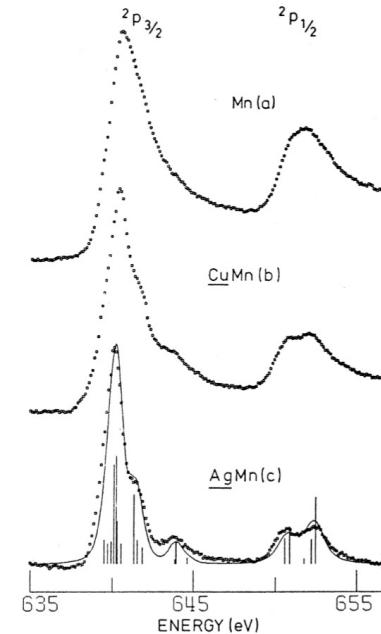
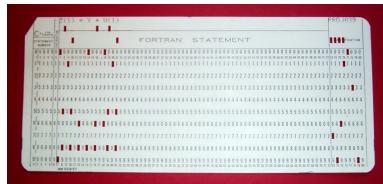
Article

Cowan Code: 50 Years of Growing Impact on Atomic Physics

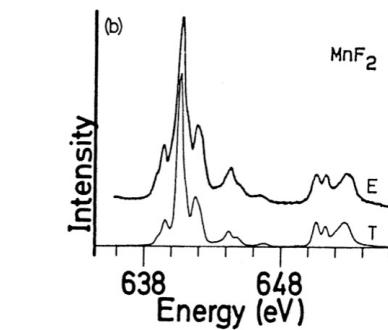
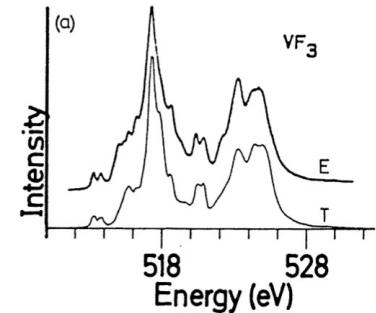
Alexander Kramida

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B.T. Thole *et al.*,
Phys. Rev. B, 31, 1985



F.M.F. de Groot *et al.*,
Phys. Rev. B, 1990

QUANTY: A MODERN APPROACH TO MULTIPLETS CALCULATIONS

The screenshot shows a Jupyter notebook cell with the following code:

```
XAS.L2,3
Once the ground-state is calculated one can calculate the spectra. This example shows the Ni 2p to 3d excitations in NiO. Note that these excitations have an energy of more than 800 electron Volt, which is much higher than the chemically relevant energy scales. Non-the-less these kind of spectroscopy contain useful information on the local ground-state wave-function and the low energy effective Hamiltonian.

This tutorial compares calculated spectra to experiment. In order to make the plots you need to download the experimental data. You can download them in a zip file here nio\_data.zip. Please unpack this file and make sure to have the folders NIO_Experiment and NIO_Radial in the same folder as you do the calculations. And as always, if used in a publication, please cite the original papers that published the data.

The input file to do these calculation is:
XAS.Quantity
-- some example code
-- This tutorial calculates the 2p to 3d x-ray absorption spectra of Ni in NiO using
-- crystal field theory

-- Within crystal-field theory the solid is approximated by a single atom in an effective
-- potential. Although an extremely crude approximation it is useful for some cases.
-- For correlated transition metal insulators it captures the right symmetry of the
-- localized open d-shell. It is useful to determine magnetic g-factors, energies of d-d
-- excitations or core level x-ray absorption. (2p to 3d excitations L23 edges)

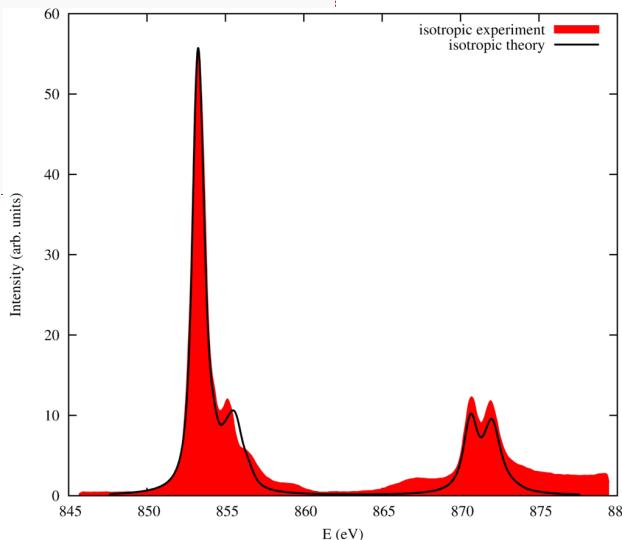
-- One should notice that the effective crystal-field potential is an affective potential
-- it is there to mimic the interaction with neighboring ligand atoms. In real materials
-- there do not exist such large electro static potentials.

-- In order to do crystal-field theory for NiO we need to define a Ni d-shell.
-- A d-shell has 10 elements and we label again the even spin-orbitals to be spin down
-- and the odd spin-orbitals to be spin up. In order to calculate 2p to 3d excitations we
-- also need a Ni 1p shell. We thus have a total of 10+6=16 fermions, 6 Ni-2p and 10 Ni-3d
-- spin-orbitals
NP=16
Np=6
IndexDn_2p={(0,2,4)}
IndexUp_2p={(1,3,5)}
IndexDn_3d={(6,8,10,12,14)}
IndexUp_3d={(7,9,11,13,15)}

The resulting spectra are: (Experimental data from Alders et al. Phys. Rev. B 57, 11623 (1998) DOI)
```

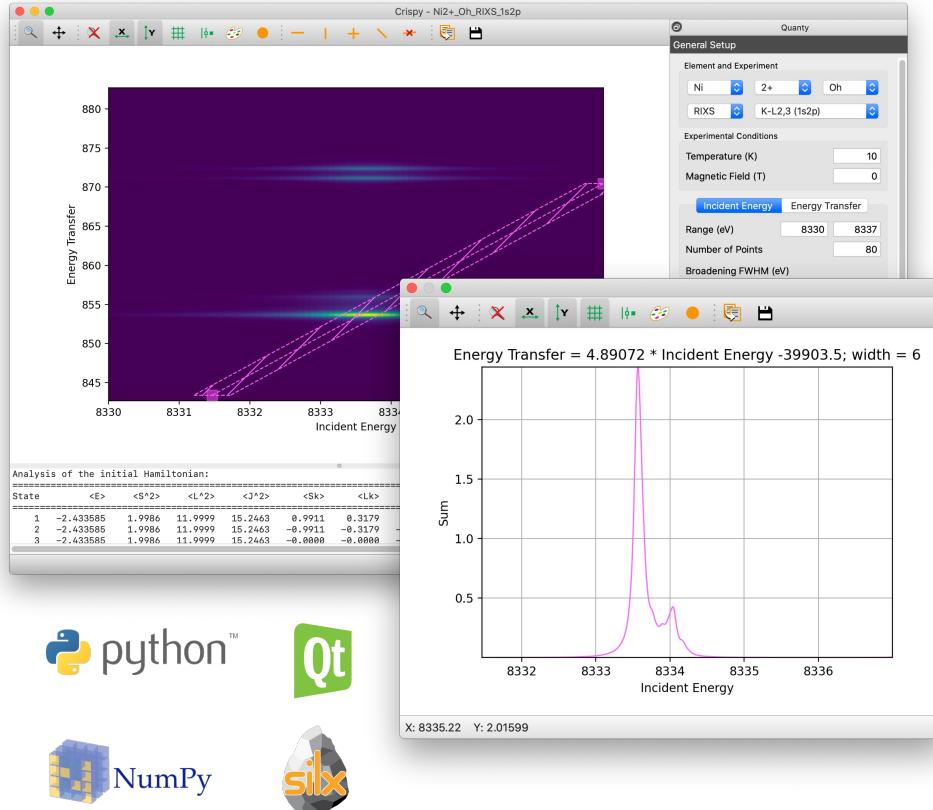
Quanty is a powerful and versatile library, but...

- You will have to write code to perform calculations.
- The program is very forgiving, and it can take a long time to spot an error.



<https://quanty.org>

CRISPY: A GRAPHICAL USER INTERFACE FOR MULTIPLETS CALCULATIONS



Calculations:

- transition metals, lanthanides, and actinides
- XAS, XMCD, X(M)LD, XES, XPS, and RIXS
- a large number of edges
- O_h , D_{4h} , C_{3v} , T_d , and D_{3h} symmetries

Additional features:

- logging console to display the progress
- dialog showing the details of a calculation
- interactive broadening using FFT
- save and load functionality
- easy-to-use installers for Windows and macOS
- Jupyter notebook interface

<https://github.com/mretegan/crispy>

SEMI-EMPIRICAL MULTIPLETS: THE HAMILTONIAN

$$H = H_{kin} + H_{en} + H_{ee} + H_{so} + H_{cf} + H_{hyb} + H_{Zeeman} + H_{ex}$$

Free ion (spherical) Crystal Field Magnetic Field Hybridization Exchange

$$H_{kin} = - \sum_i \frac{\hbar^2 \nabla_i^2}{2m}$$

Kinetic energy of the electrons

$$H_{en} = - \sum_i \sum_I \frac{Z_I e^2}{|r_i - R_I|}$$

Electron–nuclear interaction

$$H_{ee} = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|r_i - r_j|}$$

Electron–electron interaction

$$H_{so} = \sum_i \xi(r_i) \mathbf{l}_i \cdot \mathbf{s}_i$$

Spin–orbit interaction

$$H_{cf} = \sum_{k=0}^{\infty} \sum_{m=-k}^k r^k A_{k,m} C_{k,m}(\theta, \phi)$$

Crystal field potential

Electronic repulsions: direct and exchange integrals

The Slater radial integrals are reduced from their Hartree–Fock values using empirical reduction factors.

$0.7 \leq \kappa \leq 0.9$ ionic character

$0.5 \leq \kappa \leq 0.6$ covalent character

Spin-orbit coupling constants

They are usually close to the Hartree–Fock atomic values.

Crystal field parameters

Initial values are usually taken from other spectroscopies or calculations

10Dq for octahedral symmetry (O_h)

Dq, Ds, Dt with a tetragonal distortion (D_{4h})

Hybridization (configuration interaction) parameters

Many ad hoc parameters: $\Delta, U_{dd}, U_{pd}, V(e_g), V(t_{2g})$