Data analysis of XAFS data

1. XAFS data analysis and related software

2. From XAS to XAFS: data treatment procedures
3. Training: EXAFS data refinement
4. Training: XANES data analysis

https://tinyurl.com/SRSelettra2021

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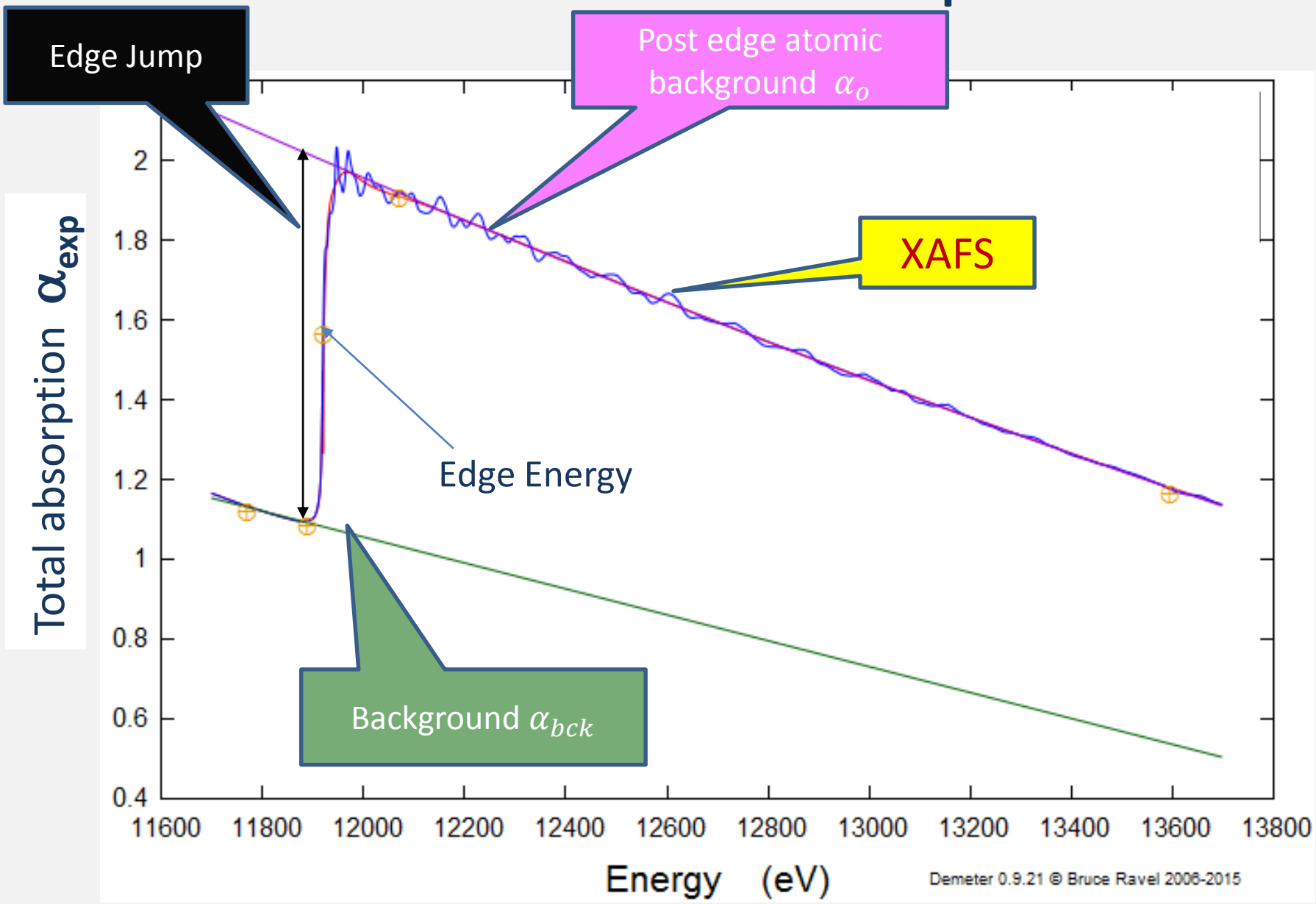
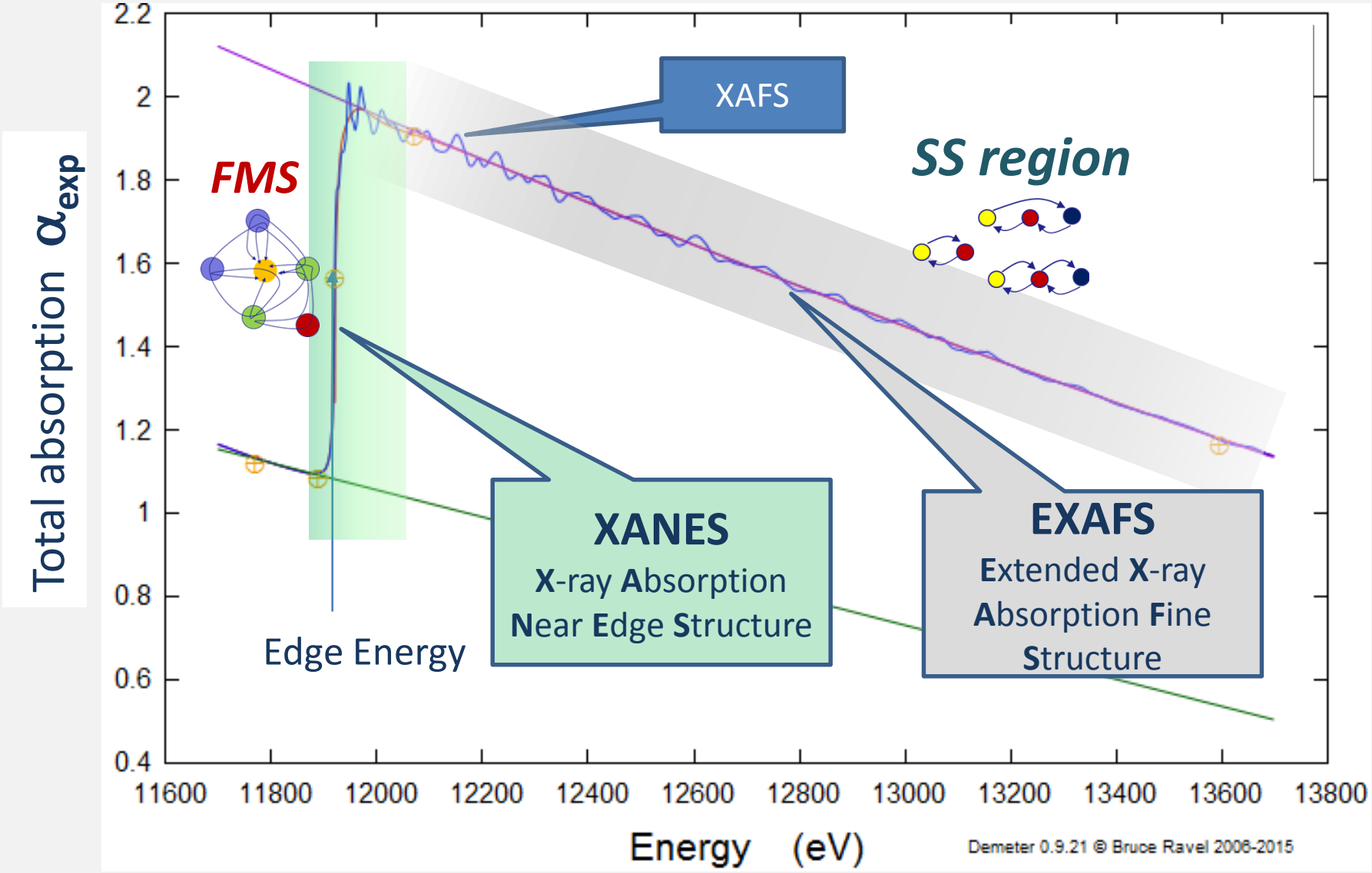
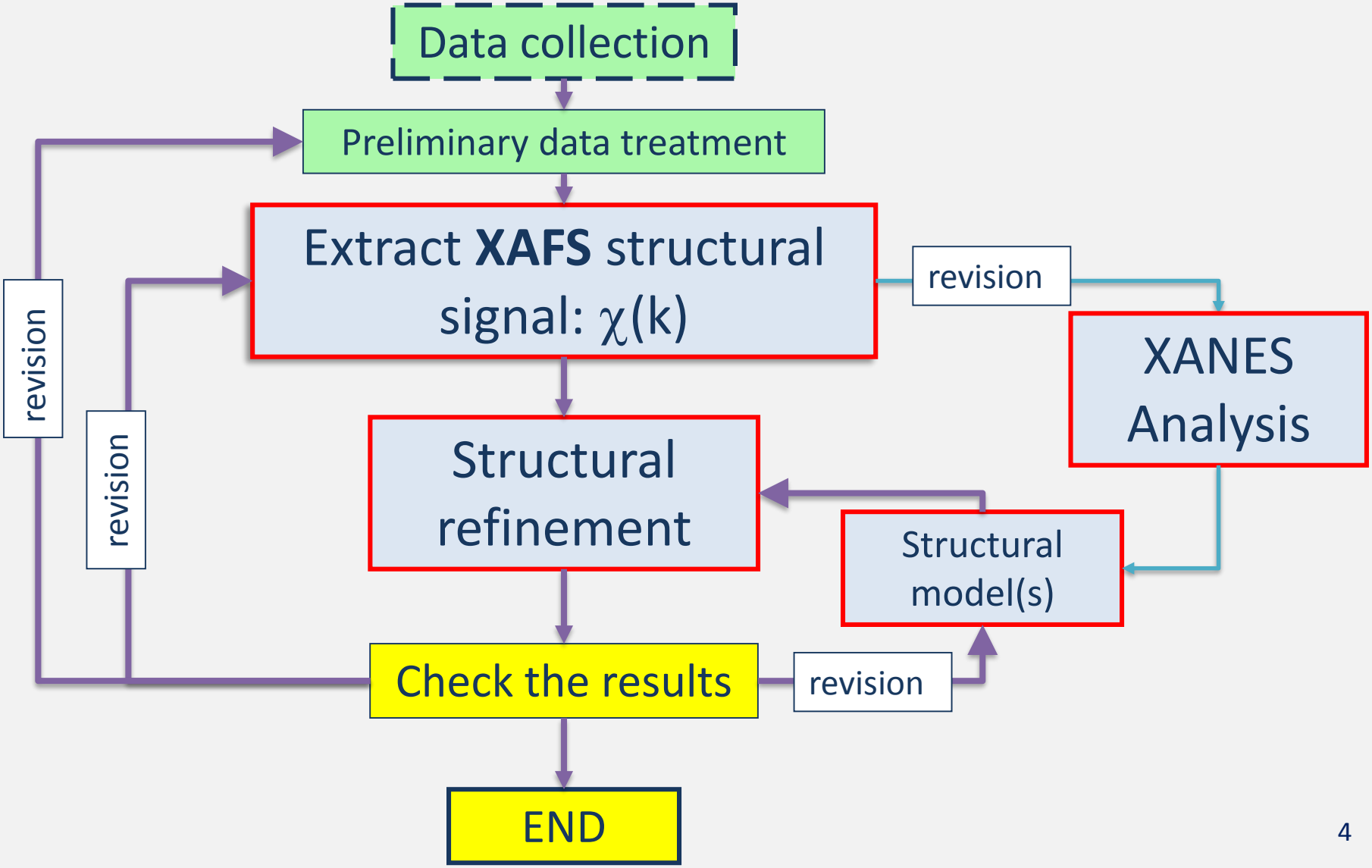
Characteristics of a XAS spectrum



Characteristics of a XAS spectrum



XAFS data ANALYSIS: from the experimental data to structural details



Software

Mandatory

- *Data manipulation software (EXCEL, ORIGIN, Gnuplot, FitYk, ….)*
- *XAFS data analysis software*

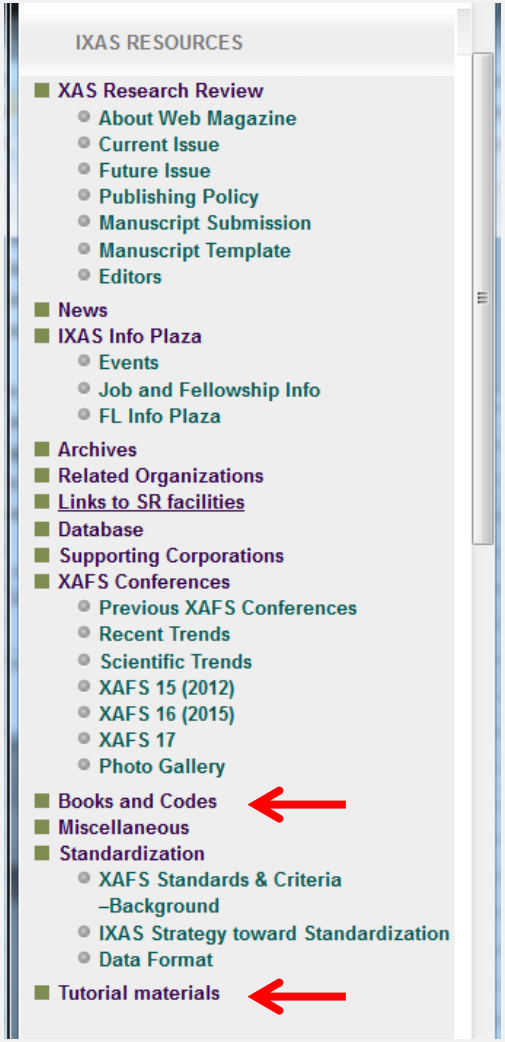
Useful:

- Database of crystallographic structures
- Atomic Structure visualization programs
- Coordination geometry calculation programs

XAFS data analysis Software

IXAFS organization

http://www.ixasportal.net/ixas/



http://feffproject.org/

bruceravel.github.io/demeter/

Simple and easy to use data analysis software, freeware, based on FEFF6 and IFEFFIT

Download and install it

Google search:
demeter EXAFS

GnXAS Software

INTRODUCTION to GNXAS

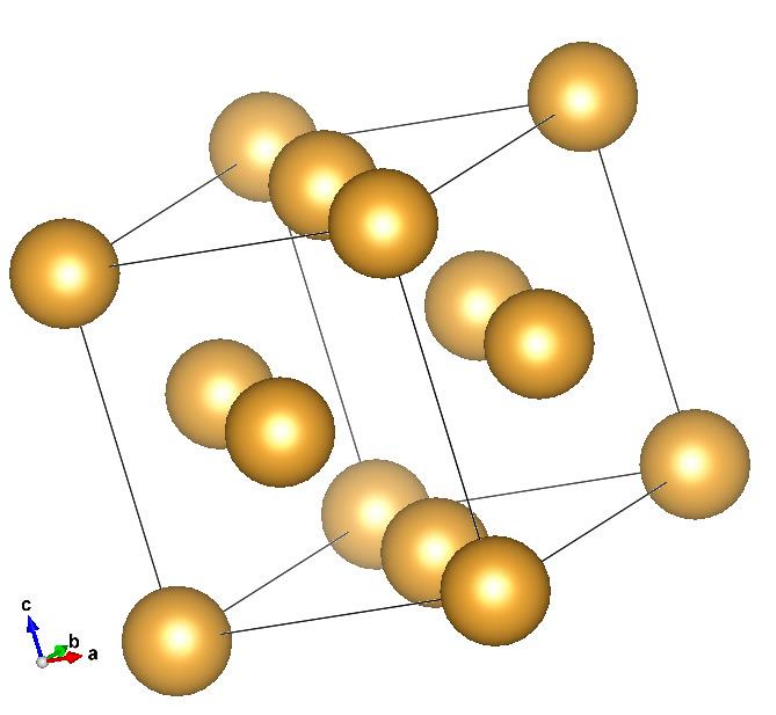
http://gnxas.unicam.it/pag_gnxas.html

The GNXAS package is and advanced software for EXAFS data analysis based on multiple-scattering (MS) calculations and a rigorous fitting procedure of the raw experimental data. The main characteristic of the software are:

- atomic phase shifts calculations in the muffin-tin approximation based on atom self-consistent relativistic calculations. Account for the neighbors is taken.
- Inclusion of inelastic losses through complex Hedin-Lundqvist potential.
- Calculation of MS signals associated with two, three, and four atom configurations using advanced algorithms.
- Use of an advanced fitting procedure that allows:
  - to fit simultaneously any number of spectra containing any number of edges,
  - to use directly the raw data without any pre-analysis,
  - to account for complex background multi-electron excitation features,
  - to use various model peaks for the pair, triplet and quadruplet distribution functions, including non Gaussian models and extremal cases. In all cases absolute parameters can be fitted,
  - to treat liquid phase or disordered systems and extract reliable g(r) functions in the short range,
  - to perform a rigorous statistical error analysis and plot two-dimensional correlation maps,
  - To provide a flexible scientific tool for EXAFS data analysis where the user has access to every stage of the calculation. **GNXAS is not a black box.**

Crystallographic structures DBs

http://www.webelements.com/



Gold: crystal structures

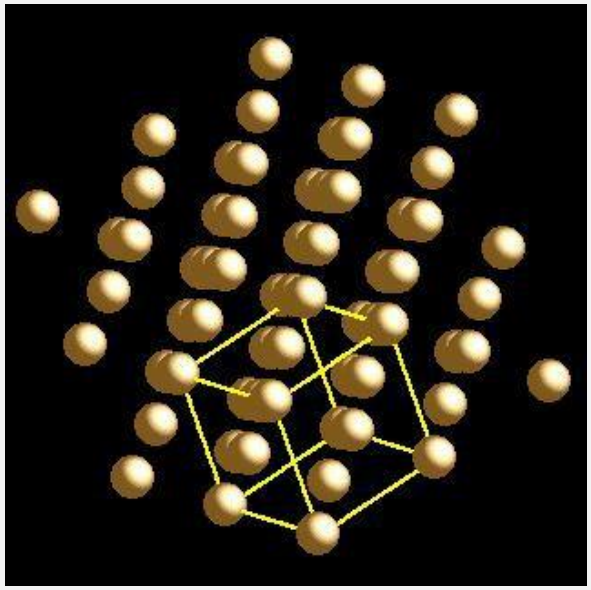
Space group: **Fm-3m**

Space group number: **225**

Structure: **ccp (cubic close-packed)**

Cell parameters:

- *a*: 407.82 pm
- *b*: 407.82 pm
- *c*: 407.82 pm
- α: 90.000°
- β: 90.000°
- γ: 90.000°



Crystallographic structures DBs

- Crystallography Open Database (COD)

www.crystallography.net

Often Synchrotron Facilities have access to commercial databases. Use them during beam-time!

- WWW-MINCRYST

database.iem.ac.ru/mincryst/

- American Mineralogist Crystal Structure DB
- rruff.geo.arizona.edu/AMS/amcsd.php

- ICSD ($): inorganic chemistry database (guest)

FIZ Karlsruhe

- Google Scholar

….

Structure Visualizers

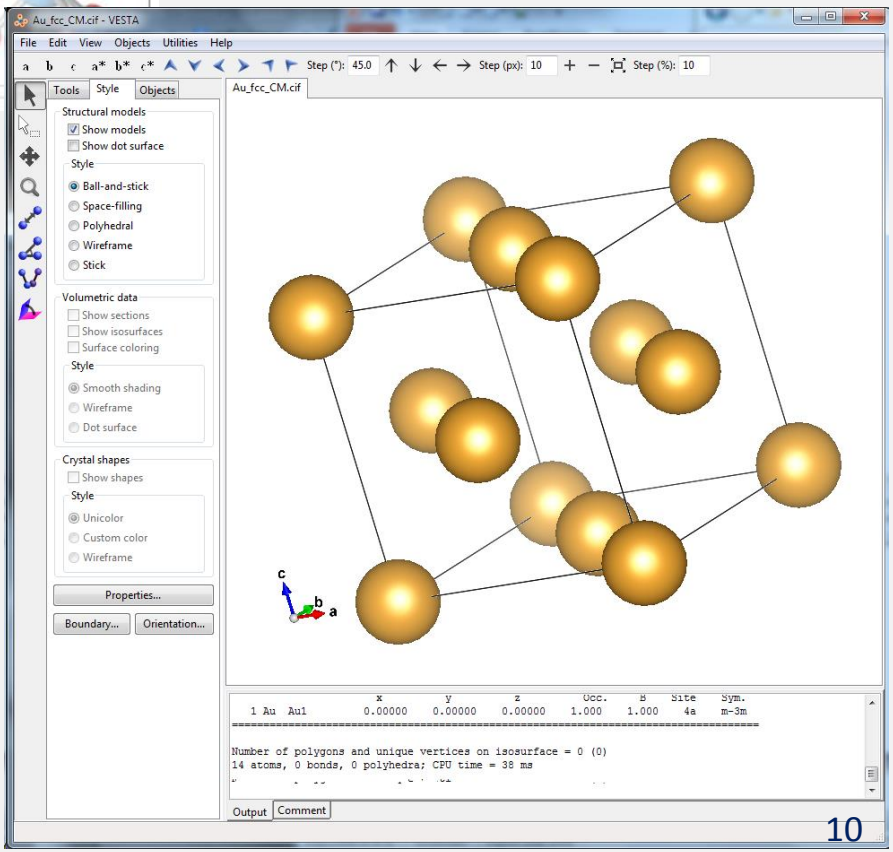
VESTA

Visualization for Electronic and STructural Analysis

Download it

http://jp-minerals.org/soft/en/

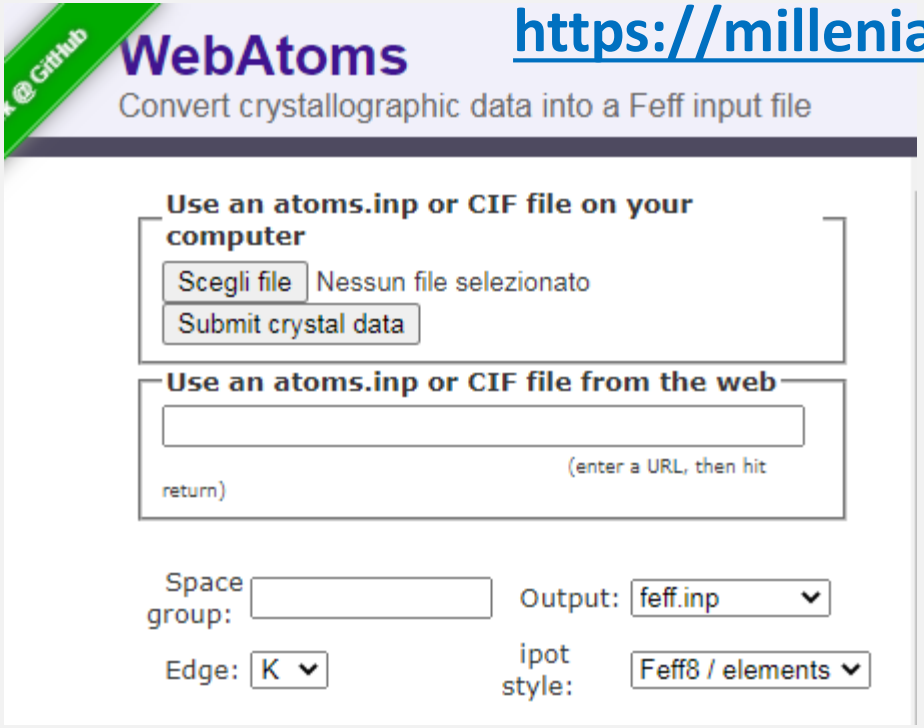
Google search:
Vesta Download



Coordination geometry

Neighbour geometry around the absorber

ATOMS package
included in the *Demeter* (Arthemis) package



https://millenia.cars.aps.anl.gov/webatoms/

Note: VESTA may read or save in ATOMS format