XAFS
Training on data Analysis

1. XAFS data analysis software

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

tinyurl.com/meneghini-sils2017

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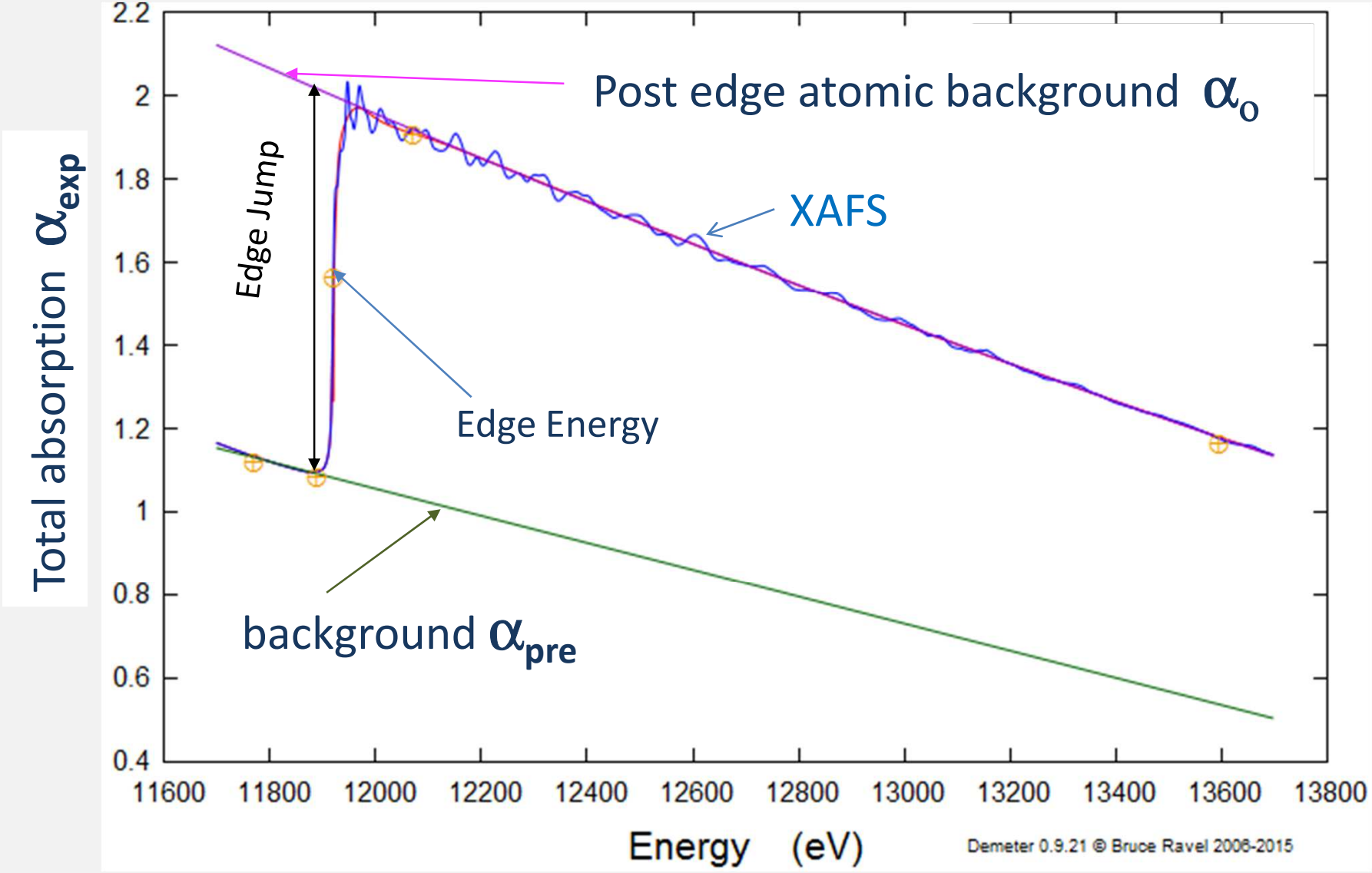
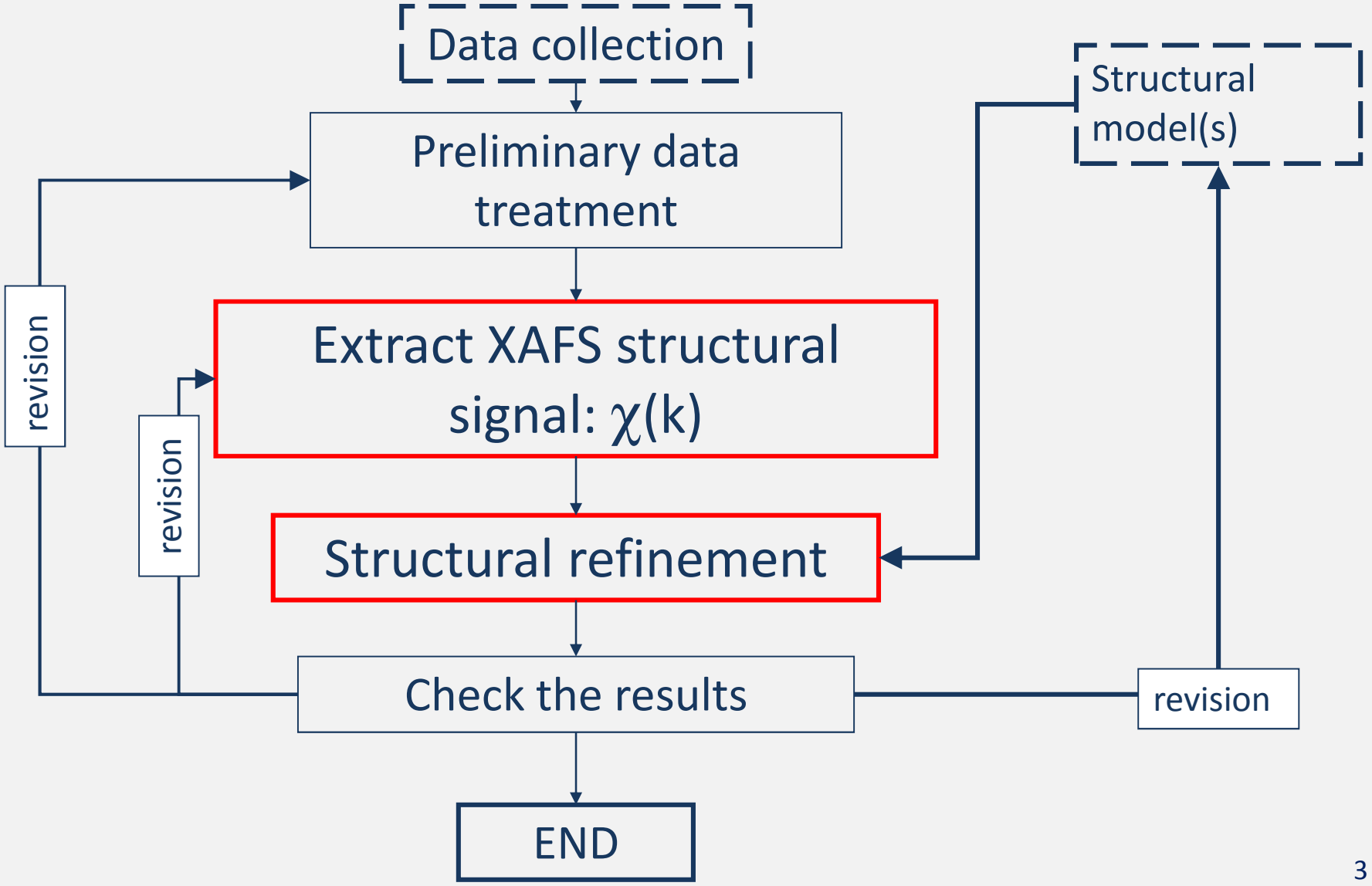
Characteristics of a XAS spectrum



XAFS data ANALYSIS: from the experimental data to structure



Software

Mandatory

- **XAFS data analysis software**

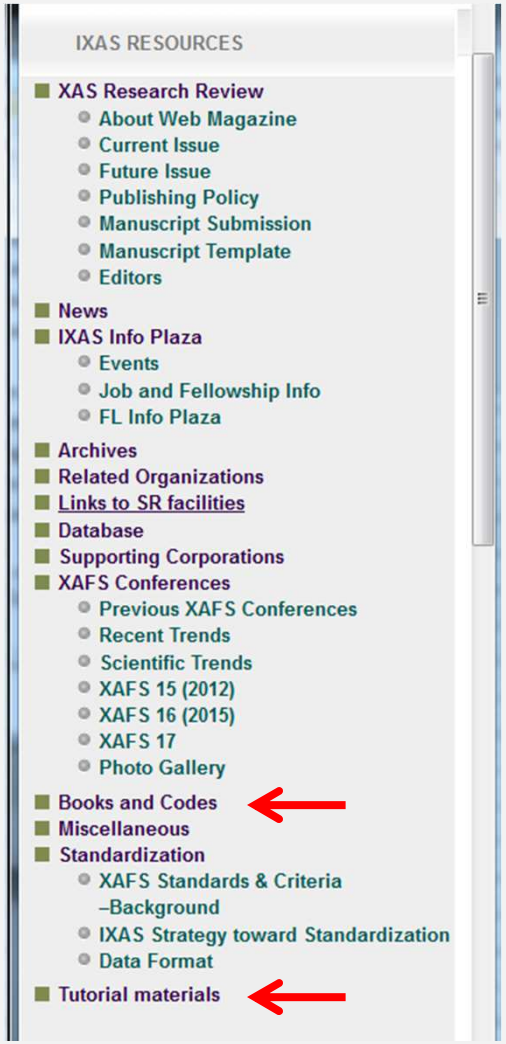
Useful:

- Database of crystallographic structures
- Structure visualization programs
- Distance and geometry calculation programs

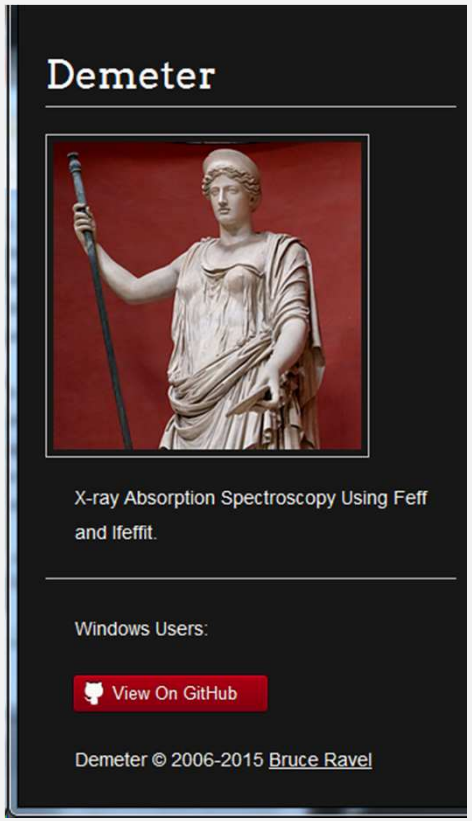
XAFS data analysis Software

IXAFS organization

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



http://feffproject.org/



bruceravel.github.io/demeter/

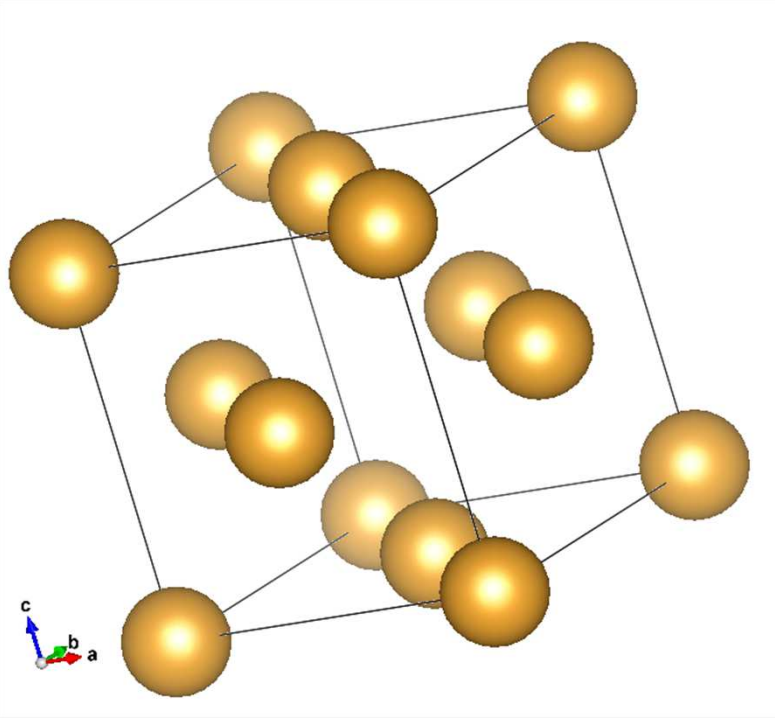
Simple and easy to use data analysis software, freeware, based on FEFF6 and IFEFFIT

Download and install it

Google search:
demeter EXAFS

Crystallographic structures DBs

http://www.webelements.com/



Gold: crystal structures

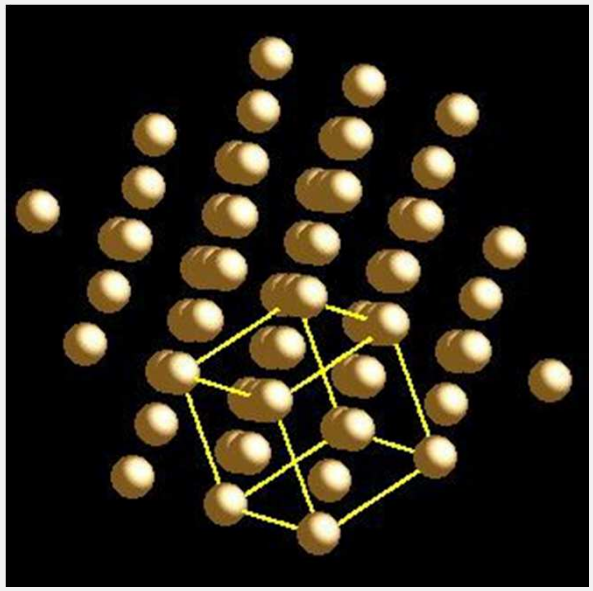
Space group: **Fm-3m**

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

Synchrotron Facilities have access to commercial databases. Use them during data collection 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

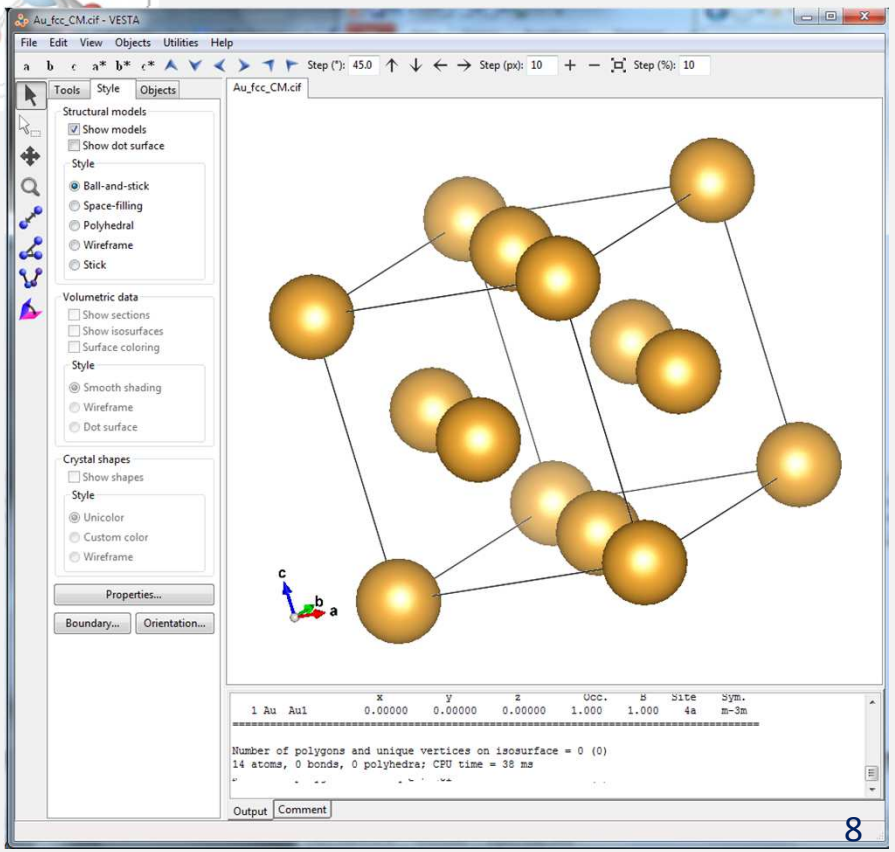
VESTA

Visualization for Electronic and STructural Analysis

Download it

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

Google search:
Vesta Download

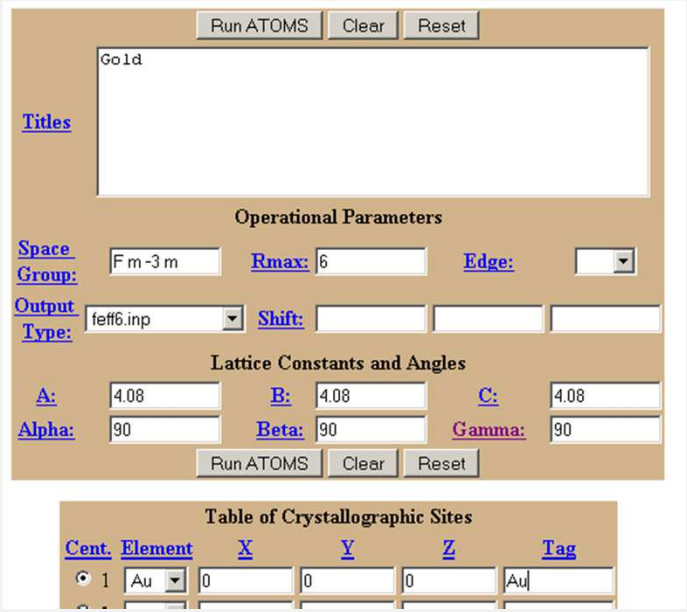


Radial distribution function

Shell distances and geometries around the absorber

ATOMS on the Web

http://millenia.cars.aps.anl.gov/cgi-bin/atoms/atoms.cgi



It is also included in the Demeter (Arthemis) package