



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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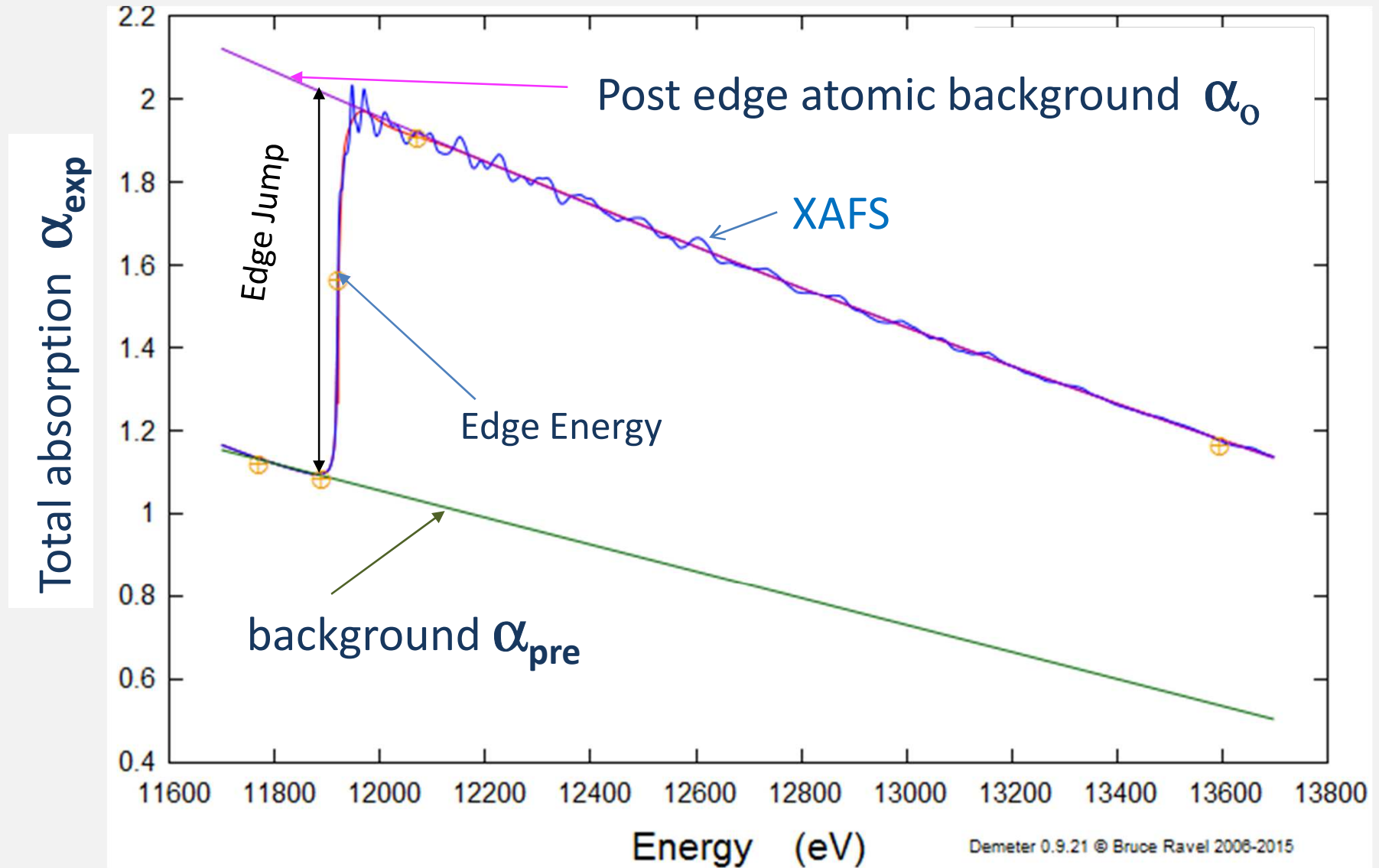
carlo.meneghini@uniroma3.it



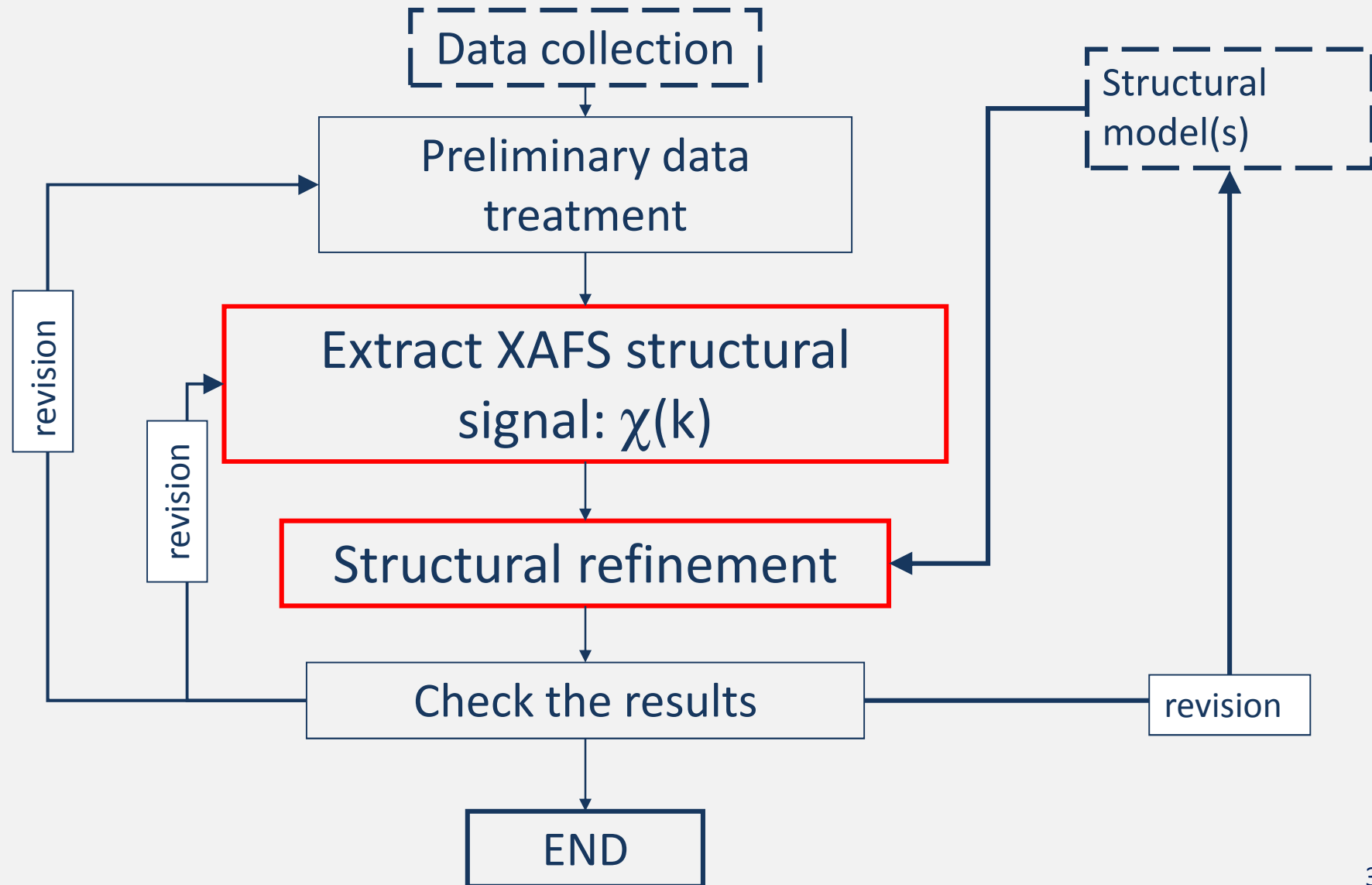
XIV School on Synchrotron Radiation:
Fundamentals, Methods and Applications
Muggia, Italy / 18-29 September 2017



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

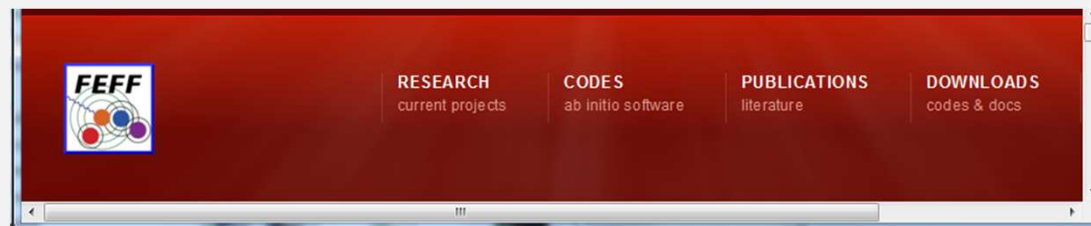
IXAFS organization

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


IXAS RESOURCES

- XAS Research Review
 - About Web Magazine
 - Current Issue
 - Future Issue
 - Publishing Policy
 - Manuscript Submission
 - Manuscript Template
 - Editors
- News
- IXAS Info Plaza
 - Events
 - Job and Fellowship Info
 - FL Info Plaza
- Archives
- Related Organizations
- [Links to SR facilities](#)
- Database
- Supporting Corporations
- XAFS Conferences
 - Previous XAFS Conferences
 - Recent Trends
 - Scientific Trends
 - XAFS 15 (2012)
 - XAFS 16 (2015)
 - XAFS 17
 - Photo Gallery
- Books and Codes ←
- Miscellaneous
- Standardization
 - XAFS Standards & Criteria –Background
 - IXAS Strategy toward Standardization
 - Data Format
- Tutorial materials ←

<http://feffproject.org/>



Demeter



X-ray Absorption Spectroscopy Using Feff and Iffeffit.

Windows Users:

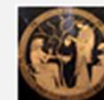
[View On GitHub](#)

Demeter © 2006-2015 [Bruce Ravel](#)

bruceravel.github.io/demeter/

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

Download and install it

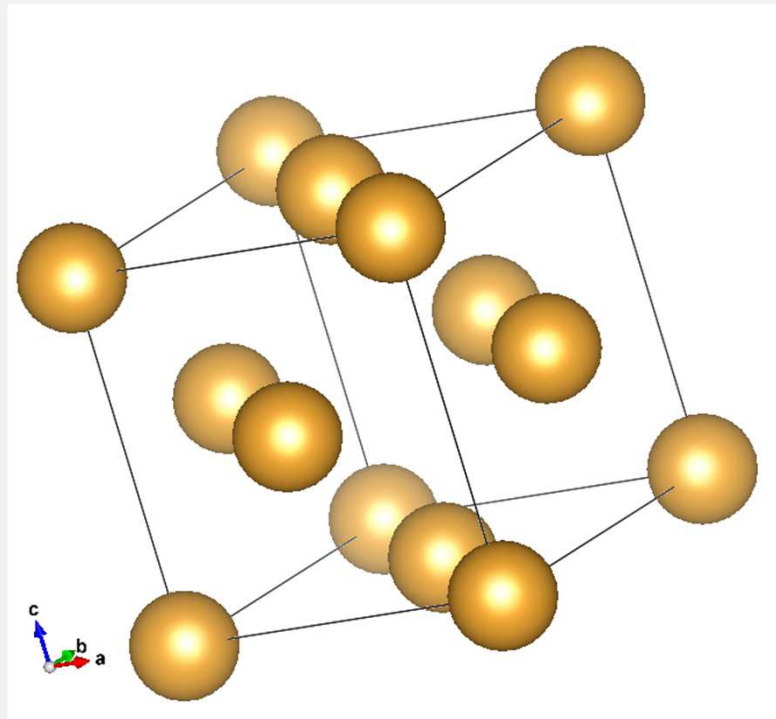


Google search:

[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

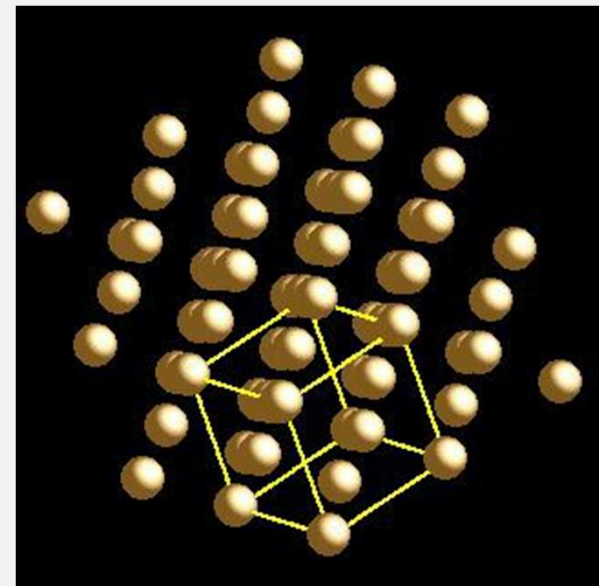
b : 407.82 pm

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

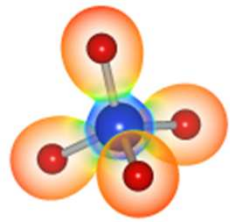
- ICSD (\$): inorganic chemistry database (guest)

FIZ Karlsruhe

- Google Scholar

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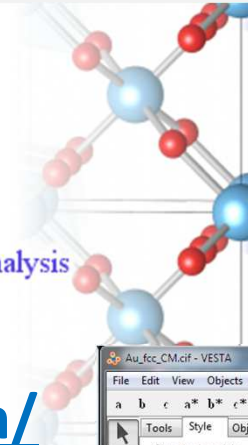
Structure Visualizers



VESTA
Visualization for Electronic and STructural Analysis

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

Google search:
Vesta Download



The screenshot shows the VESTA software window titled 'Au_fcc_CM.cif - VESTA'. The interface includes a menu bar (File, Edit, View, Objects, Utilities, Help), a toolbar, and a main 3D view area. The 3D view displays a gold (Au) crystal structure in a ball-and-stick style. The left sidebar contains several panels: 'Structural models' (with 'Show models' checked), 'Style' (with 'Ball-and-stick' selected), 'Volumetric data' (with 'Show sections', 'Show isosurfaces', and 'Surface coloring' unchecked), and 'Crystal shapes' (with 'Show shapes' unchecked). The bottom status bar shows the following data:

	x	y	z	Occ.	b	Site	Sym.
1 Au	1	1	1	1.000	1.000	4a	m-3m

Number of polygons and unique vertices on isosurface = 0 (0)
14 atoms, 0 bonds, 0 polyhedra; CPU time = 38 ms



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>

Run ATOMS Clear Reset

Gold

Titles

Operational Parameters

Space Group: Fm-3m Rmax: 6 Edge:

Output Type: feff6.inp Shift:

Lattice Constants and Angles

A: 4.08 B: 4.08 C: 4.08

Alpha: 90 Beta: 90 Gamma: 90

Run ATOMS Clear Reset

Table of Crystallographic Sites

Cent.	Element	X	Y	Z	Tag
1	Au	0	0	0	Au

It is also included in the Demeter (Arthemis) package