Theory of XANES and EXAFS

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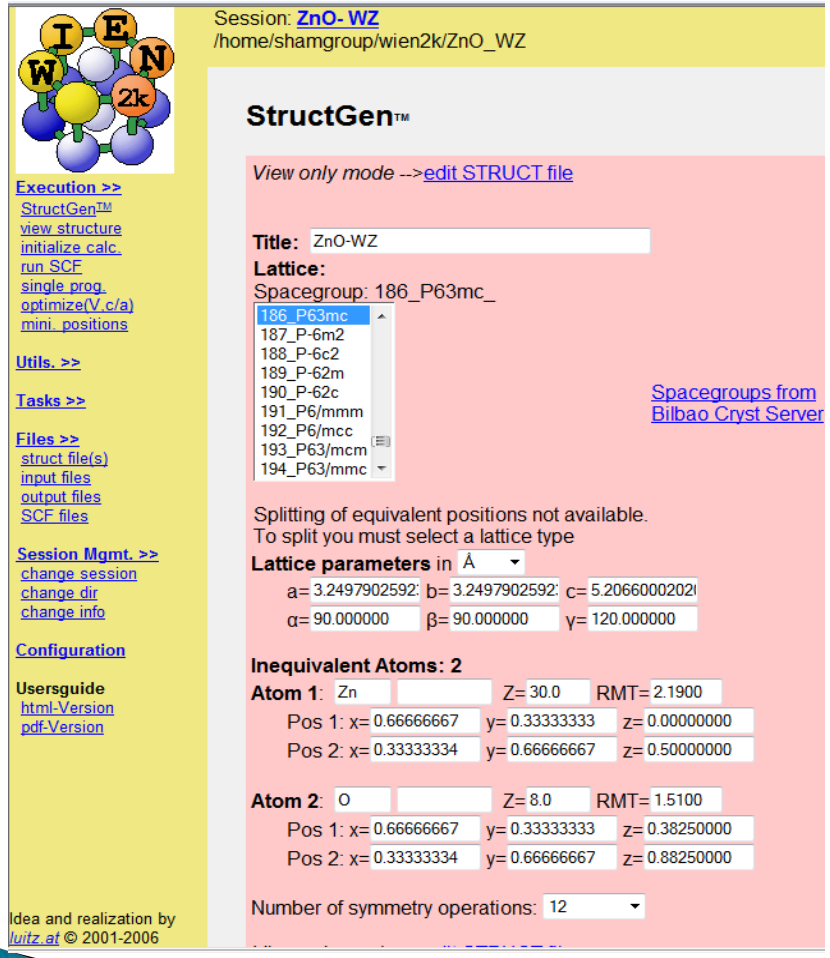
Group Work Shop 2013

XANES and EXAFS Theory

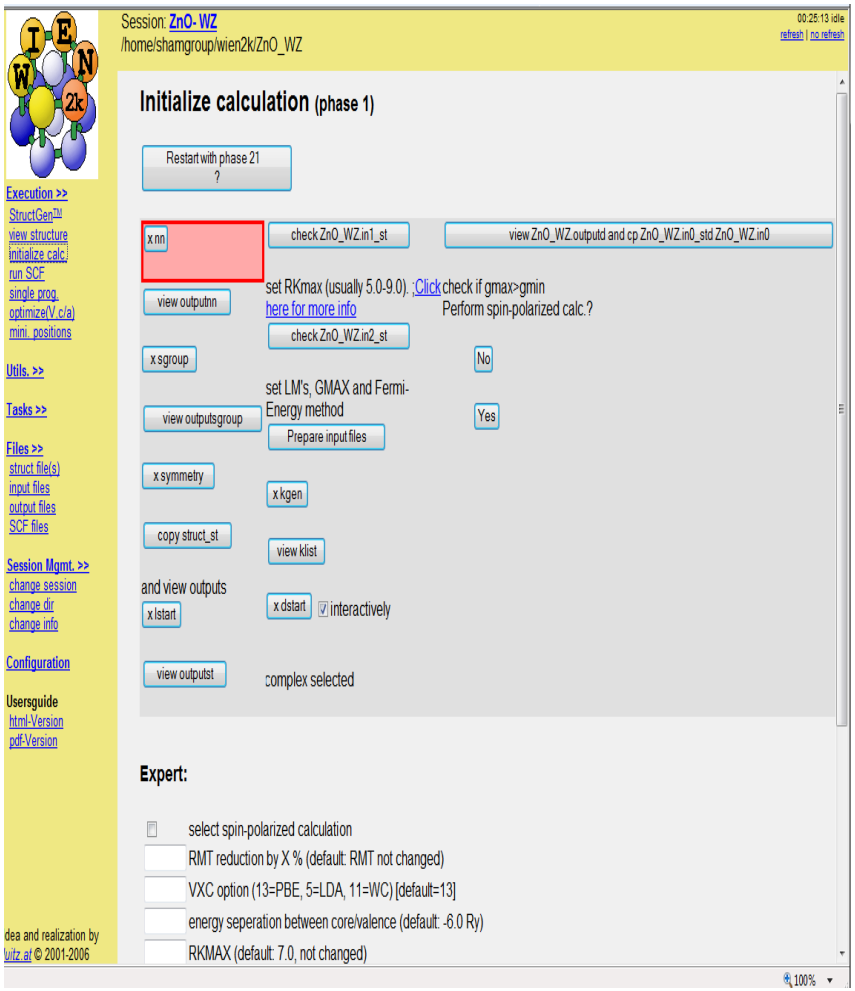
- Density Functional Theory:
  - Computer code (wien2k)
    - Local Density Approximation
    - Generalized Gradient Approximation
- Real Space Multiple Scattering Theory:
  - Computer code (FEFF9)
- Artemis
- Athena

- Workstations:
  - Duxeon.chem.uwo.ca
    - 129.100.60.115
  - xeony.chem.uwo.ca
    - 129.100.60.33
  - Lockin-name: yyiu
  - Lockin-name: shamgroup
- http://129.100.60.115:7890
  - yyiu
- http://129.100.60.115:1234
  - shamgroup
- http://129.100.60.33:7890
  - yyiu

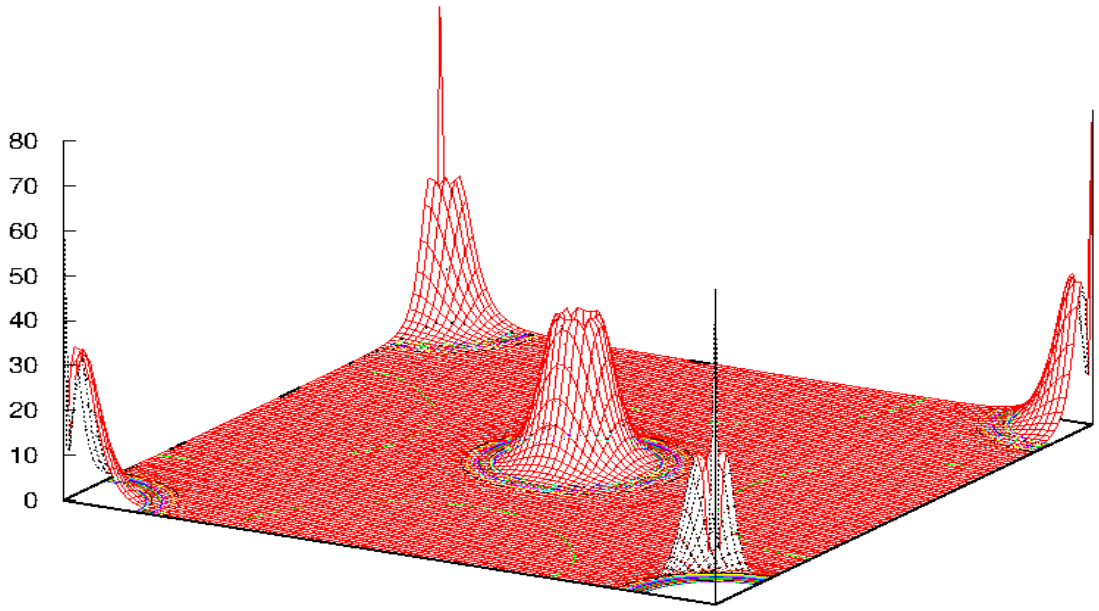
Structure Generation of WIEN2k



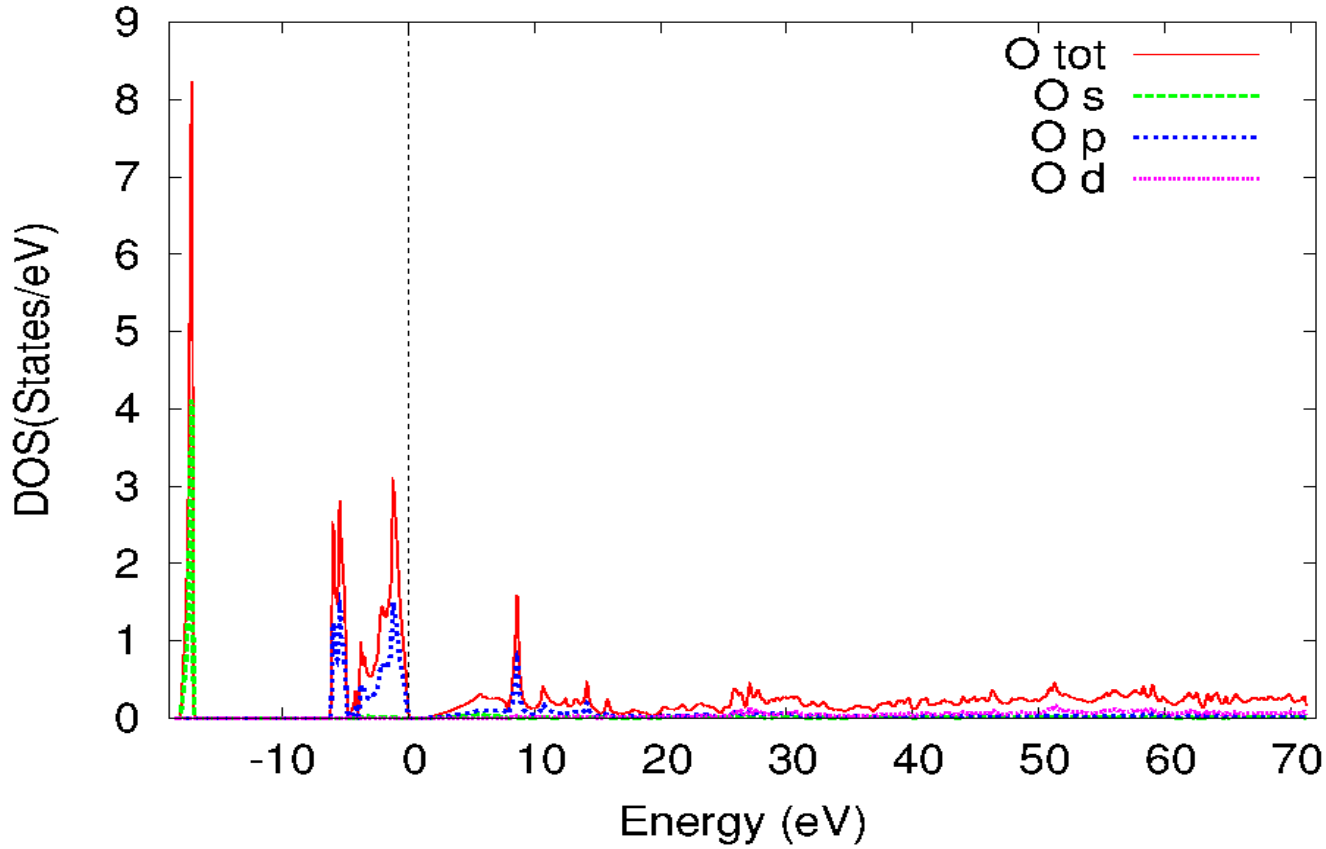
WIEN Initialized Calculation



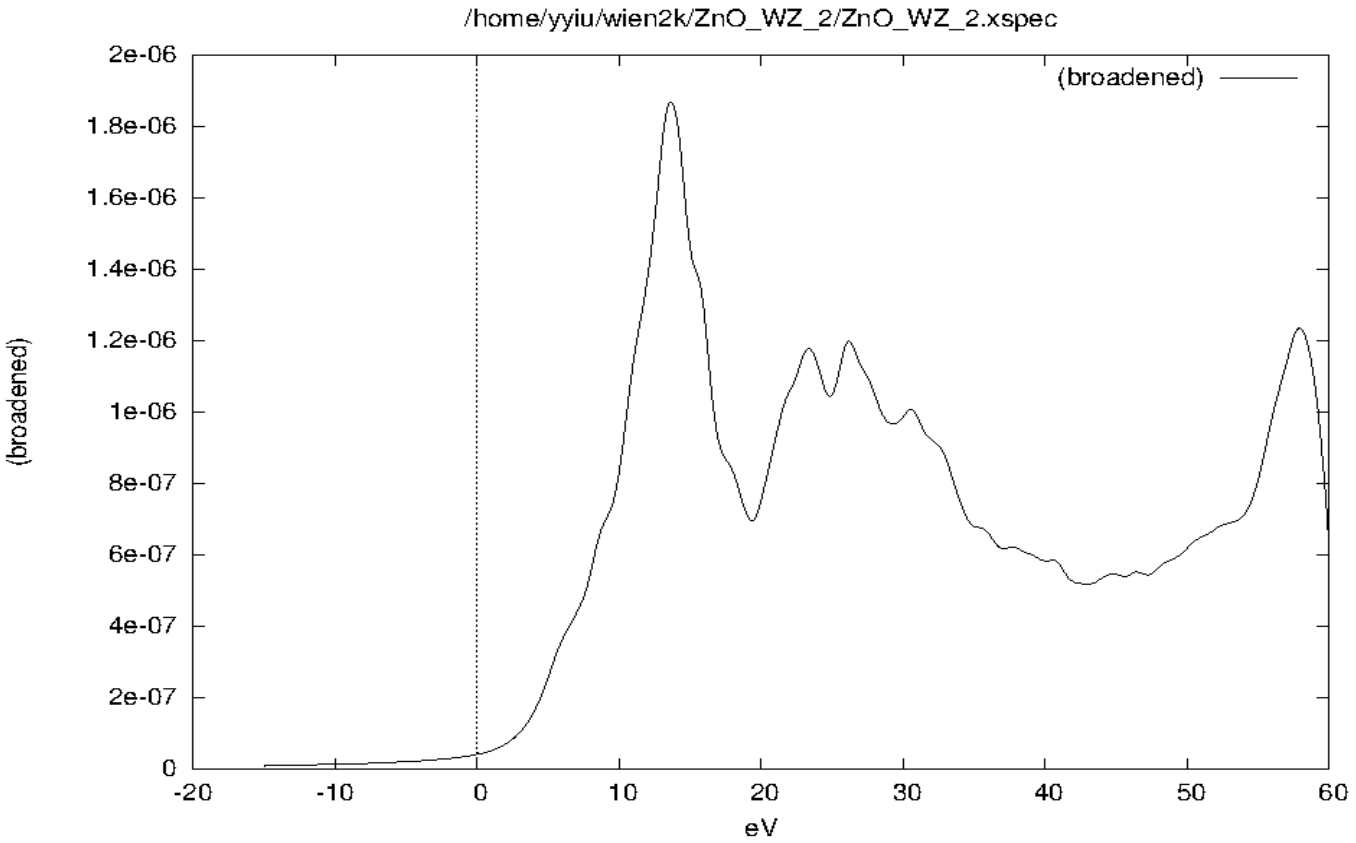
Electron density of ZnSe (plane 100)



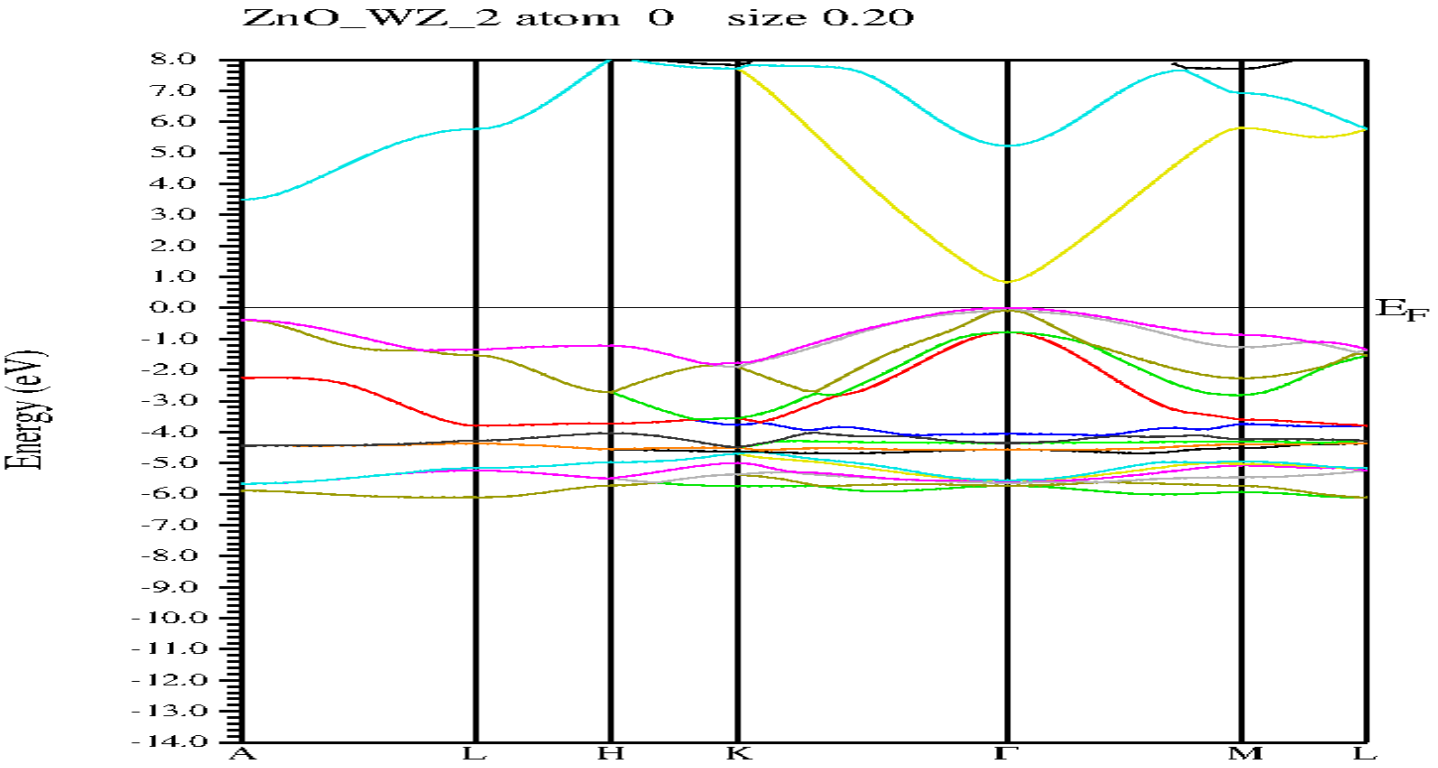
O Partial Density of States of ZnO (WZ)



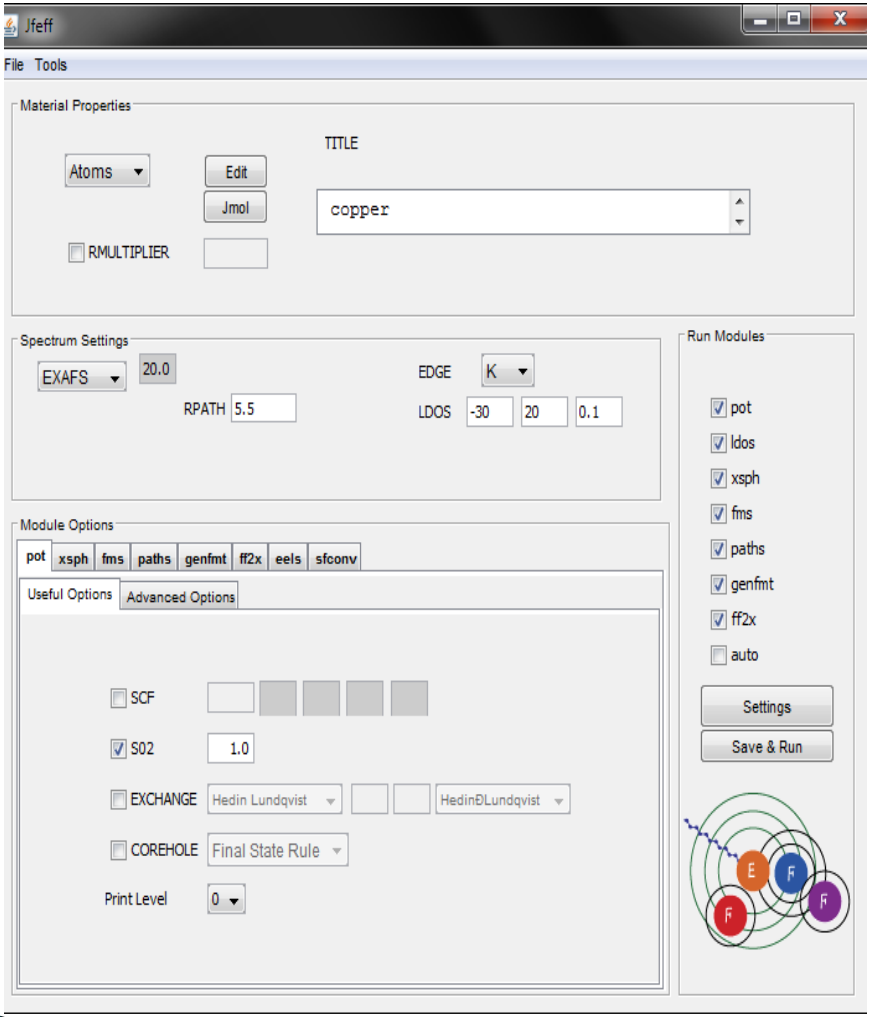
Zn K-edge of ZnO (WZ)



Band structure of ZnO (WZ)



FEFF9

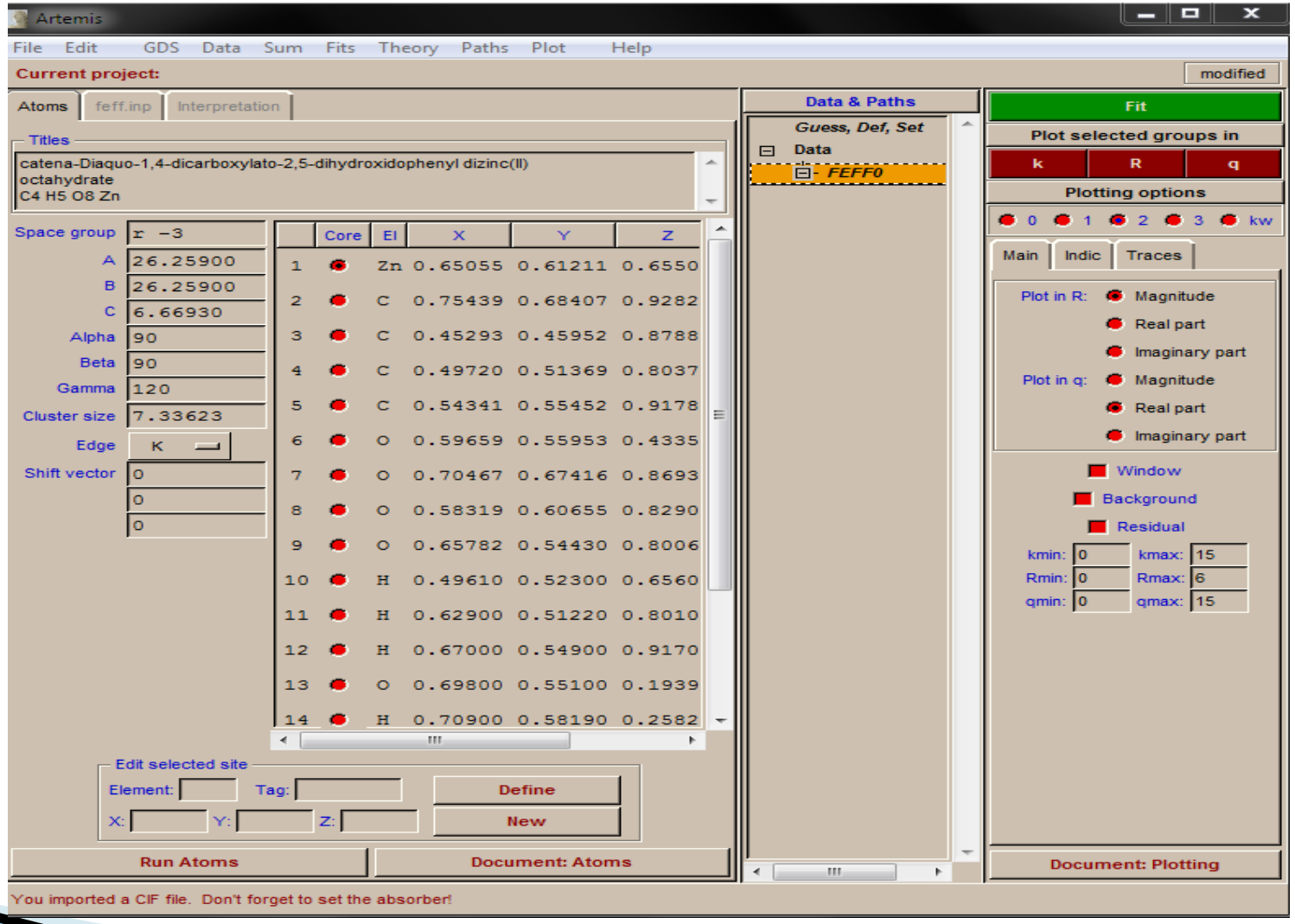


HOLE 1 1.0 * Ca K edge (4038.50 eV), second number is S0^2
* mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1 1 1
PRINT 1 0 0 0 0 0
RMAX 8.0
LDOS -10 50 0.1
SCF 3.7 0 30 0.05 10
FMS 5.1
RPATH 1.0
*AFOLP 1.0
XANES 6.0 0.05 0.2
*CRITERIA curved plane
*DEBYE temp debye-temp
NLEG 4
POTENTIALS
* ipot Z element
0 20 Ca
1 20 Ca
2 74 W
3 8 O

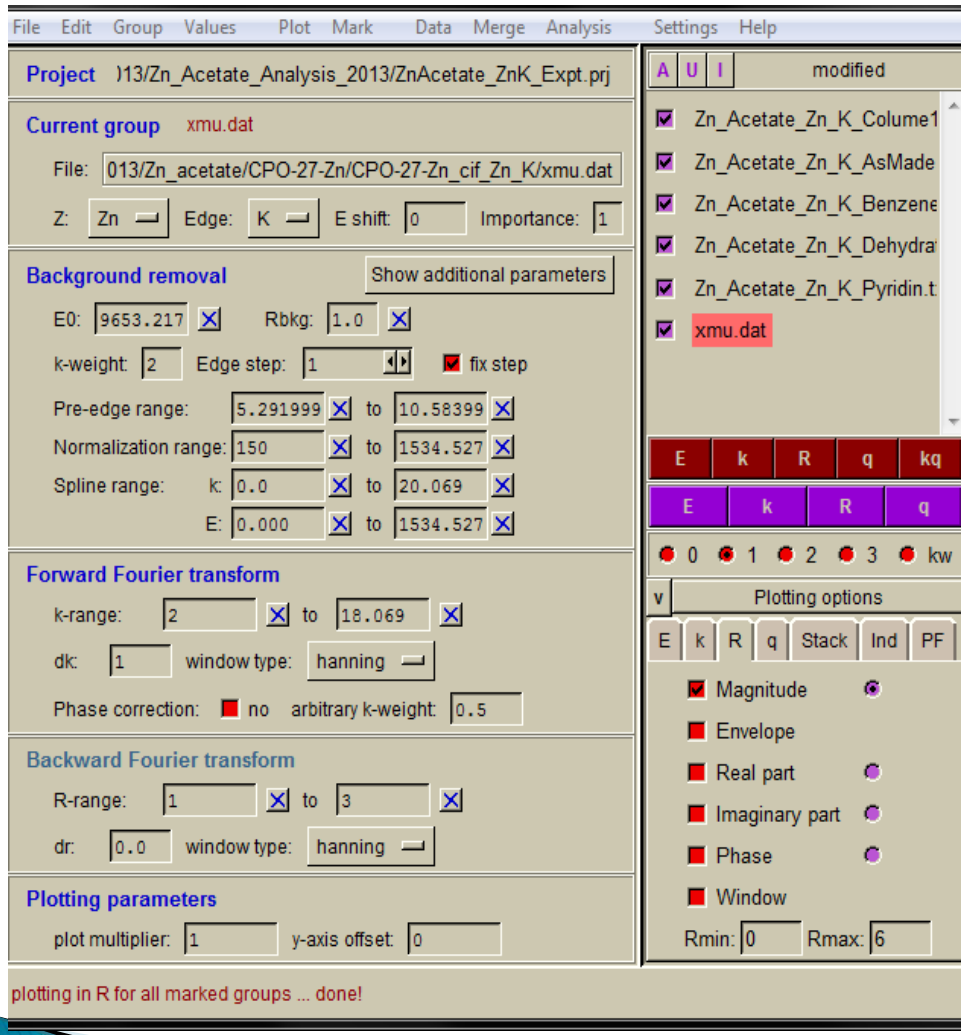
ATOMS * this list contains 317 atoms

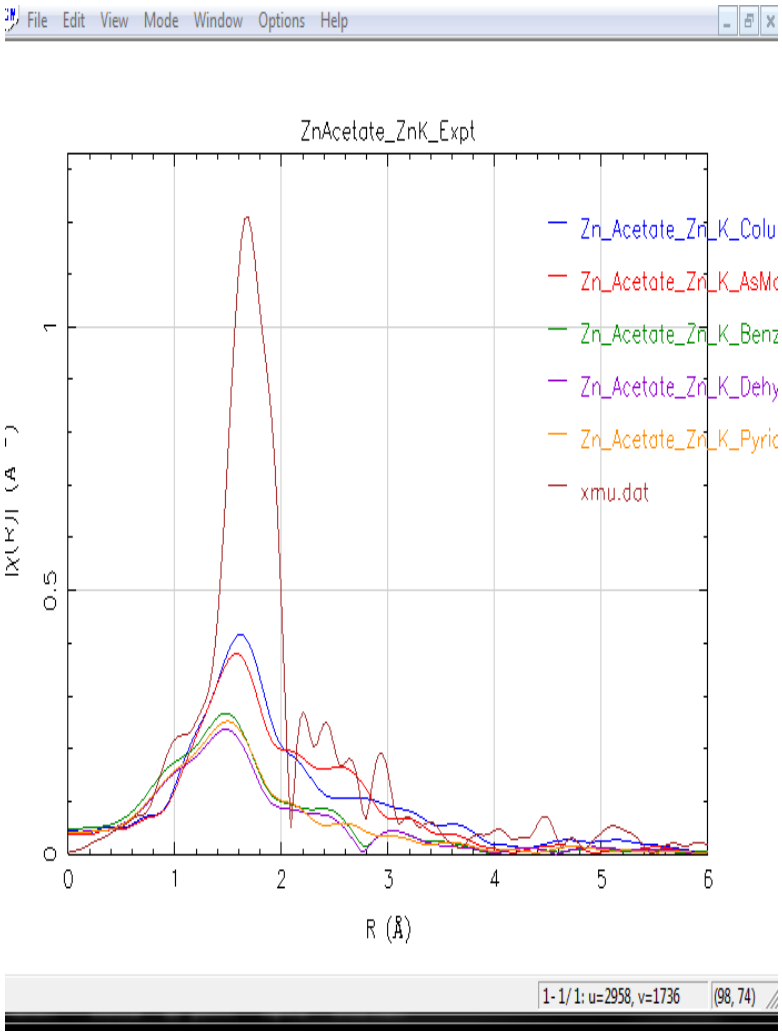
* x	y	z	ipot	tag	distance
0.00000	0.00000	0.00000	0	Ca1	0.00000
0.79222	1.35636	0.97947	3	O1_1	1.85113
-0.79222	-1.35636	-0.97947	3	O1_1	1.85113
0.51853	-0.04561	1.86453	3	O2_1	1.93583

Artemis


Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
Current project:
modified
Atoms
feff.inp
Interpretation
Titles
catena-Diaquo-1,4-dicarboxylato-2,5-dihydroxidophenyl dizinc(II)
octahydrate
C4 H5 O8 Zn
Space group r -3
A 26.25900
B 26.25900
C 6.66930
Alpha 90
Beta 90
Gamma 120
Cluster size 7.33623
Edge K
Shift vector 0 0 0
Core El X Y Z
1 Zn 0.65055 0.61211 0.6550
2 C 0.75439 0.68407 0.9282
3 C 0.45293 0.45952 0.8788
4 C 0.49720 0.51369 0.8037
5 C 0.54341 0.55452 0.9178
6 O 0.59659 0.55953 0.4335
7 O 0.70467 0.67416 0.8693
8 O 0.58319 0.60655 0.8290
9 O 0.65782 0.54430 0.8006
10 H 0.49610 0.52300 0.6560
11 H 0.62900 0.51220 0.8010
12 H 0.67000 0.54900 0.9170
13 O 0.69800 0.55100 0.1939
14 H 0.70900 0.58190 0.2582
Edit selected site
Element: Tag: Define
X: Y: Z: New
Run Atoms
Document: Atoms
Data & Paths
Guess, Def, Set
Data
FEFF0
Fit
Plot selected groups in
k R q
Plotting options
0 1 2 3 kw
Main Indic Traces
Plot in R: Magnitude
Real part
Imaginary part
Plot in q: Magnitude
Real part
Imaginary part
Window
Background
Residual
kmin: 0 kmax: 15
Rmin: 0 Rmax: 6
qmin: 0 qmax: 15
Document: Plotting
You imported a CIF file. Don't forget to set the absorber!

Athena


File Edit Group Values Plot Mark Data Merge Analysis Settings Help
Project)13/Zn_Acetate_Analysis_2013/ZnAcetate_ZnK_Expt.prj
Current group xmu.dat
File: 013/Zn_acetate/CPO-27-Zn/CPO-27-Zn_cif_Zn_K/xmu.dat
Z: Zn Edge: K E shift: 0 Importance: 1
Background removal
Show additional parameters
E0: 9653.217 Rbkg: 1.0
k-weight: 2 Edge step: 1 fix step
Pre-edge range: 5.291999 to 10.58399
Normalization range: 150 to 1534.527
Spline range: k: 0.0 to 20.069
E: 0.000 to 1534.527
Forward Fourier transform
k-range: 2 to 18.069
dk: 1 window type: hanning
Phase correction: no arbitrary k-weight: 0.5
Backward Fourier transform
R-range: 1 to 3
dr: 0.0 window type: hanning
Plotting parameters
plot multiplier: 1 y-axis offset: 0
A U I modified
Zn_Acetate_Zn_K_Colume1
Zn_Acetate_Zn_K_AsMade
Zn_Acetate_Zn_K_Benzene
Zn_Acetate_Zn_K_Dehydra
Zn_Acetate_Zn_K_Pyridin.t
xmu.dat
E k R q kq
E k R q
0 1 2 3 kw
Plotting options
E k R q Stack Ind PF
Magnitude
Envelope
Real part
Imaginary part
Phase
Window
Rmin: 0 Rmax: 6
plotting in R for all marked groups ... done!


File Edit View Mode Window Options Help
ZnAcetate_ZnK_Expt
Zn_Acetate_Zn_K_Colu
Zn_Acetate_Zn_K_AsMc
Zn_Acetate_Zn_K_Benz
Zn_Acetate_Zn_K_Dehy
Zn_Acetate_Zn_K_Pyric
xmu.dat
|χ(R)| (Å⁻³)
0
0.5
1
0 1 2 3 4 5 6
R (Å)
1-1/1: u=2958, v=1736
(98, 74)

References

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