

Theory of XANES and EXAFS

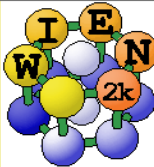
Yun-Mui Yiu
Group Work Shop 2013

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](http://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



Session: **ZnO- WZ**
/home/shamgroup/wien2k/ZnO_WZ

StructGen™

View only mode --> [edit STRUCT file](#)

Title: ZnO-WZ

Lattice:
Spacegroup: 186_P63mc_

- 186_P63mc_ ▲
- 187_P-6m2
- 188_P-6c2
- 189_P-62m
- 190_P-62c
- 191_P6/mmm
- 192_P6/mcc
- 193_P63/mcm (=)
- 194_P63/mmc ▾

[Spacegroups from Bilbao Cryst Server](#)

Splitting of equivalent positions not available.
To split you must select a lattice type

Lattice parameters in Å

a= 3.2497902592 b= 3.2497902592 c= 5.2066000202
α= 90.000000 β= 90.000000 γ= 120.000000

Inequivalent Atoms: 2

Atom 1: Zn Z= 30.0 RMT= 2.1900

Pos 1:	x= 0.66666667	y= 0.33333333	z= 0.00000000
Pos 2:	x= 0.33333334	y= 0.66666667	z= 0.50000000

Atom 2: O Z= 8.0 RMT= 1.5100

Pos 1:	x= 0.66666667	y= 0.33333333	z= 0.38250000
Pos 2:	x= 0.33333334	y= 0.66666667	z= 0.88250000

Number of symmetry operations: 12 ▾

Idea and realization by [lutz.at](#) © 2001-2006

Execution >>
[StructGen™](#)
[view structure](#)
[initialize calc.](#)
[run SCF](#)
[single prog.](#)
[optimize\(V,c/a\)](#)
[mini. positions](#)

Utils. >>

Tasks >>


Files >>
[struct file\(s\)](#)
[input files](#)
[output files](#)
[SCF files](#)

Session Mgmt. >>
[change session](#)
[change dir](#)
[change info](#)

Configuration

Usersguide
[html-Version](#)
[pdf-Version](#)

WIEN Initialized Calculation



Session: **ZnO- WZ**
/home/shamgroup/wien2k/ZnO_WZ

00:25:13 idle
[refresh](#) | [no refresh](#)

Initialize calculation (phase 1)

Restart with phase 21 ?

x nn

set RKmax (usually 5.0-9.0). [Click here for more info](#) check if gmax=gmin
Perform spin-polarized calc.?

x sgroup

set LM's, GMAX and Fermi-Energy method

x symmetry

and view outputs interactively

complex selected

Expert:

select spin-polarized calculation

RMT reduction by X % (default: RMT not changed)

VXC option (13=PBE, 5=LDA, 11=WC) (default=13)

energy separation between core/valence (default: -6.0 Ry)

RKMAX (default: 7.0, not changed)

Idea and realization by [lutz.at](#) © 2001-2006

Execution >>
[StructGen™](#)
[view structure](#)
[initialize calc.](#)
[run SCF](#)
[single prog.](#)
[optimize\(V,c/a\)](#)
[mini. positions](#)

Utils. >>

Tasks >>

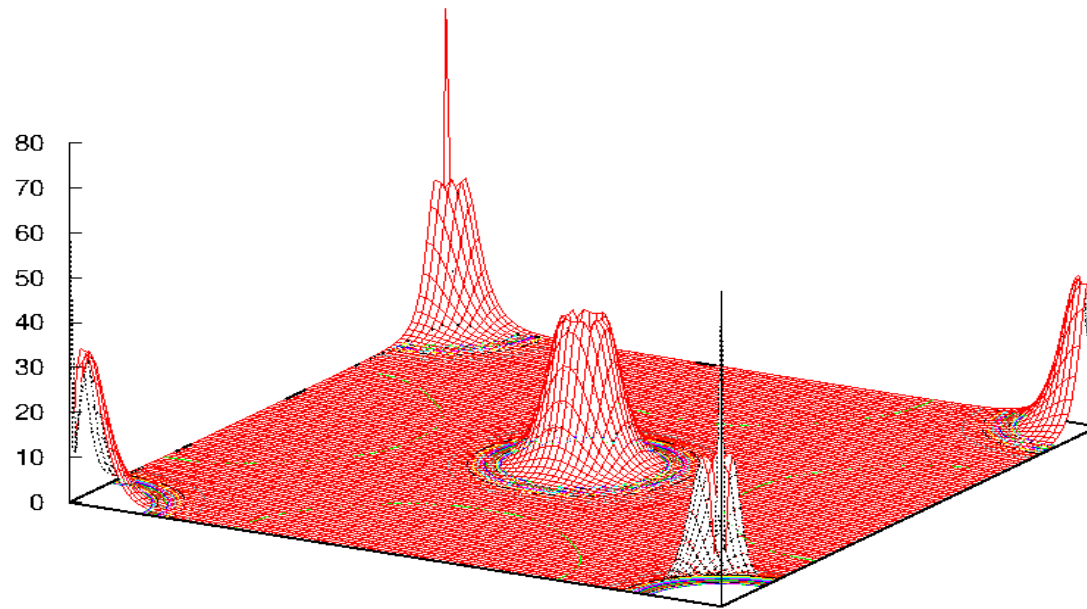
Files >>
[struct file\(s\)](#)
[input files](#)
[output files](#)
[SCF files](#)

Session Mgmt. >>
[change session](#)
[change dir](#)
[change info](#)

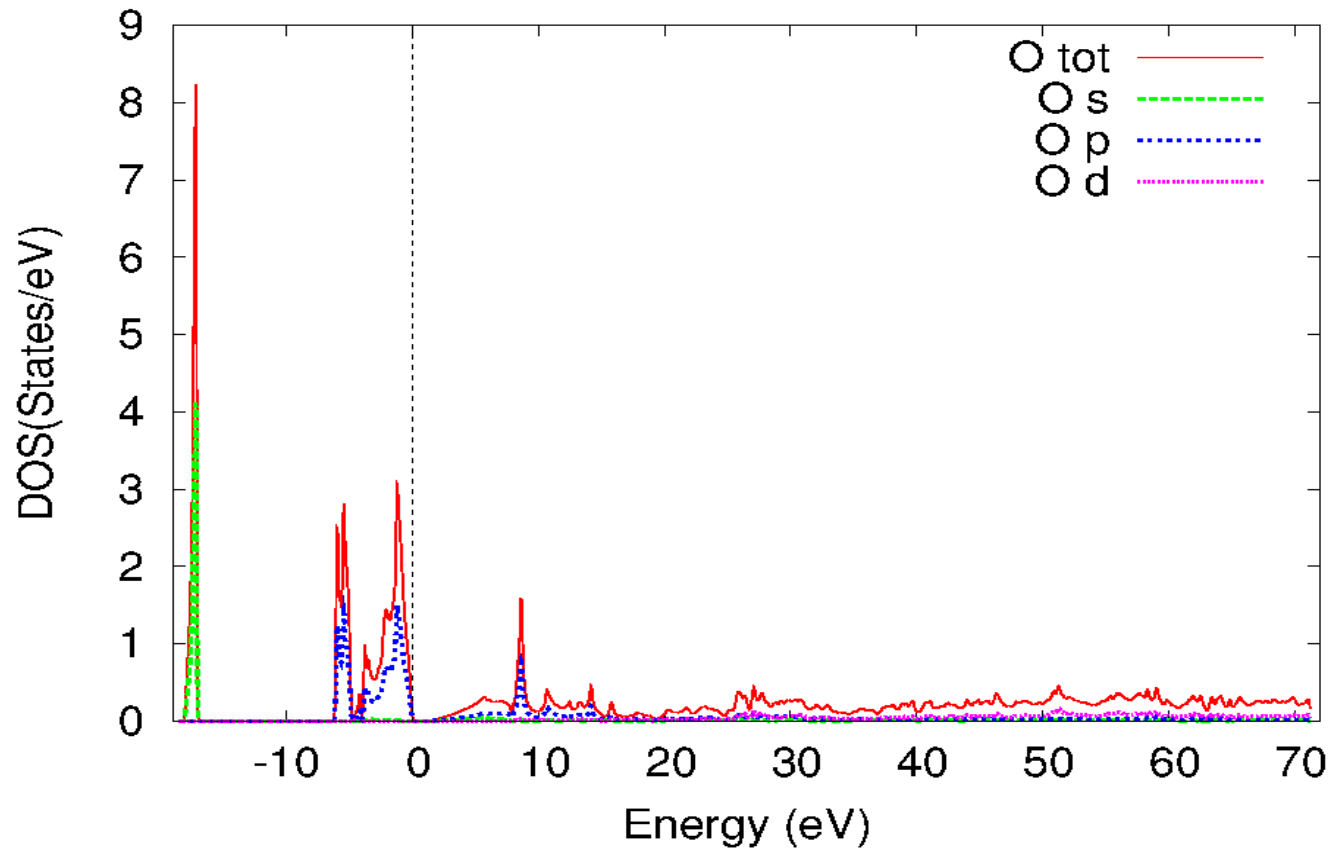
Configuration

Usersguide
[html-Version](#)
[pdf-Version](#)

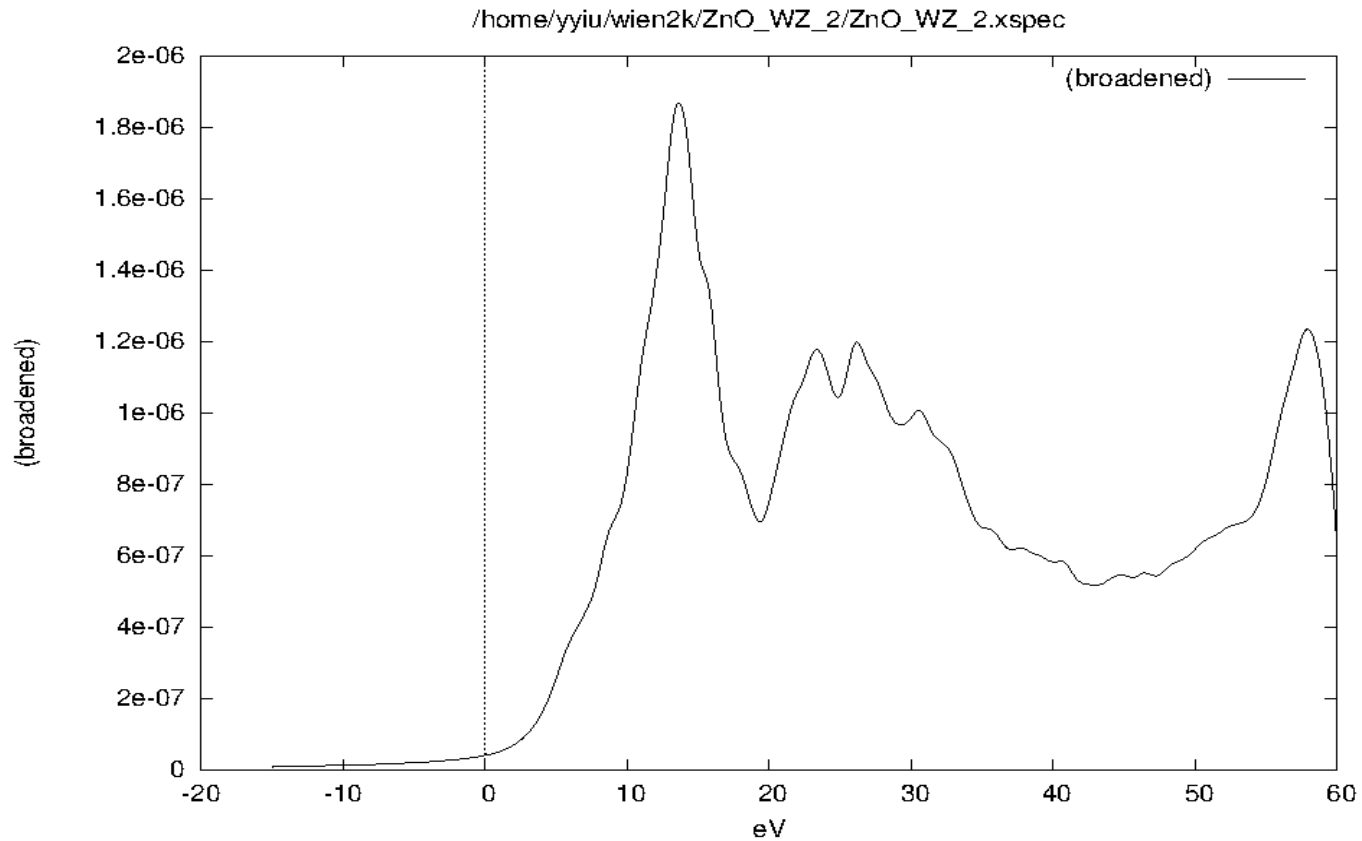
Electron density of ZnSe (plane 100)



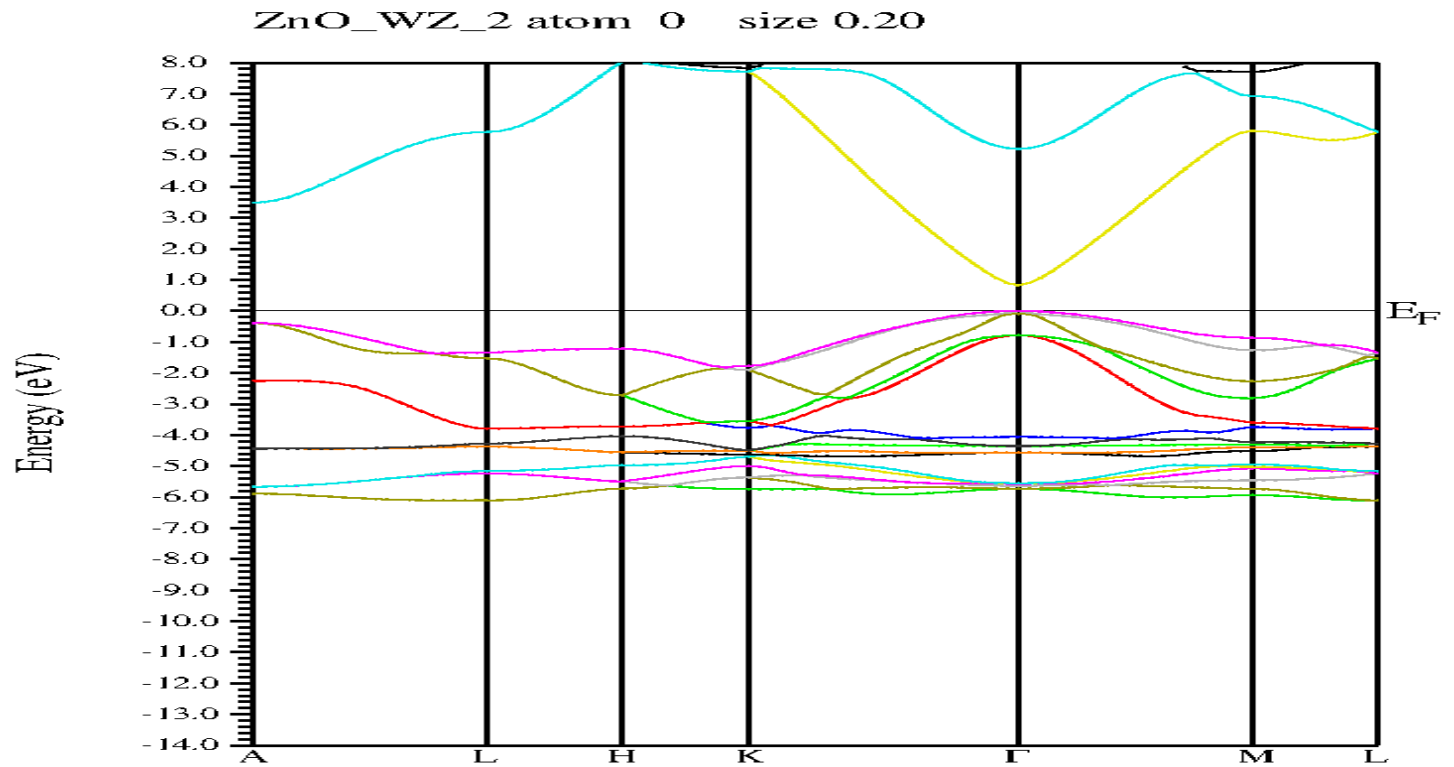
O Partial Density of States of ZnO (WZ)



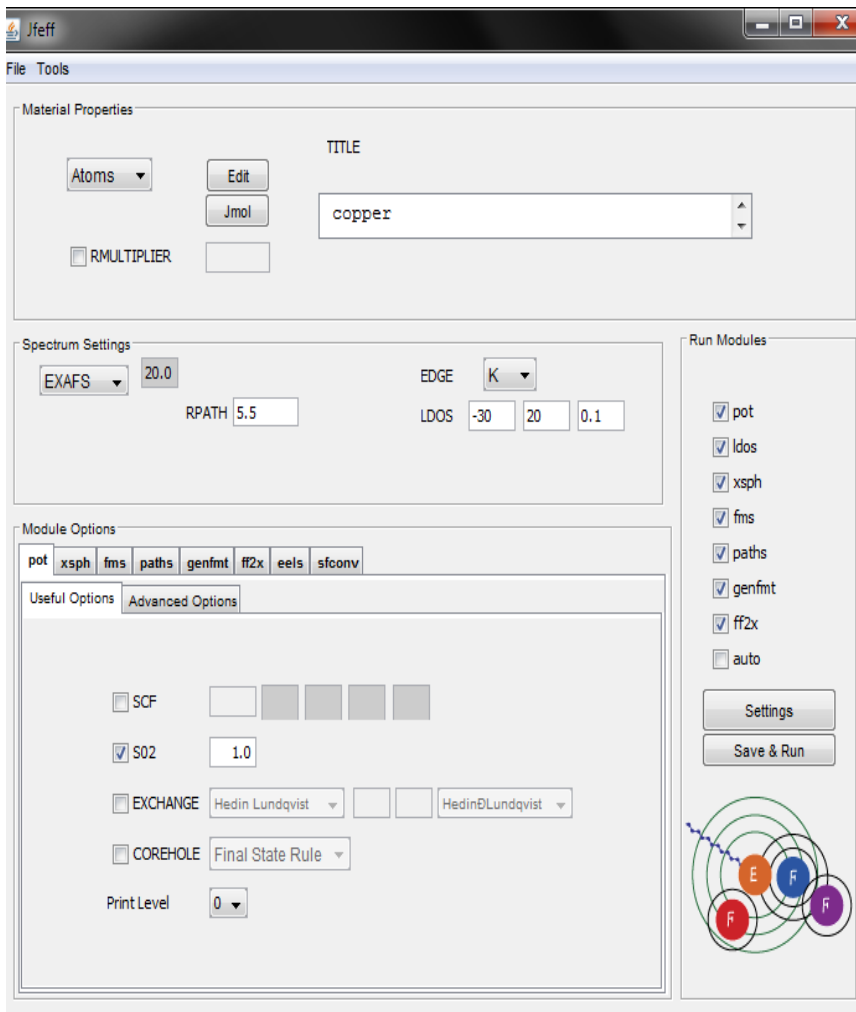
Zn K-edge of ZnO (WZ)



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 1 111
PRINT 1 0 0 000
      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 z -3

	Core	El	X	Y	Z
A	1	Zn	0.65055	0.61211	0.6550
B	2	C	0.75439	0.68407	0.9282
C	3	C	0.45293	0.45952	0.8788
Alpha	4	C	0.49720	0.51369	0.8037
Beta	5	C	0.54341	0.55452	0.9178
Gamma	6	O	0.59659	0.55953	0.4335
Cluster size	7	O	0.70467	0.67416	0.8693
Edge	8	O	0.58319	0.60655	0.8290
Shift vector	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

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

Edit selected site

Element: Tag: Define

X: Y: Z: New

Run Atoms Document: Atoms

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

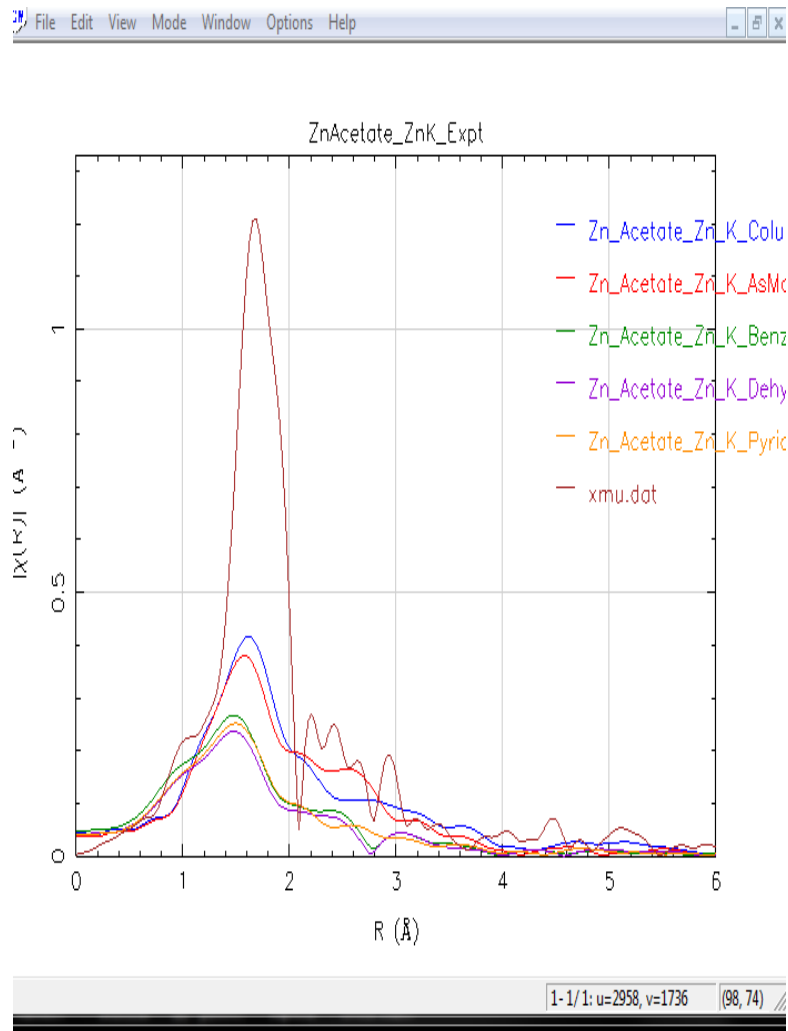
R-range: 1 to 3

dr: 0.0 window type: hanning

Plotting parameters

plot multiplier: 1 y-axis offset: 0

plotting in R for all marked groups ... done!



References

- P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
- J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992).
- P. Blaha, K. Schwarz, and P. Sorantin, and S. B. Trickey, Computer Phys. Comm., **59**, 399 (1990).
- J. Mustre de Leon, J. J. Rehr, S. I. Zabinsky, R. C. Albers, PRB **44**, 4146 (1991); S. I. Zabinsky, J. J. Rehr, A. Ankudinov, R. C. Albers, and M. J. Eller, Phys. Rev. B **52**, 2995 (1995); J. J. Rehr and R. C. Albers, Phys. Rev. B **41**, 8139 (1990); A. L. Ankudinov, B. Ravel, J. J. Rehr, and S. D. Conradson, Phys. Rev. B **58**, 7565 (1998); A. L. Ankudinow, S. D. Conradson, J. M. DeLeon, and J. J. Rehr, *Phys. Rev. B* 1998, **57**, 7518.
- J. J. Rehr and R. C. Albers, Rev. Mod. Phys. **72**, 621 (2000).
- T. L. Loucks, 'Augmented Plane Wave Method', (Benjamin, New York)', 1967.