

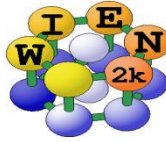


**Calculation for XANES and XAFS:
Part II. Density Functional Theory**

Y. M. Yiu

Sham's Group Meeting (Nov. 6, 2013)

WIEN2k

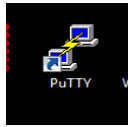


- Density Functional Theory:

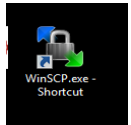
- Computer code (wien2k)
 - Local Density Approximation.
 - Generalized Gradient Approximation.
 - MBJ (Modified Becke-Johnson) exchange potential.

- <http://www.wien2k.at/>

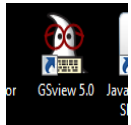
- Login Workstations: use putty.
 - <http://www.uwo.ca/its/sitelicense/putty/index.html>



- File transfer: use winscp.
 - <http://www.uwo.ca/its/sitelicense/WinSCP/index.html>



- View postscript files: use ghostview.



<http://gsview.soft32.com/>

Computer Servers

- Workstations:

- Duxeon.chem.uwo.ca

- 129.100.60.115

- xeony.chem.uwo.ca

- 129.100.60.33

- Dualo_III.chem.uwo.ca

- 129.100.61.183

- <http://129.100.60.115:1234>

- <http://129.100.60.33:1234>

- <http://129.100.61.183:7890>

- **Usersguide**

- [html-Version](#)

- [pdf-Version](#)

Density Functional Theory

• Kohn-Sham's Equation:

$$E = T[n] + \int v(r)n(r)d^3r + \iint \frac{n(r)n(r')}{|r - r'|}d^3rd^3r' + E_{xc}[n]$$

➤ where

- $T[n]$ is the kinetic energy functional of a system of N electrons,
- $v[r]$ is the potential,
- $n[r]$ is the density,
- and $E_{xc}[n]$ is the exchange and correlation energy functional of an interacting system with density $n[r]$.

Self-consistent Generalized Gradient

- The exchange-correlation energy is given by: $E_{xc}(r) = \int e_{xc}(r)n d^3r + \int e_{xc}^{GGA}(n, \nabla n) d^3r + \dots$
- Energy Minimization $\frac{\delta E(n)}{\delta n} = 0, \forall Z = \text{Const.}$
- Where $Z = \int n(r) d^3r$ and $n = \int \psi^*(r)\psi(r) d^3r$

Full Potential Augmented Plane Wave Method

$$\varphi_{k_n} = \sum_{lm} \left[A_{lm} u_l(r, E_l) + B_{lm} \frac{\partial u_l(r, E_l)}{\partial r} \right] Y_{lm}(r), \forall r \in S$$

$$\varphi_{k_n} = \frac{1}{\sqrt{\omega}} e^{ik_n r}, \forall r \notin S$$

where $\mathbf{k}_n = \mathbf{k} + \mathbf{K}_n$,

\mathbf{k} is the wave vector in 1st Brillouin Zone,

\mathbf{K}_n is the reciprocal lattice vectors.

Boundary Conditions:

$$\varphi_{k_n}(S)|_{r_s} = \varphi_{k_n}(I)|_{r_s} \quad \text{and}$$

$$\frac{\partial \varphi_{k_n}(S)}{\partial r} \Big|_{r_s} = \frac{\partial \varphi_{k_n}(I)}{\partial r} \Big|_{r_s}$$

Wien2k: Procedures

- 1. Structure Generation.
- 2. Initialize Calculation:
 - x nn
 - x sgroup
 - x symmetry
 - x lstart
 - x xkgen (1000 k points)
 - x dstart
- 3. Run scf.
- 4. Calculation of Properties.

Session | CIS_B4_3 | 14:10:04
home/yju/wien2k/CIS_B4_3

w2web, the fully web-enabled interface to WIEN2k

Session Name: CIS_B4_3
Session ID: 413804
Directory: /home/yju/wien2k/CIS_B4_3
Last changed: Fri Sep 13 16:22:23 2013

Comments:

spin polarized calculation
 AFM calculation
 complex calculation (no inversion)
 parallel calculation

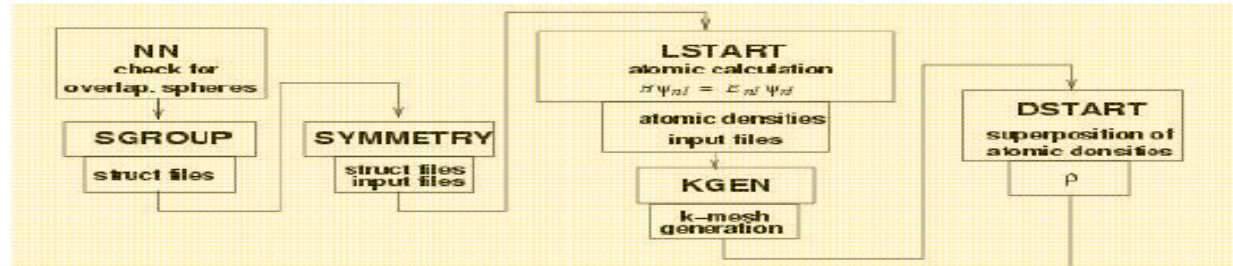
Change session information

w2web

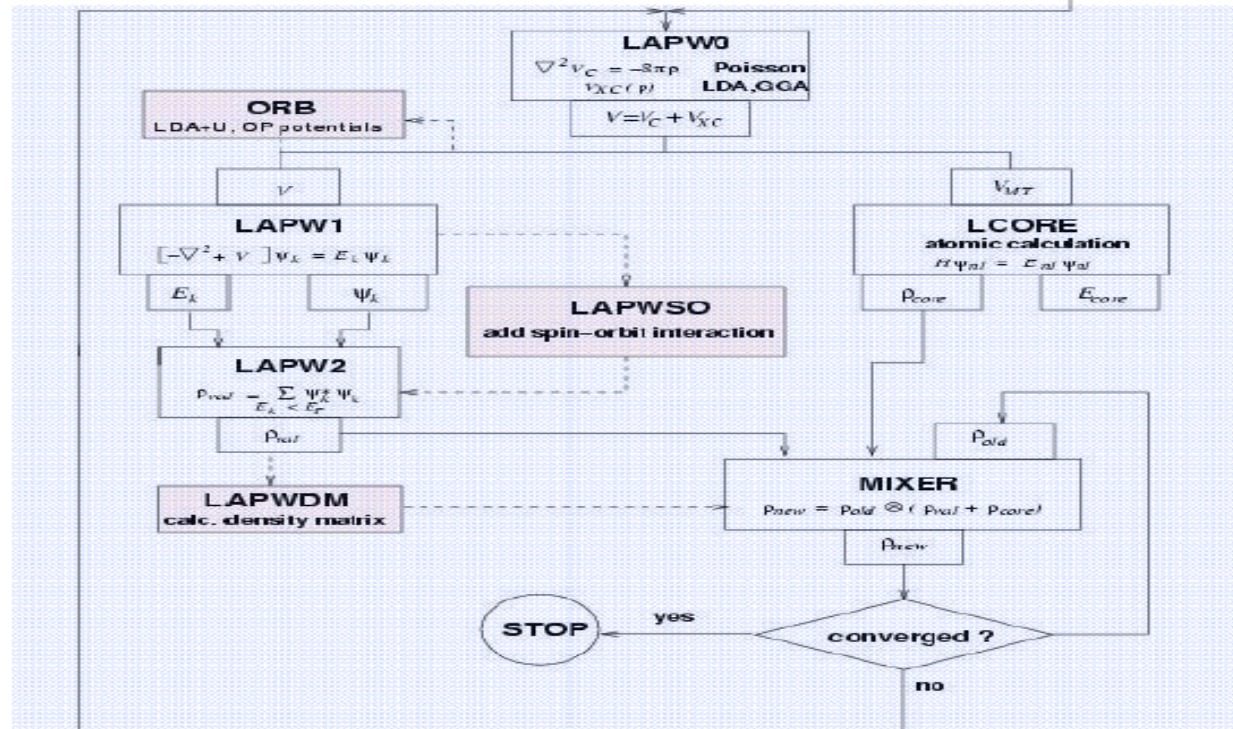
CIS_B4_3

Flaw Chart of wien2k

Initialization



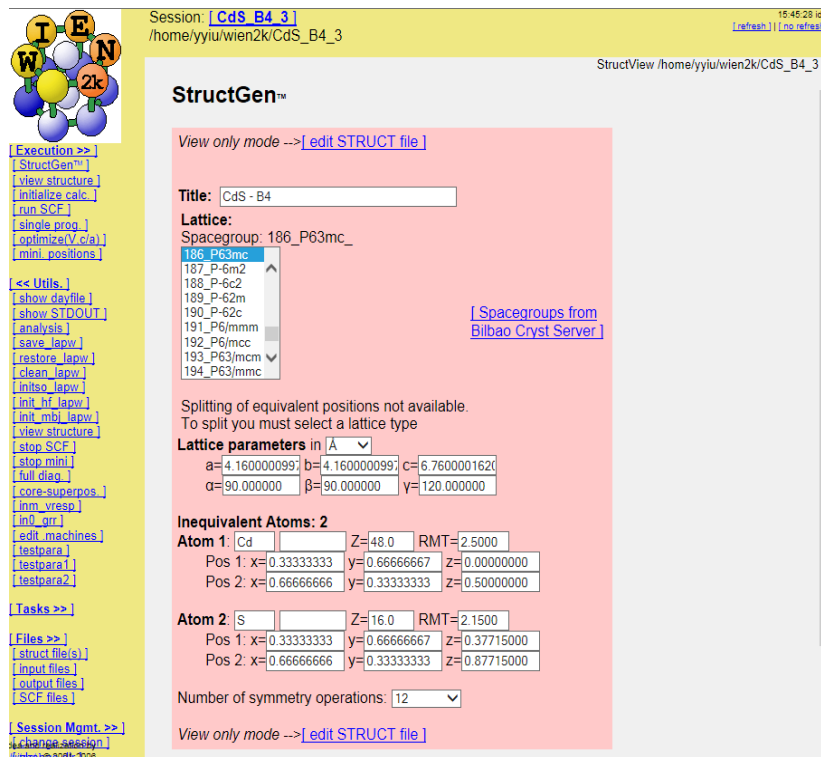
SCF



Structure Generation

1. Use .cif file to generate case.struct file:
cif2struct
2. Use case.struct: need space group
symmetry.

Save StructGen



Session: [CdS_B4_3] /home/yjiu/wien2k/CdS_B4_3

StructView /home/yjiu/wien2k/CdS_B4_3

StructGen™

View only mode --> [edit STRUCT file]

Title: CdS - B4

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=4.160000099; b=4.160000099; c=6.7600001620
α=90.00000000; β=90.00000000; γ=120.00000000

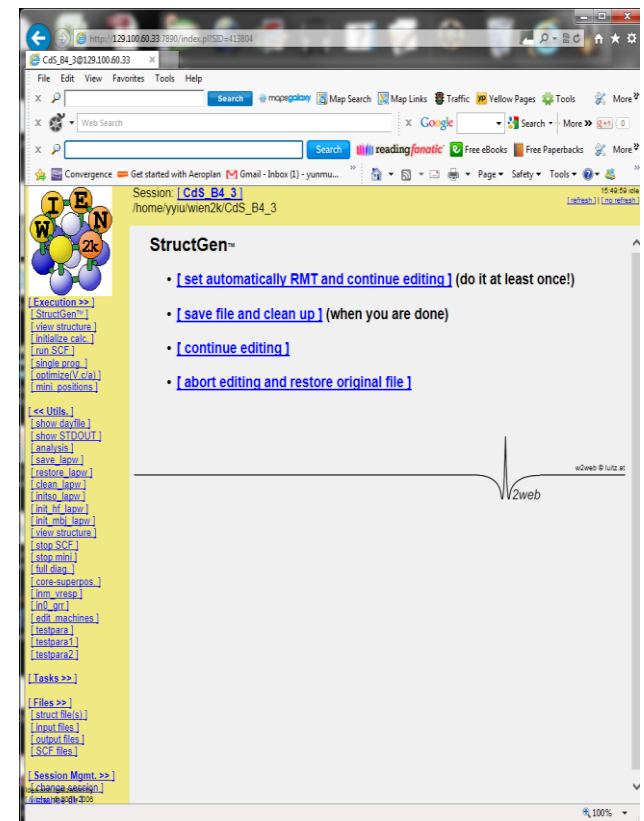
Inequivalent Atoms: 2

Atom 1: Cd Z=48.0 RMT=2.5000
Pos 1: x=0.33333333 y=0.66666667 z=0.00000000
Pos 2: x=0.66666666 y=0.33333333 z=0.50000000

Atom 2: S Z=16.0 RMT=2.1500
Pos 1: x=0.33333333 y=0.66666667 z=0.37715000
Pos 2: x=0.66666666 y=0.33333333 z=0.87715000

Number of symmetry operations: 12

View only mode --> [edit STRUCT file]



Session: [CdS_B4_3] /home/yjiu/wien2k/CdS_B4_3

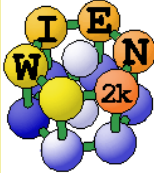
StructGen™

- [set automatically RMT and continue editing] (do it at least once!)
- [save file and clean up] (when you are done)
- [continue editing]
- [abort editing and restore original file]

w2web © Lutz at

v2web

Initialize Calculation



Session: [CdS_B4_3](#)
/home/yuiu/wien2k/CdS_B4_3

15:51:6
[\[refresh\]](#) | [\[no ref\]](#)

Initialize calculation (phase 1)

set RKmax (usually 5.0-9.0). ; [\[Click here for more info\]](#) Perform spin-polarized calc. ?

set LM's, GMAX and Fermi-Energy method

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, 19=PBESol) [default=13]
- energy separation between core/valence (default: -6.0 Ry)
- RKMAX (default: 7.0, [\[Click here for more info\]](#))
- use TEMP with smearing by X Ry (default: TETRA)
- set mixing to X (default: 0.2)
- use X k-points in full BZ (default: 1000; [\[Click here for more info\]](#))

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

[\[<< Utils.\]](#)
[\[show dayfile\]](#)
[\[show STDOUT\]](#)
[\[analysis\]](#)
[\[save lapw\]](#)
[\[restore lapw\]](#)
[\[clean lapw\]](#)
[\[initso lapw\]](#)
[\[init hf lapw\]](#)
[\[init mbj lapw\]](#)
[\[view structure\]](#)
[\[stop SCF\]](#)
[\[stop mini\]](#)
[\[full diag.\]](#)
[\[core-superpos.\]](#)
[\[inm_vresp\]](#)
[\[in0_grr.\]](#)
[\[edit machines\]](#)
[\[testpara\]](#)
[\[testpara1\]](#)
[\[testpara2\]](#)

[\[Tasks >>\]](#)

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

[\[Session Mgmt. >>\]](#)
[\[change session\]](#)
[\[quit\]](#)

SCF (Self-consistent Field)

- The SCF cycle consists of the following steps:
 - **LAPW0 (POTENTIAL)** generates potential from density
 - **LAPW1 (BANDS)** calculates valence bands (eigen-values and eigenvectors)
 - **LAPW2 (RHO)** computes valence densities from eigenvectors
 - **LCORE** computes core states and densities
 - **MIXER** mixes input and output densities



Session: [\[Li2PO2N-s1\]](#) 10:52:18 ide
/home/yyiu/wien2k/Li2PO2N-s1 [\[refresh\]](#) [\[no.refresh\]](#)

Show dayfile

```
> stop

ec cc and fc_conv 1 1 1
:CHARGE convergence: 0 0.0000 .0027754
:ENERGY convergence: 1 0.0001 .0000309700000000
> mixer (19:42:02) 0.4u 0.1s 0:00.64 81.2% 0+0k 0+11656io OpF+0w
> lcore (19:42:02) 0.0u 0.0s 0:00.07 85.7% 0+0k 0+448io OpF+0w
> lapw2 (19:34:27) 441.8u 12.2s 7:34.46 99.9% 0+0k 0+9760io OpF+0w
> lapw1 (04:33:46) 53911.5u 96.1s 15:00:40.75 99.9% 0+0k 0+1953632io OpF+0w
> lapw0 (04:33:36) 9.9u 0.1s 0:10.11 100.0% 0+0k 0+7296io OpF+0w

cycle 10 (Wed Sep 18 04:33:36 EDT 2013) (31/90 to go)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000 .0013890
:ENERGY convergence: 0 0.0001 .0002078900000000
> mixer (04:33:35) 0.4u 0.1s 0:00.64 84.3% 0+0k 0+11656io OpF+0w
> lcore (04:33:35) 0.0u 0.0s 0:00.07 100.0% 0+0k 0+448io OpF+0w
> lapw2 (04:26:01) 441.1u 12.4s 7:33.92 99.9% 0+0k 0+9760io OpF+0w
> lapw1 (13:35:16) 53336.3u 84.4s 14:50:45.06 99.9% 0+0k 0+1953752io OpF+0w
> lapw0 (13:35:06) 9.9u 0.0s 0:10.07 99.9% 0+0k 0+7296io OpF+0w

cycle 9 (Tue Sep 17 13:35:06 EDT 2013) (32/91 to go)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000 .0069388
:ENERGY convergence: 0 0.0001 .0018485550000000
> mixer (13:35:05) 0.4u 0.0s 0:00.63 80.9% 0+0k 0+11656io OpF+0w
> lcore (13:35:05) 0.0u 0.0s 0:00.07 85.7% 0+0k 0+448io OpF+0w
> lapw2 (13:27:30) 441.7u 12.5s 7:34.53 99.9% 0+0k 0+9760io OpF+0w
> lapw1 (22:38:21) 53240.3u 85.0s 14:49:09.58 99.9% 0+0k 0+1953200io OpF+0w
> lapw0 (22:38:11) 9.9u 0.0s 0:10.06 100.0% 0+0k 0+7296io OpF+0w

cycle 8 (Mon Sep 16 22:38:11 EDT 2013) (33/92 to go)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000 .0115038
:ENERGY convergence: 0 0.0001 .0040139750000000
> mixer (22:38:10) 0.3u 0.1s 0:00.63 76.1% 0+0k 0+11656io OpF+0w
> lcore (22:38:10) 0.0u 0.0s 0:00.06 116.6% 0+0k 0+448io OpF+0w
> lapw2 (22:30:36) 440.7u 12.5s 7:33.53 99.9% 0+0k 0+9760io OpF+0w
> lapw1 (07:22:36) 54343.1u 103.0s 15:08:00.05 99.9% 0+0k 0+1960320io OpF+0w
```

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

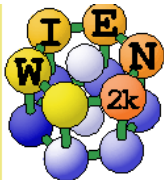
[\[<< Utils.\]](#)
[\[show dayfile\]](#)
[\[show STDOUT\]](#)
[\[analysis\]](#)
[\[save lapw\]](#)
[\[restore lapw\]](#)
[\[clean lapw\]](#)
[\[initiso lapw\]](#)
[\[init hf lapw\]](#)
[\[init mbi lapw\]](#)
[\[view structure\]](#)
[\[stop SCF\]](#)
[\[stop mini\]](#)
[\[full diag.\]](#)
[\[core-superpos.\]](#)
[\[im_wresp\]](#)
[\[in0_ort\]](#)
[\[edit machines\]](#)
[\[testpara\]](#)
[\[testpara1\]](#)
[\[testpara2\]](#)

[\[Tasks >>\]](#)

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

[\[Session Mgmt. >>\]](#)
[\[change session\]](#)
[\[change session\]](#)

Electron density plots



[Execution >>]
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V.c/a)]
[mini_positions]

[Utils. >>]

[<< Tasks]
[El_Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]

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

[Session Mgmt. >>]
[change session]
[change dir.]
[change info]

[Configuration]

Usersguide
[html-Version]
[pdf-Version]

idea and realization by
[luitz.et] © 2001-2006

Session: [CdS_B4_3]
/home/yyiu/wien2k/CdS_B4_3

16:03:31 ide
[refresh] [no.refresh]

Electron density plots

You must have a valid CdS_B4_3 vector file (from an scf calculation).
If you don't have it, you must run "x lapw1" with an appropriate input.

Select E-range for lapw2 for a density without semicore or within an E-window.
For proper values check energy-parameters and eigenvalues or band-ranges in the corresponding scf-files

edit CdS_B4_3.scf1

edit CdS_B4_3.scf2

x lapw2 Calculate clmval with Emin and Emax so

For difference densities only !

default valence states:

non-default valence states:

edit CdS_B4_3.inst put P for all your states

x lstart -sigma Calculate atomic valence densities x lstart Calculate atomic valence densities as defined above

Calculate density with XCrysden (or create CdS_B4_3.in5c" / execute lapw5 below)

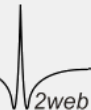
edit CdS_B4_3.in5c Edit input-file

x lapw5 Calculate density

Preview density with XCrysden

rhoplot Plot Density or download [CdS_B4_3.rho] for plotting with your own plotting program


w2web @ luitz.et



100%

case.in5

- Direction: [100]
 - 1 0 0 1
 - 1 1 0 1
 - 1 0 1 1
- Direction: [110]
 - 1 0 0 1
 - 0 1 0 1
 - 1 0 1 1
- Direction: [111]
 - 1 1 1 2
 - 1 0 0 1
 - 0 0 1 2



Session: [Li2PO2N-s3](#)
/home/yuiu/wien2k/Li2PO2N-s3

File:
/home/yuiu/wien2k/Li2PO2N-s3/Li2PO2N-s3.in5c

```
1 1 1 2      # x, y, z, divisor   of origin
1 0 0 1      # x, y, z, divisor   of x-end
0 0 1 2      # x, y, z, divisor   of y-end
3 2 3        # number of shells
100 100      # number of points in x and y dir, (ratio close to lenght
RHO          # RHO|DIFF|OVER; ADD|SUB or blank
ANG VAL NODEBUG # ANG|ATU; VAL|TOT; DEBUG|NODEBUG
ORTHO        # optional: ORHO|NONORTHO plotting direction
```

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

[\[Utils. >> \]](#)

[\[<< Tasks \]](#)
[\[El. Dens. \]](#)
[\[DOS \]](#)
[\[XSPEC \]](#)
[\[TELNES3 \]](#)
[\[OPTIC \]](#)
[\[Bandstructure \]](#)

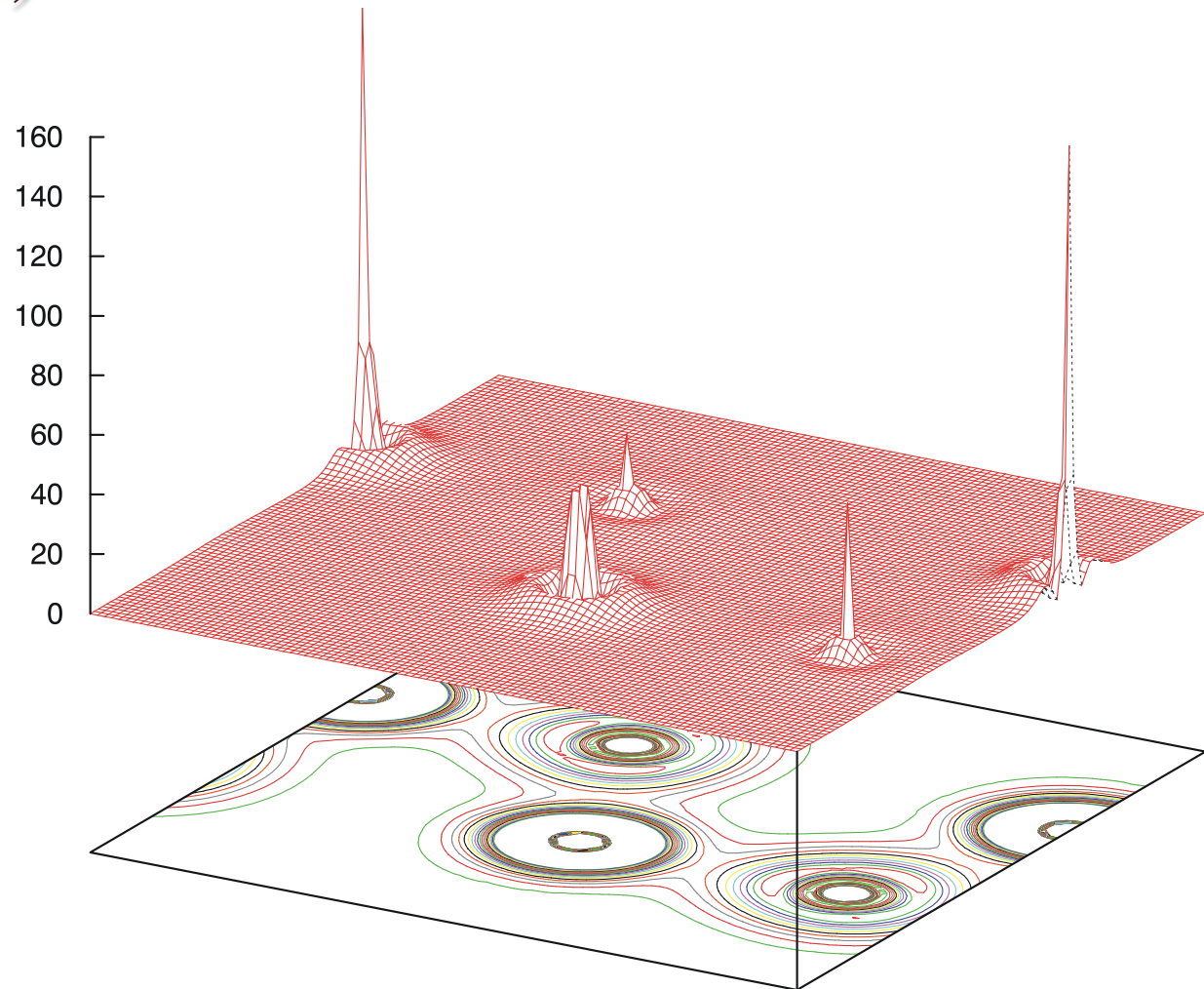
[\[Files >> \]](#)
[\[struct file\(s\) \]](#)
[\[input files \]](#)
[\[output files \]](#)
[\[SCF files \]](#)

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

[\[Configuration \]](#)

Usersguide
wien2k version 6.0.1
Copyright 2006

Electron density of CdS_B4 (plane 111)



XSPEC: XANES

Session: [CdS_B4_3](#) /home/yjiu/wien2k/CdS_B4_3

XSPEC

If you want to include states with higher energy

[edit CdS_B4_3.in1c](#) Edit in1c

[x.lapw1](#) Calculate eigenvalues interactively


[x.lapw2 -qt](#) Calculate partial charges interactively

[edit CdS_B4_3.inxs](#) Edit input-file for XSPEC

[x.xspec](#) Calculate X-ray spectra interactively

[plot](#) Plot XSPEC or download XSPEC ASCII files for plotting with your own plotting program

[\[CdS_B4_3.corewfx\]](#) [\[CdS_B4_3.m1\]](#) [\[CdS_B4_3.m2\]](#) [\[CdS_B4_3.xspec\]](#) [\[CdS_B4_3.Cd.K.7p28.xspec\]](#)
[\[CdS_B4_3.Cd.L3.2p5.xspec\]](#) [\[CdS_B4_3.S.K.p59.xspec\]](#) [\[CdS_B4_3.S.L3.p1.xspec\]](#)



W2web © 1/12/07

See and realization by [W2web](#) © 2001-2008

Session: [CdSse_B3_mBJ](#) /home/yjiu/wien2k/CdSse_B3_mBJ

File: /home/yjiu/wien2k/CdSse_B3_mBJ/CdSse_B3_mBJ.in1c

[continue with xspec](#) [Save](#) [Download this file:](#)

```

WFFIL EF=.6490335799 (WFFIL, WFPRI, ENFIL, SUPWF)
7.00 10 4 (R-MT*K-MAX; MAX L IN WF, V-NMT)
0.30 4 0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW)
1 0.30 0.000 CONT 1
1 -4.49 0.001 STOP 1
2 0.30 0.005 CONT 1
0 0.30 0.000 CONT 1
0.30 3 0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW)
0 -0.97 0.002 CONT 1
0 0.30 0.000 CONT 1
1 0.30 0.000 CONT 1
0.30 5 0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW)
2 0.30 0.000 CONT 1
2 -3.57 0.001 STOP 1
0 -0.97 0.002 CONT 1
0 0.30 0.000 CONT 1
1 0.30 0.000 CONT 1
K-VECTORS FROM UNIT:4 -9.0 6.5 42 emin / de (emax=Ef+de) / :
    
```

W2web © 1/12/07

See and realization by [W2web](#) © 2001-2008

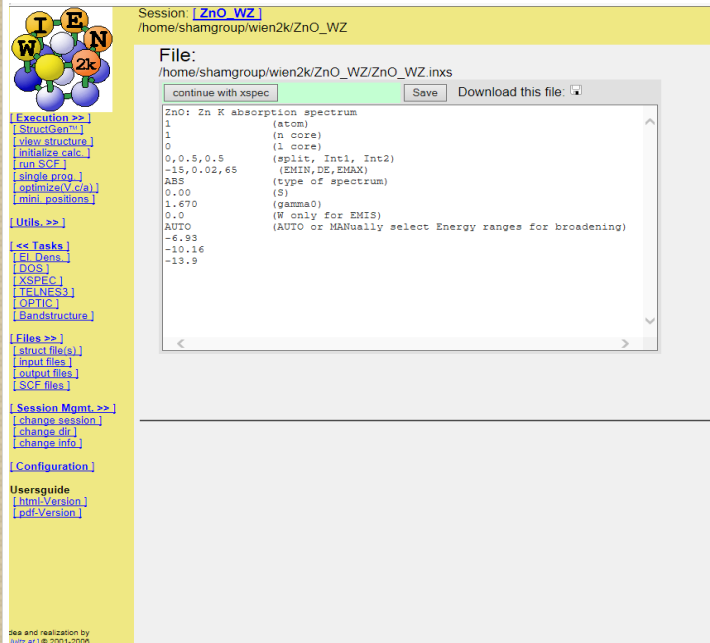
Download XANES Input and Output Files

Input file: case.inxs

S (spectrometer broadening FWHM in eV);

gamma0 (broadening parameter for the life-time broadening of the core states);

W (broadening parameter for the life-time broadening of valence states).

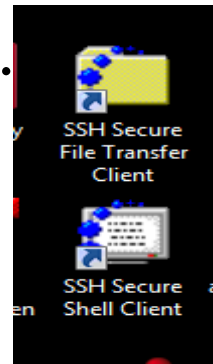
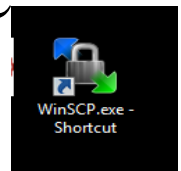
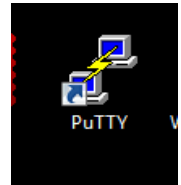


The screenshot shows the WIEN software interface. At the top, it displays the session name 'ZnO_WZ' and the file path '/home/shamgroup/wien2k/ZnO_WZ'. The main window shows the XANES input file 'case.inxs' with the following parameters:

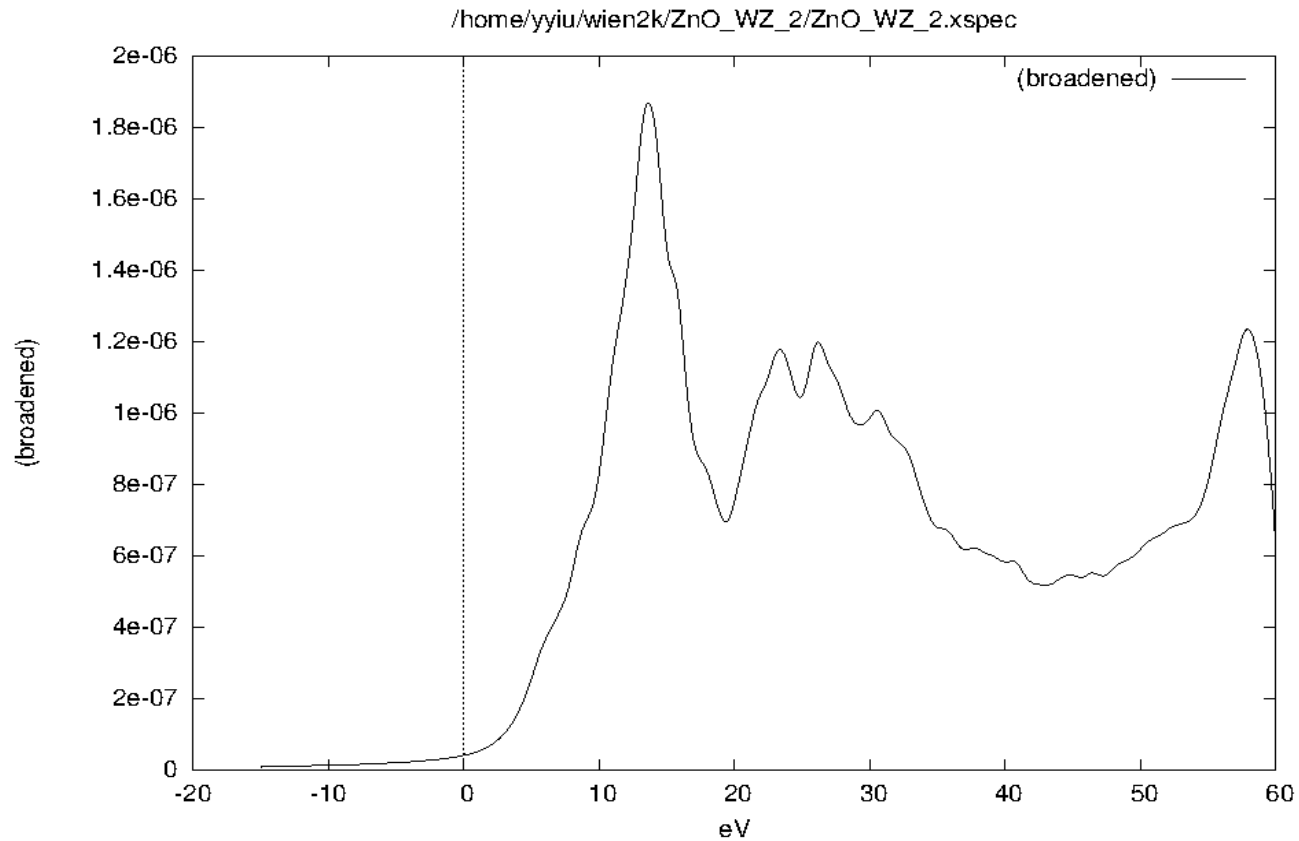
```
ZnO: Zn K absorption spectrum
1      (atom)
1      (n core)
0      (l core)
0,0.5,0.5 (split, Int1, Int2)
-15,0.02,65 (EMIN,DE,EMAX)
ABS      (type of spectrum)
0.00     (S)
1.670    (gamma0)
0.0      (W only for EMIS)
AUTO     (AUTO or MANUALLY select Energy ranges for broadening)
-6.93    (Emin)
-10.16   (Emax)
-13.9    (Emin)
```

The interface also includes various utility menus on the left side, such as 'Execution >>', 'Tools >>', 'Files >>', and 'Session Mgmt. >>'.

- Use putty to login:
 - cd wien2k/case
 - cp case.xspec case_atom_edge.xspec
- Use winscp for file transfer.
- Old login and file transfer: ssh shell.



Zn K-edge of ZnO (WZ)



Density of States (DOS)

SESSION: [CdS_B4_3] /home/lyyiu/wien2k/CdS_B4_3

Density of states

x lapw2 -qtl Calculate partial charges so interactively

Optional alternative to "x lapw2 -qtl" (f-states, SO-DOS, rotations)!
 edit CdS_B4_3.inq Edit input-file for QTL

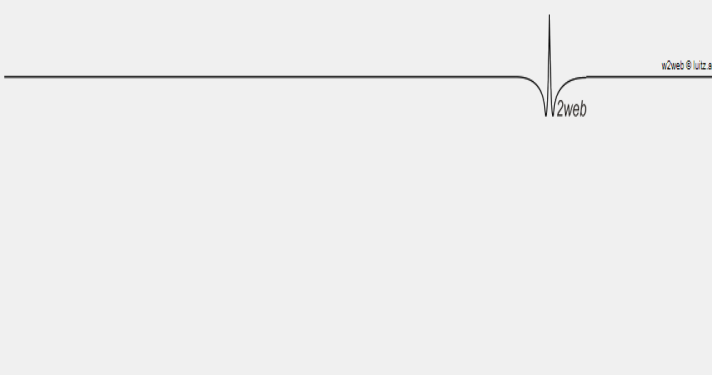
x qtl Calculate partial charges with QTL program so interactively

The required input file CdS_B4_3.int can be generated by:
 configure CdS_B4_3.int configure input-file for TETRA edit CdS_B4_3.int Edit input-file for TETRA

x tetra Calculate partial DOS interactively
 edit CdS_B4_3.output Check output of TETRA

dosplot Plot DOS or download DOS ASCII-data files for plotting with your own plotting program
[CdS_B4_3.dos1] [CdS_B4_3.dos1ev] [CdS_B4_3.dos2] [CdS_B4_3.dos2ev]
[CdS_B4_3.Cd.dos1ev.dos1ev] [CdS_B4_3.Cd.dos2ev.dos2ev] [CdS_B4_3.S.dos1ev.dos1ev] [CdS_B4_3.S.dos2ev.dos2ev]

save_lapw -dos with name:



idea and realization by [lutz et al.](#) © 2001-2006

SESSION: [ZnO_WZ] /home/shamgroup/wien2k/ZnO_WZ

File:

continue with DOS

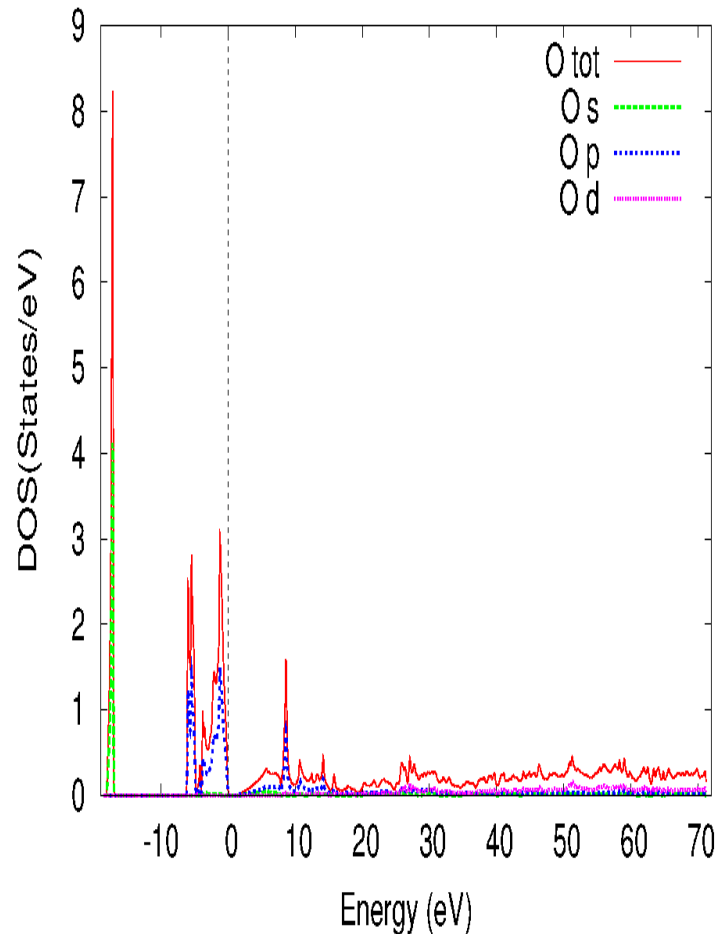
Header from ZnO_WZ.qtl:

| ATOM | COLUMN | | | |
|------------|---|--|--|--|
| ATOM Zn: 1 | tot, s, p, FZ, EX+PY, d, DZ2, DX2Y2+DXY, DXZ+DYZ, f | | | |
| ATOM O: 2 | tot, s, p, FZ, EX+PY, d, DZ2, DX2Y2+DXY, DXZ+DYZ, f | | | |

| ZnO_WZ | | | | | |
|--------|---------|---------------|-------|------------------------------|--|
| -1.100 | 0.00250 | 6.00 | 0.003 | #Emin, DE, Emax, Gauss-Broad | |
| 11 | | | | #Number of DOS | |
| 0 | 1 | total-DOS | | | |
| 1 | 1 | tot-Zn | | | |
| 1 | 2 | Zn s | | | |
| 1 | 3 | Zn p | | | |
| 1 | 4 | Zn pz | | | |
| 1 | 5 | Zn px+py | | | |
| 1 | 6 | Zn d | | | |
| 1 | 7 | Zn dz2 | | | |
| 1 | 8 | Zn dx2y2+dxxy | | | |
| 1 | 9 | Zn dxz+dxyz | | | |
| 1 | 10 | Zn f | | | |

idea and realization by [lutz et al.](#) © 2001-2006

O Partial Density of States of ZnO (WZ)



- Rename DOS
Output Files:
 - `cd wien2k/case`
 - `cp case.dos1ev case_atom.dos1ev`
 - `cp case.dos2ev case_atom.dos2ev`
- Download DOS
Output Files.

Band structure

Session: [CdS_B4_3] /home/yjiu/wien2k/CdS_B4_3

Band structure

Generate k-mesh using XCrystden (save klist as xcrystden.klist)

hpc create CdS_B4_3.klist_band [Brillouinzones from Bilbao Cryst Server]

x lapw1 -band Calculate Eigenvalues orb interactively

needed only for continuous lines in the plot (not for non-symmorphic spacegroups!)

x irrep Calculate irreducible representations so interactively

for band character plots only!

x lapw2 -band -qtl Calculate partial charges ("qtl"-file) so interactively

edit CdS_B4_3.insp Insert correct EF

x spaghetti Calculate bandstructure so interactively

plot bandstructure Plot bandstructure or download Xmgrace files for plotting with xmgrace [CdS_B4_3.bands.agr]

save_lapw -band with name:

Execution >> [StructGen] [view structure] [initialize calc.] [run SCF] [single prog.] [optimize(V,c,a)] [mini_positions]

Utils >> [El Dens.] [DOS] [XSPEC] [TELNES3] [OPTIC] [Bandstructure]

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

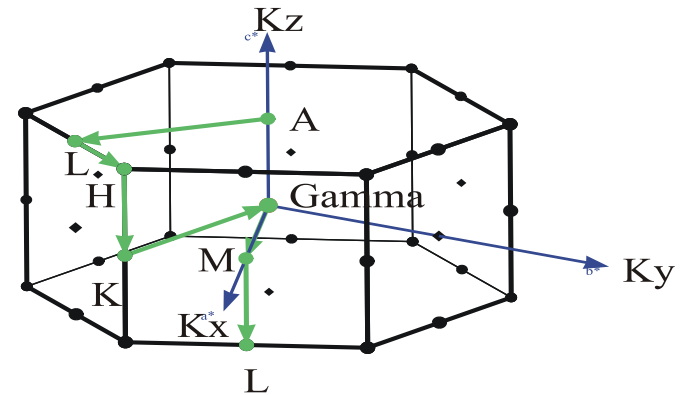
Session Mgmt. >> [change session] [change dir.] [change info]

Configuration

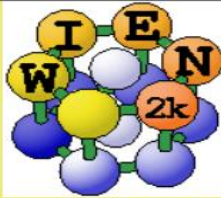
Usersguide

- xcrysden plots: choose Brillouin Zone direction, and save as case.lpr.
- View file by ghostview or CorelDraw.

Primitive Brillouin Zone CdS - B4



Band Structure Plot



Session: [\[CdS B4 3 \]](#)
[/home/yyiu/wien2k/CdS_B4_3](#)

[\[Execution >> \]](#)

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

[\[Utils. >> \]](#)

[\[Tasks >> \]](#)

[\[Files >> \]](#)

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

[\[Session Mgmt. >> \]](#)

- [\[change session \]](#)
- [\[change dir \]](#)
- [\[change info \]](#)

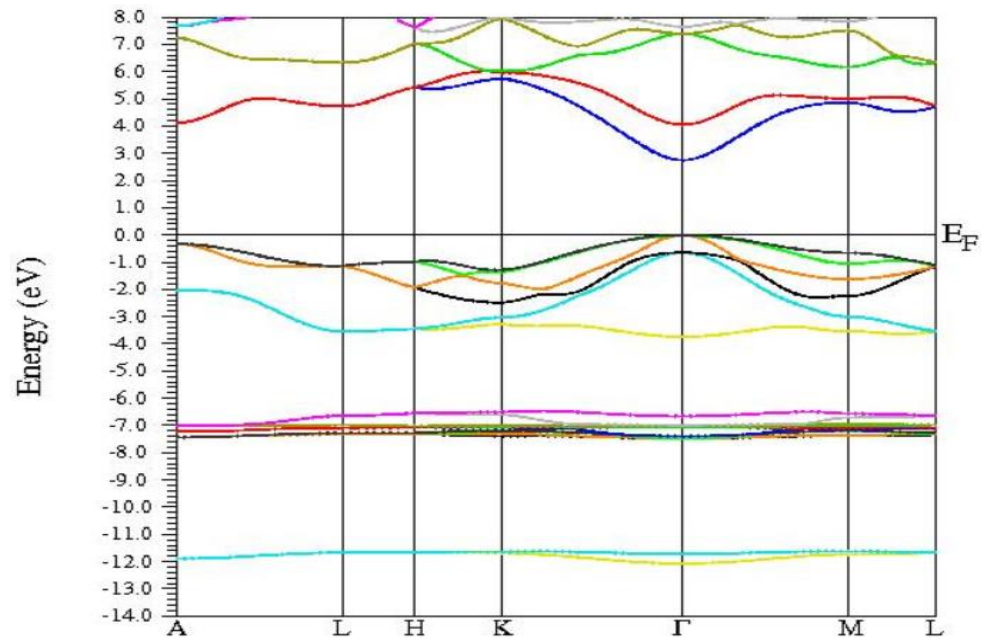
[\[Configuration \]](#)

Jsersguide

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

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

CdS_B4_3 atom 0 size 0.20



[\[Download hardcopy in PostScript format \]](#)

[\[Show full menu \]](#)

MBJ (Modified Becke-Johnson) exchange potential

- Modified B-J Potential:

$$v_{x,\sigma}^{MBJ}(\vec{r}) = cv_{x,\sigma}^{BR}(\vec{r}) + (3x - 2) \frac{1}{\pi} \sqrt{\frac{5}{12}} \sqrt{\frac{2t_\sigma(\vec{r})}{\rho_\sigma(\vec{r})}}$$

$$\frac{xe^{-2x/3}}{x-2} = \frac{2}{3} \pi^{2/3} \rho_\sigma^{5/3} \left\{ \frac{1}{6} \left(\nabla^2 \rho_\sigma - 2\gamma \left[\sum_{i=1}^{\sigma} |\nabla \psi_i|^2 - \frac{(\nabla \rho_\sigma)^2}{4\rho_\sigma} \right] \right) \right\}^{-1} \quad \boxed{\gamma = 1}$$

- Becke-Roussel Potential

$$v_{x,\sigma}^{BR}(\vec{r}) = -\frac{1}{b_\sigma(\vec{r})} \left[1 - e^{-x_\sigma(\vec{r})} - \frac{1}{2} x_\sigma(\vec{r}) e^{-x_\sigma(\vec{r})} \right]$$

- where

$$b_\sigma = \left[\frac{x_\sigma^3 e^{-x_\sigma}}{8\pi\rho_\sigma} \right]^{1/3}$$

$$\rho_\sigma = \sum_{i=1}^{N_\sigma} |\psi_{i,\sigma}|^2$$

$$t_\sigma = \frac{1}{2} \sum_{i=1}^{N_\sigma} \vec{\nabla} \psi_{i,\sigma}^* \vec{\nabla} \psi_{i,\sigma}$$

$$c = A + B \left(\frac{1}{V_{\text{cell}}} \int_{\text{cell}} \frac{|\nabla \rho(\vec{r}')|}{\rho(\vec{r}')} d^3 r' \right)^{1/2}$$

$$A = -0.012$$

$$B = 1.023 \text{ bohr}^{1/2}$$

MBJ (Modified Becke-Johnson) exchange potential SCF calculation

- run a regular initialization and SCF calculation using LDA or PBE.
- **init_mbj_lapw:**
 - **cp \$WIENROOT/SRC_templates/template.inm_vresp case.inm_vresp.**
 - edit **case.in0** and set "R2V" option (instead of "NR2V") such that the XC potential is written in **case.r2v**.
- **run_lapw -NI -i 1:** to generate the required **case.r2v** and **case.vresp** files.
- "save" the LDA (or PBE) calculation.
- run **init_mbj_lapw** again:
 - edit **case.in0** and change the functional to option **indxc=28** (this is mBJ).
 - **cp case.in0 case.in0_grr**
 - choose **indxc=50** in **case.in0_grr**. This option will calculate the average of $\nabla\rho/\rho$ over the unit cell.
- edit **case.inm** and choose the PRATT mixing scheme. First use mixing factor (eg. 0.2 or 0.1).
- run the mBJ SCF calculation.
- run DOS properties.

Simple Commands for Unix or Linux

In x-window or use putty:

- top: list of the process, CTRL c to quit.
- cd: change directory.
- cp : copy file.
- vi filename: simple text editor.
 - esc (toggle between commands)
 - x (delete character)
 - dd (delete line)
 - i (insert)
 - ZZ (save file)
 - :q! (exit without saving file)
- emacs: text editor.
- Run command: `./run_lapw -NI -i 1`
- When done:
 - cd wien2k
 - cp clean_lapw case/
 - cd case
 - ./clean_lapw
 - logout

Or use http:
Utils
clean_lapw

Summary

- Use wien2k program to calculate self-consistently:
 - Local Density Approximation.
 - Generalized Gradient Approximation.
 - MBJ (Modified Becke-Johnson) exchange potential:
 - Better band gap energy.
- Properties to be calculated:
 - Electron density: lapw5.
 - XANES: xspec.
 - DOS (Densities of States): tetra.
 - Band structure: spaghetti.

References

- N. F. M. Henry and K. Lonsdale: “International Tables For X-ray Crystallography”, Kynoch Press, (Birmingham, England), (1965).
- 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).
- T. L. Loucks, “Augmented Plane Wave Method”, (Benjamin, New York), (1967).
- J. C. Fuggle and J. E. Inglesfield, “Unoccupied Electronic States: Fundamentals for XANES, EELS, IPS, and BIS”, Springer-Verlag, Berlin Heidelberg (1992).
- A. D. Becke and E. R. Johnson, J. Chem. Phys. **124**, 221101 (2006); doi: 10.1063/1.2213970.
- F. Tran and P. Blaha, PRL **102**, 226401 (2009); DOI: 10.1103/PhysRevLett.102.226401.
- David Koller, Fabien Tran, and Peter Blaha, Phys. Rev. B **85**, 155109 (2012); DOI: 10.1103/PhysRevB.85.155109.