The Augmented Spherical Wave Package

Hands on Session III

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Electronic Structure in a Nutshell

Outline

Outline

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Organization I

General

- the one and only input file
- upward compatible
- all other files are automatically created and deleted
- 17 categories (cols. 1-8)
- max. 16 tokens per category (cols. 9-80)
- “free format” (no tabs)
- compatible to CTRL files of LMTO 47

Organization II

Categories

- HEADER
- VERSION
- IO
- OPTIONS
- STRUC (mandatory)
- CLASS (mandatory)
- SITE (mandatory)
- SYMGRP
- PACK

Categories

- ENVEL
- BZSMP
- CHARGE
- CONTROL
- MIXING
- SUPCELL
- SYMLIN
- PLOT

Categories HEADER and VERSION

title — character

- 1st line for the title
- 1st line will be used in plots
- 19 additional lines for comments etc.

ASW-2.3 — double

- version number of CTRL
- do NOT change when using old CTRLs
- different interpretation of fractional coordinates in versions prior to ASW-2.0

Category IO

HELP=T/F — logical

switch to print the HELP file

SHOW=T/F — logical

switch to echo CTRL to output

VERBOS=30 — integer

verbosity level for printing to output

WRITE=CBAK — character

name of file to which a copy of CTRL is written

Category OPTIONS

REL=T/F — logical

switch between non-relativistic and scalar-relativistic calculations

NSPIN=1/2 — integer

number of spin channels

AFSYM=T/F — logical

switch to use antiferromagnetic symmetry if present

OVLCHK=T/F — logical

switch to perform overlap check

Category OPTIONS (cont.)

XCPAR=VWN-VWN/P-S character

Character string for the XC-parametrization

- P=KSG: Kohn, Sham, and Gaspar (exchange only)
- P=GLW: Gunnarsson, Lundqvist, and Wilkins
- P=JMW: Janak, Moruzzi, and Williams
- P=VBH: von Barth and Hedin
- P=MJW: Moruzzi, Janak, and Williams
- P=PZ: Perdew and Zunger
- P=VWN: Vosko, Wilk, and Nusair
- P=PW: Perdew and Wang

Category OPTIONS (cont.)

XCPAR=VWN-VWN/P-S character

Character string for the XC-parametrization
(Spin interpolation)

- S=GLW: Gunnarsson, Lundqvist, and Wilkins
- S=VBH: von Barth and Hedin
- S=VWN: Vosko, Wilk, and Nusair
- S=PW: Perdew and Wang

Category OPTIONS (cont.)

GGA=PBE — character

Character string for the GGA-parametrization

- PW86: Perdew and Wang 1986 (GGA-I)
- PW: Perdew and Wang 1991 (GGA-II)
- EV: Engel and Vosko 1993
- PBE: Perdew, Burke, and Ernzerhof 1996
- ZY: Zhang and Yang 1998
- WC: Wu and Cohen 2005

Category STRUC mandatory

UNITS=ANGS/BOHR character

units to be used in categories STRUC and SUPCELL

ALAT= mandatory, double

lattice constants in UNITS

PLAT= double

primitive translations in units of ALAT

BLAT=/CLAT= double

lattice constants in UNITS

Category STRUC (cont.) mandatory

BBYA=/CBYA= double

ratios of lattice constants BLAT/ALAT, CLAT/ALAT

ALPHA=/BETA=/GAMMA=90 double

angles between lattice vectors

CNTR=P/C/B/A/I/F/R character

centering type of the Bravais lattice

Category CLASS mandatory

ATOM= mandatory, character

class labels $\Longrightarrow$ define names of atomic files

Z= mandatory, double

atomic numbers

R= double

atomic sphere radius in atomic units (a_B)

LMXL= integer

maximum angular momentum for the lower waves
Cu: LMXL=2

Category CLASS (cont.) mandatory

LMXI= integer

maximum angular momentum for the intermediate waves
Cu: LMXL=3

CONF= integer

principal quantum numbers for all orbitals
Cu: CONF=4 4 3 4

QVAL= double

number of valence electrons for each orbital
Cu: QVAL= 1.0 0.0 10.0 0.0

MVAL= double

magnetic moment for each orbital

Category SITE mandatory

CARTP=T/F logical

switch to treat atomic positions as Cartesian

CHOUT=T/F logical

switch to change interpretation of atomic positions

ATOM= mandatory, character

class labels $\Longleftrightarrow$ same as in category CLASS

POS= mandatory, double

positions of basis atoms

SPIN=UP/DN character

character string fo spin direction

Category SYMGRP

GENPOS=T/F — logical

switch to complete atomic basis using symmetry

CARTR=T/F — logical

switch to treat rotation axes as Cartesian

CARTT=T/F — logical

switch to treat fractional translations as Cartesian

ORIGIN=1 — integer

choice of origin

Category SYMGRP (cont.)

SGSYM= character

space group symbol
Cu: SGSYM=Fm-3m

SGNUM= integer

space group number
Cu: SGNUM=225

SYMOPS= character

characters for space group generators
Cu: SYMOPS=I R4X R3D

Category PACK

FILLNG=1.0 — double

filling factor for atomic sphere volumes

OBYDMX=0.15 — double

maximum allowed overlap/distance

NCEMAX=1024 — integer

maximum number of allowed empty sphere classes

RADMAX= — double

maximum atomic sphere radius of empty spheres

Category BZSMP

NKBAB=6 — integer

k-point spacing for Brillouin zone integration

BZINT=SMS/HPS/LTM — character

character string indicating the BZ integration scheme

EMIN=-2.0/EMAX=1.0 — double

minimum/maximum energy for DOS calculation

NDOS= — integer

number of divisions of the interval EMAX-EMIN

Category BZSMP (cont.)

SAVDOS=T/F — logical

switch to save calculated partial DOSs

SAVCOOP=T/F — logical

switch to save calculated COOPs

SAVFERM=T/F — logical

switch to save calculated Fermi surface data

SAVOPT=T/F — logical

switch to save calculated partial optical spectra

Category CHARGE

NETA=2 — integer

number of envelope functions for the interstitial electron density
never ever change!

EETA=-1.0, -3.0 — double

energies of envelope functions for the interstitial electron density

SAVRHO=T/F — logical

switch to save calculated electron density

Category CONTROL

NITBND=99 — integer

maximum number of iterations

CNVG=1.0D-08 — double

convergence tolerance for atomic multipole moments

CNVGET=1.0D-08 — double

convergence tolerance for total energy (Ryd)

Category SYMLIN

NPAN= — integer

number of symmetry lines (panels)

NPTS= — integer

maximum total number of **k**-points

ORBWGT=T/F — logical

switch to calculate orbital weights

CARTE=T/F — logical

switch to treat endpoints as Cartesian

LABEL= — character

labels of endpoints

Category PLOT

CARTV=T/F — logical

switch to treat plot vectors as Cartesian

ORIGIN= — double

origin of plot space

RPLOT1=/RPLOT2=/RPLOT3= — double

plot vectors specifying the plot space

NPDIV1=/NPDIV2=/NPDIV3= — integer

number of divisions of the plot space

Outline

Background I

Rutile-Related Transition-Metal Dioxides

	d^0	d^1	d^2	d^3	d^4	d^5	d^6
3d	TiO_2 (S)	VO_2^* (M–S)	CrO_2 (F–M)	MnO_2 (AF–S)			
4d		NbO_2^* (M–S)	MoO_2^* (M)	TcO_2^* (M)	RuO_2 (M)	RhO_2 (M)	
5d		TaO_2 (?)	WO_2^* (M)	ReO_2^* (M)	OsO_2 (M)	IrO_2 (M)	PtO_2^* (M)

* deviations from rutile, M = metal, S = semiconductor
F/AF = ferro-/antiferromagnet

Background II

Previous Work (ASW calculations!)

K. Schwarz

CrO_2 predicted as a half-metallic ferromagnet

J. Phys. F: Met. Phys. **16**, L211 (1986)

S. Matar, G. Demazeau, J. Sticht, V. Eyert, and J. Kübler

Etude de la structure électronique et magnétique de CrO_2

J. Phys. I France **2**, 315 (1992); ibid. **4**, 1259 (1994)

S. Matar, V. Eyert, J. Sticht, J. Kübler, and G. Demazeau

Band theoretical investigation of substituted CrO_2 within the local density approximation

J. Phys. I France **4**, 1199 (1994)

Preparing for the Application I

Create a directory tree

- create e.g. /home/user/appl/cro2 (chromium dioxide)
- create e.g. /home/user/appl/cro2/nm (spin-deg. calcs.)
- create e.g. /home/user/appl/cro2/fe (spin-pol. calcs.)
- create e.g. /home/user/appl/cro2/af (spin-pol. calcs.)

Preparing for the Application II

Spin-Degenerate Calculations

A minimum CTRL file

```
HEADER  CrO2 rutile
        data by A. A. Bolzan et al.,
        Acta Cryst. B53, 373 (1997).
VERSION ASW-2.3
IO      HELP=F SHOW=T VERBOS=30 CLEAN=T
STRUC   ALAT=8.35618 CLAT=5.511575 CNTR=P
CLASS   ATOM=CR Z=24
        ATOM=O  Z= 8
SITE    CARTP=F
        ATOM=CR POS= 0.000000  0.000000  0.000000
        ATOM=O  POS= 0.302400  0.302400  0.000000
SYMGRP  GENPOS=T SGSYM=P4_2/mnm
```

A Standard CTRL File I

Spin-Degenerate Calculations

```
HEADER  CrO2 rutile
        data by A. A. Bolzan, C. Fong, B. J. Kennedy, C. J. Howard,
        Acta Cryst. B53, 373 (1997).
VERSION ASW-2.3
IO      HELP=F SHOW=T VERBOS=30 CLEAN=T
OPTIONS REL=T OVLCHK=T
STRUC   ALAT=8.35618 CLAT=5.511575 CNTR=P
CLASS   ATOM=CR Z=24 R=2.16612899 LMXL=2 CONF=4 4 3 4
                QVAL= 1.0  0.0  5.0  0.0
        ATOM=O  Z= 8 R=1.87483912 LMXL=1 CONF=2 2 3
                QVAL= 2.0  4.0  0.0
SITE    CARTP=F
        ATOM=CR POS= 0.000000  0.000000  0.000000
        ATOM=CR POS= 0.500000  0.500000  0.500000
        ATOM=O  POS= 0.302400  0.302400  0.000000
        ATOM=O  POS=-0.302400 -0.302400  0.000000
        ATOM=O  POS=-0.197600  0.197600  0.500000
        ATOM=O  POS= 0.197600 -0.197600  0.500000
...
```

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A Standard CTRL File II

Spin-Degenerate Calculations

```
SYMGRP
BZSMP   NKBAB=6 BZINT=LTM EMIN=-1.5 EMAX=1.5 NDOS=3000
        NORD=3 WIDTH=0.01 SAVDOS=F SAVCOOP=F
CHARGE  NETA=2 EETA=-1.0 -3.0 SAVRHO=T
CONTROL START= QUIT= FREE=F NITBND=99 CNVG=1.0D-08 CNVGET=1.0D-08
        NITATM=50 CNVGQA=1.0D-10
MIXING  NMIXB=5 BETAB=0.5 INCBB=T NMIXA=5 BETAA=0.5
SYMLIN  NPAN=7 NPTS=400 CARTE=F
        LABEL=g ENDPT= 0.0  0.0  0.0
        LABEL=M ENDPT= 0.5  0.5  0.0
        LABEL=X ENDPT= 0.0  0.5  0.0
        LABEL=g ENDPT= 0.0  0.0  0.0
        LABEL=Z ENDPT= 0.0  0.0  0.5
        LABEL=A ENDPT= 0.5  0.5  0.5
        LABEL=R ENDPT= 0.0  0.5  0.5
        LABEL=Z ENDPT= 0.0  0.0  0.5
...
```

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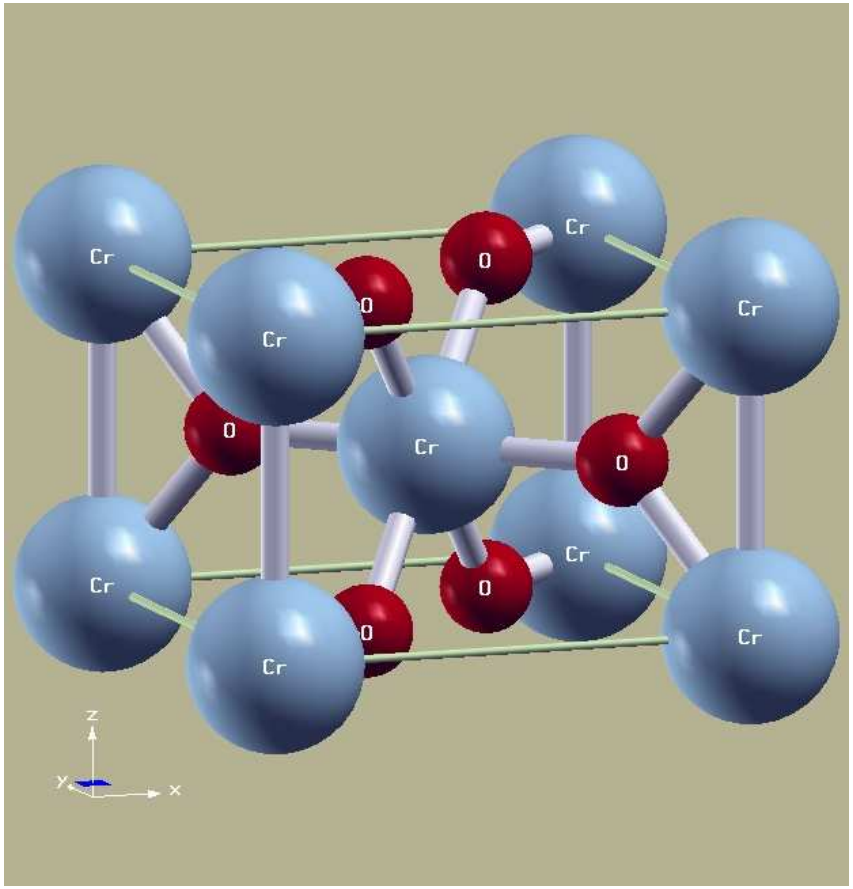
Plotting the Crystal Structure



Pyrite

- $P4_2/mnm$ (D_{4h}^{14})
- Cr (2a): $(0,0,0)$, $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
- O (4f): $\pm(u,u,0)$, $\pm(\frac{1}{2}+u,\frac{1}{2}-u,\frac{1}{2})$
- rotated CrO_6 octahedra

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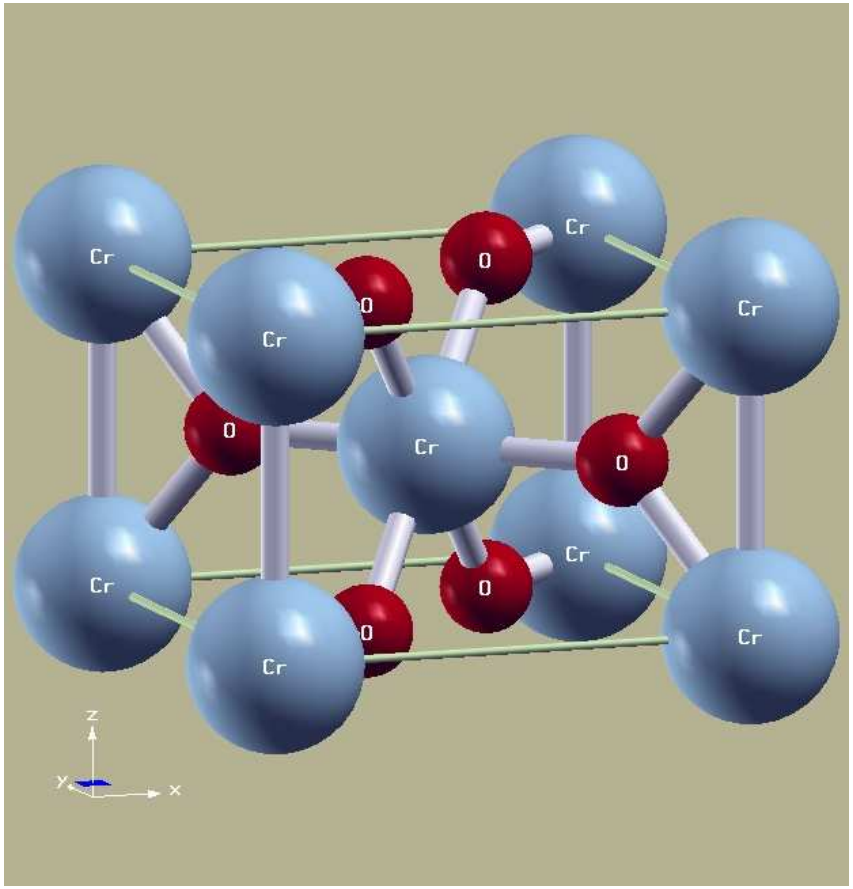
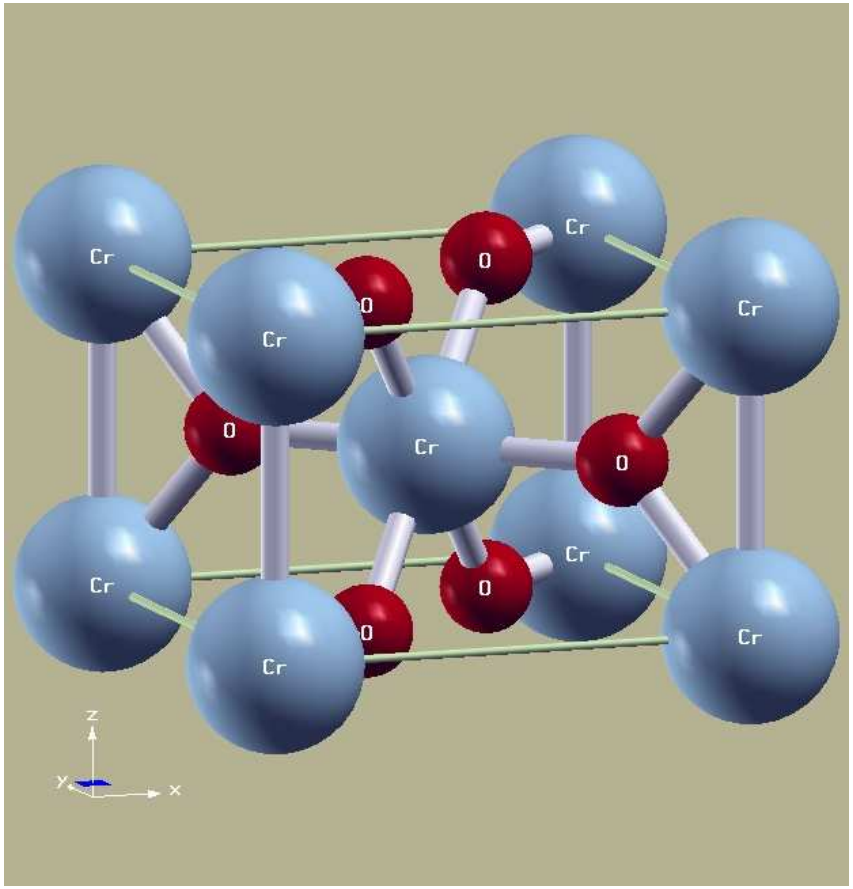
Plotting the Crystal Structure

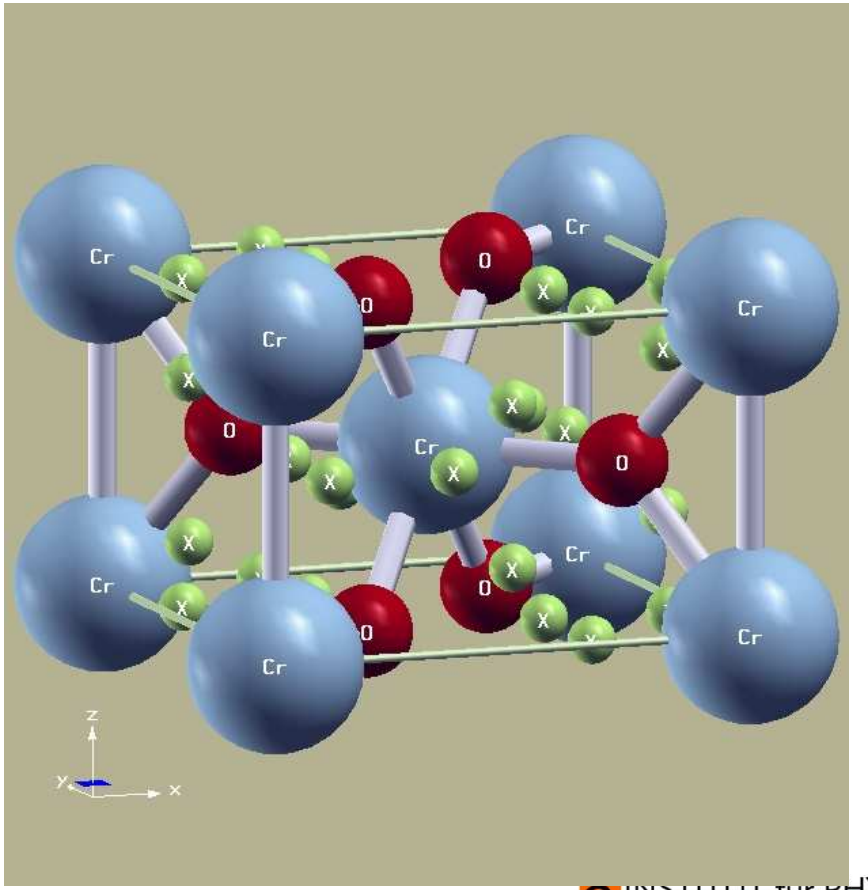


Rutile

- open crystal structure
- space filling with only Cr and O spheres
  $\Longrightarrow$ large sphere overlaps
- apply Sphere Geometry Optimization algorithm
  $\Longrightarrow$ run mnpac.x

Filling Space





The Updated CTRL File I

Category CLASS

```
CLASS   ATOM=CR Z=24 R=2.16612899 LMXL=2 CONF=4 4 3 4
                QVAL= 1.0  0.0  5.0  0.0
        ATOM=O  Z= 8 R=1.87483912 LMXL=1 CONF=2 2 3
                QVAL= 2.0  4.0  0.0
        ATOM=E1 Z= 0 R=1.65252923 LMXL=1 CONF=1 2 3
                QVAL= 0.0  0.0  0.0
        ATOM=E2 Z= 0 R=1.76771917 LMXL=1 CONF=1 2 3
                QVAL= 0.0  0.0  0.0
        ATOM=E3 Z= 0 R=0.85735960 LMXL=0 CONF=1 2
                QVAL= 0.0  0.0
```

The Updated CTRL File II

Category SITE

```
SITE    CARTP=T
...
        ATOM=E1 POS= 0.500000  0.000000 -0.250000
        ATOM=E1 POS= 0.500000  0.000000  0.250000
        ATOM=E1 POS= 0.000000 -0.500000 -0.250000
        ATOM=E1 POS= 0.000000 -0.500000  0.250000
        ATOM=E2 POS= 0.318691 -0.318691  0.000000
        ATOM=E2 POS=-0.318691  0.318691  0.000000
        ATOM=E2 POS=-0.181309 -0.181309 -0.500000
        ATOM=E2 POS= 0.181309  0.181309 -0.500000
        ATOM=E3 POS= 0.313120 -0.055474  0.000000
        ATOM=E3 POS=-0.313120  0.055474  0.000000
        ATOM=E3 POS=-0.186880 -0.444526 -0.500000
        ATOM=E3 POS= 0.186880  0.444526  0.500000
        ATOM=E3 POS= 0.055474 -0.313120  0.000000
        ATOM=E3 POS=-0.055474  0.313120  0.000000
        ATOM=E3 POS=-0.444526 -0.186880 -0.500000
        ATOM=E3 POS= 0.444526  0.186880 -0.500000
```

Running the Main Programs
Spin-Degenerate Calculations

Complete set of calculations: mnall.x

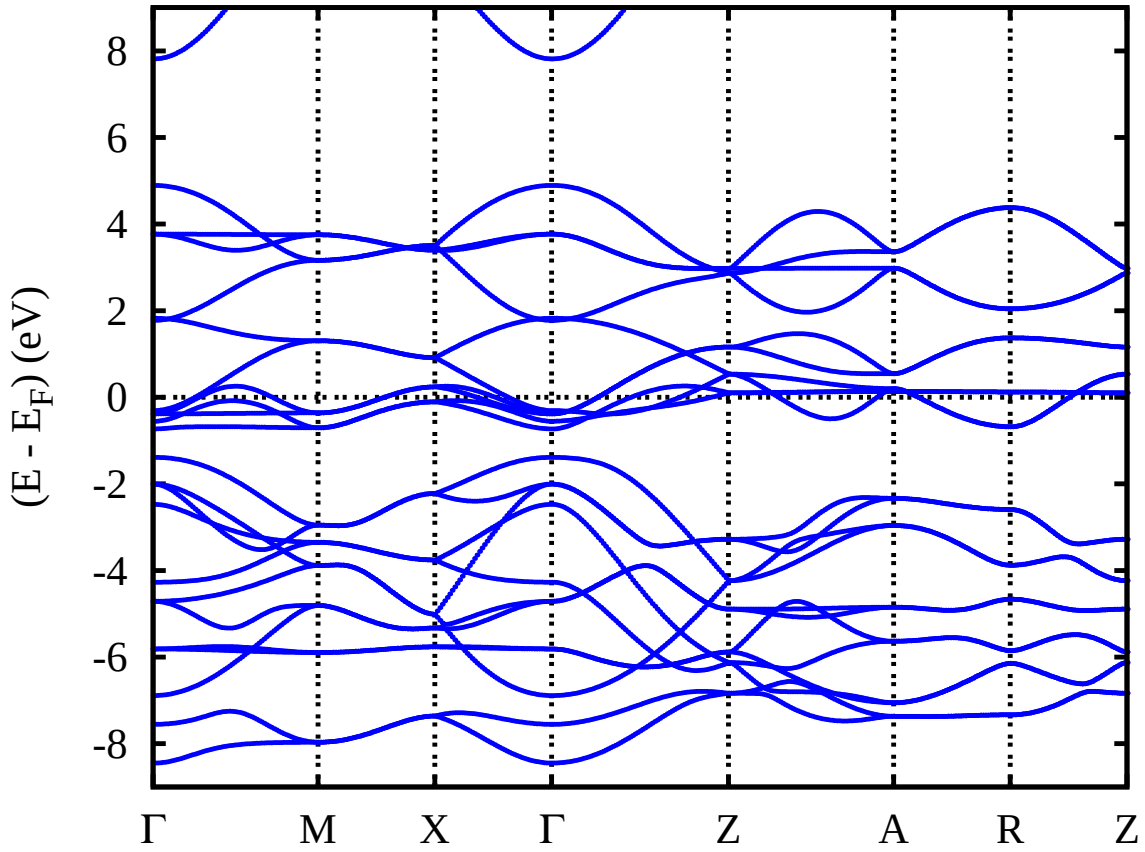
scf-cycle + band structure + DOS, COOP, Fermi surface

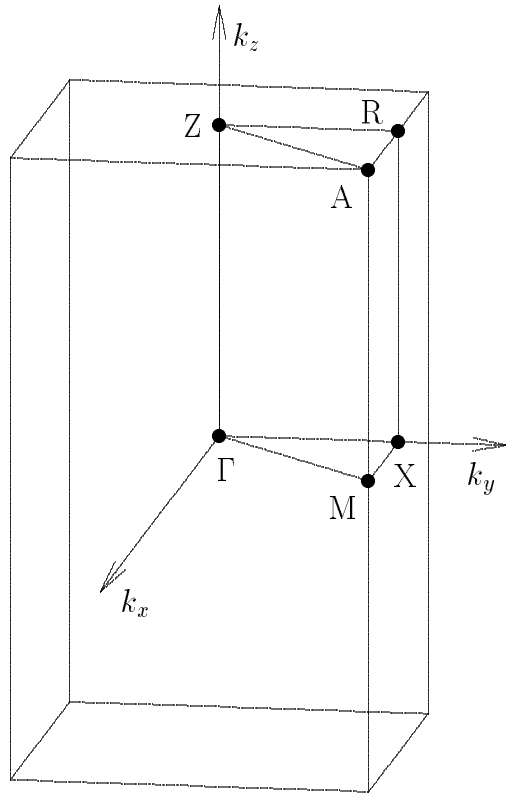
Summary Generated by Shell Script monic

```
ASW-2.3, program MNSCF started on asterix at Fri, 19 Jan 2007, 18:02:01.
Calculation converged after  13 iteration(s).
                     Start of Iteration   13
   396 irreducible k-points generated from    4116 ( 14, 14, 21).
          Fermi energy - MTZ =     0.772987 Ryd
The system is a metal:
          DOS at Fermi energy:   125.105425 1/Ryd
          Gamma * (f.u./cell):    21.674149 mJ/(mole*K**2)
Mean-square residual:                   0.751970D-24
Total free atom energies     :  -4790.190932 Ryd
Total variational energy     :  -4794.068403 Ryd
Cohesive energy              :      3.877470 Ryd
 qdiff =       0.00000000  <        0.00000001
 ediff =       0.00000000  <        0.00000001
ASW-2.3, program MNSCF ended on asterix at Fri, 19 Jan 2007, 18:16:24.
```

Running the Plot Programs I

Band Structure: plbnd.x/plbnd.run





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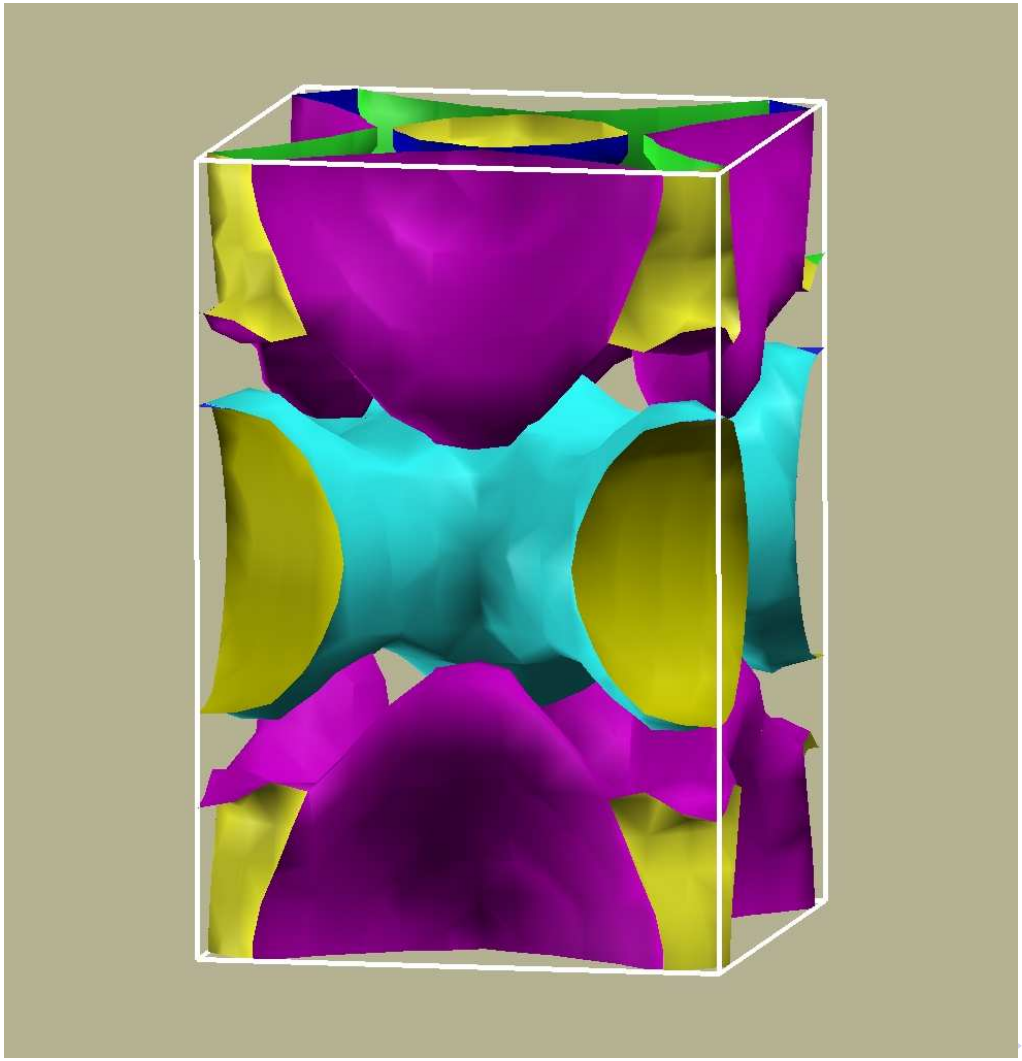
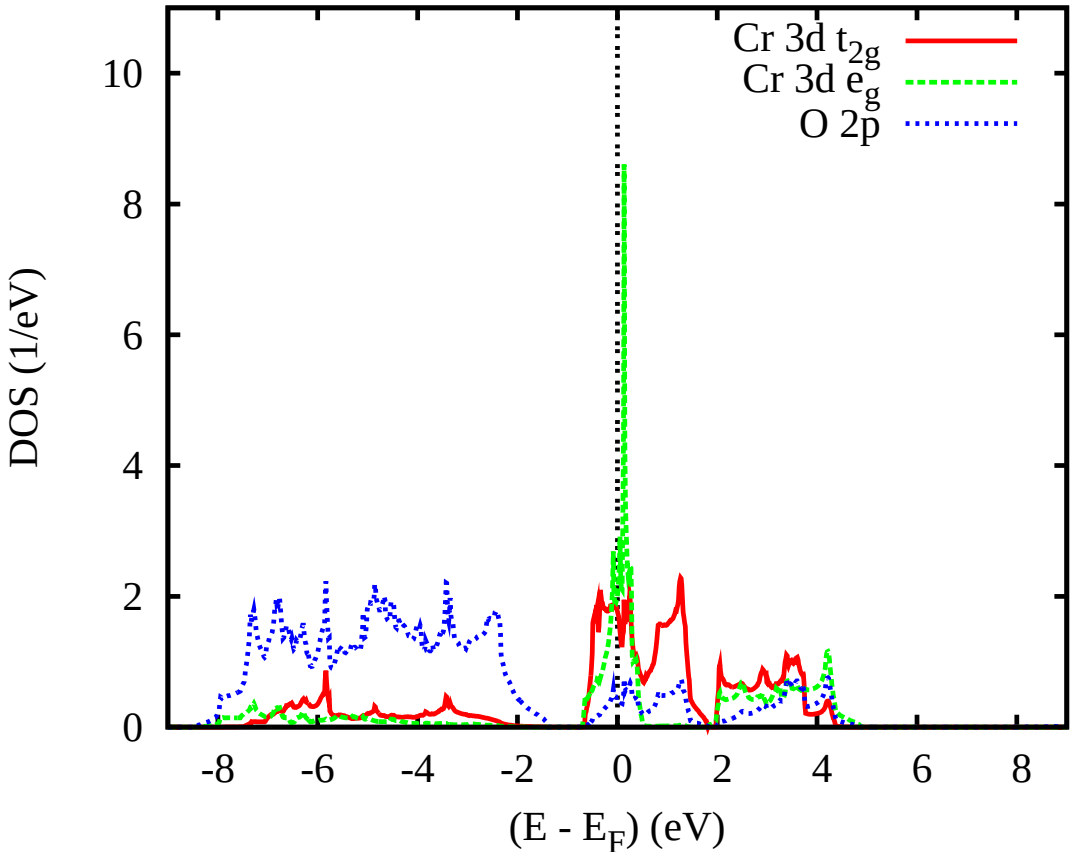
Running the Plot Programs II

Fermi Surface: plfrm.x



Running the Plot Programs III

Partial Densities of States: pldos.x/pldos.run



Crystal field splitting

Cr 3*d* in octahedron: t_{2g} and e_g states

without rotation

with rotation
R8(-1,-1,0)
*R4(1,-1,0)

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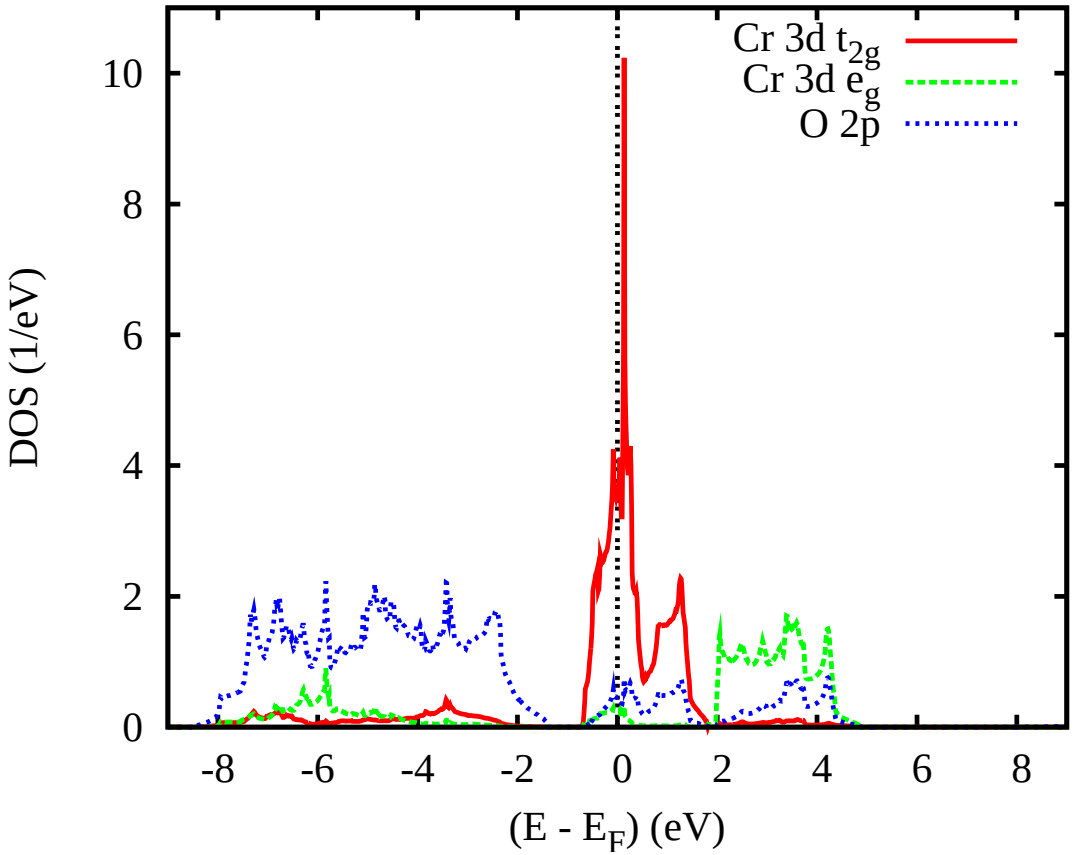
Running the Plot Programs III

Partial Densities of States: pldos.x/pldos.run



Crystal field splitting

Cr 3*d* in octahedron:
t_{2g} and e_g states

without rotation

with rotation
R8(-1,-1,0)
*R4(1,-1,0)

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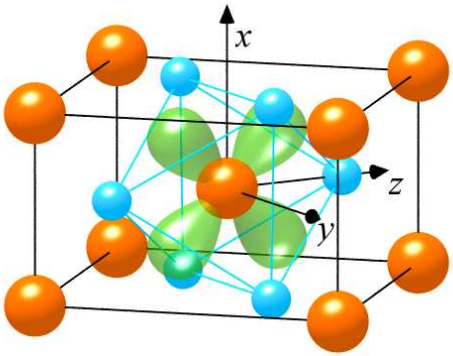
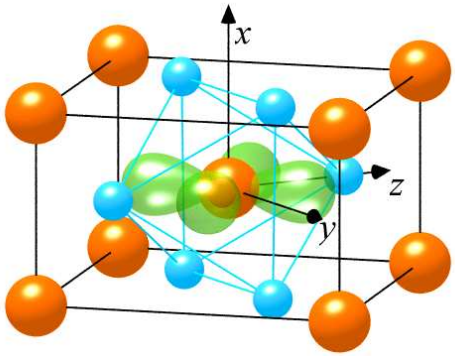
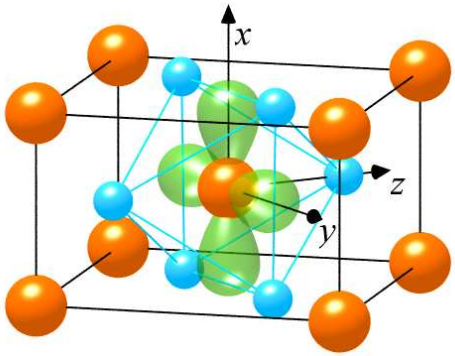
The Rotated *d* Orbitals



d_{xz}

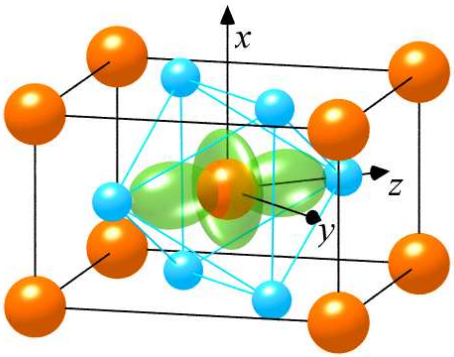


$= \text{“}\pi^*\text{”} =$

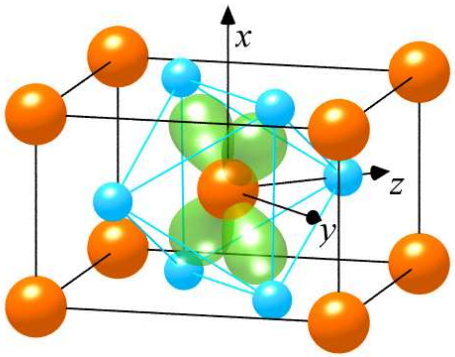


d_{yz}

$d_{x^2-y^2} = \text{“}d_{||}\text{”}$



$d_{3z^2-r^2}$



$= e_g^\sigma =$

d_{xy}

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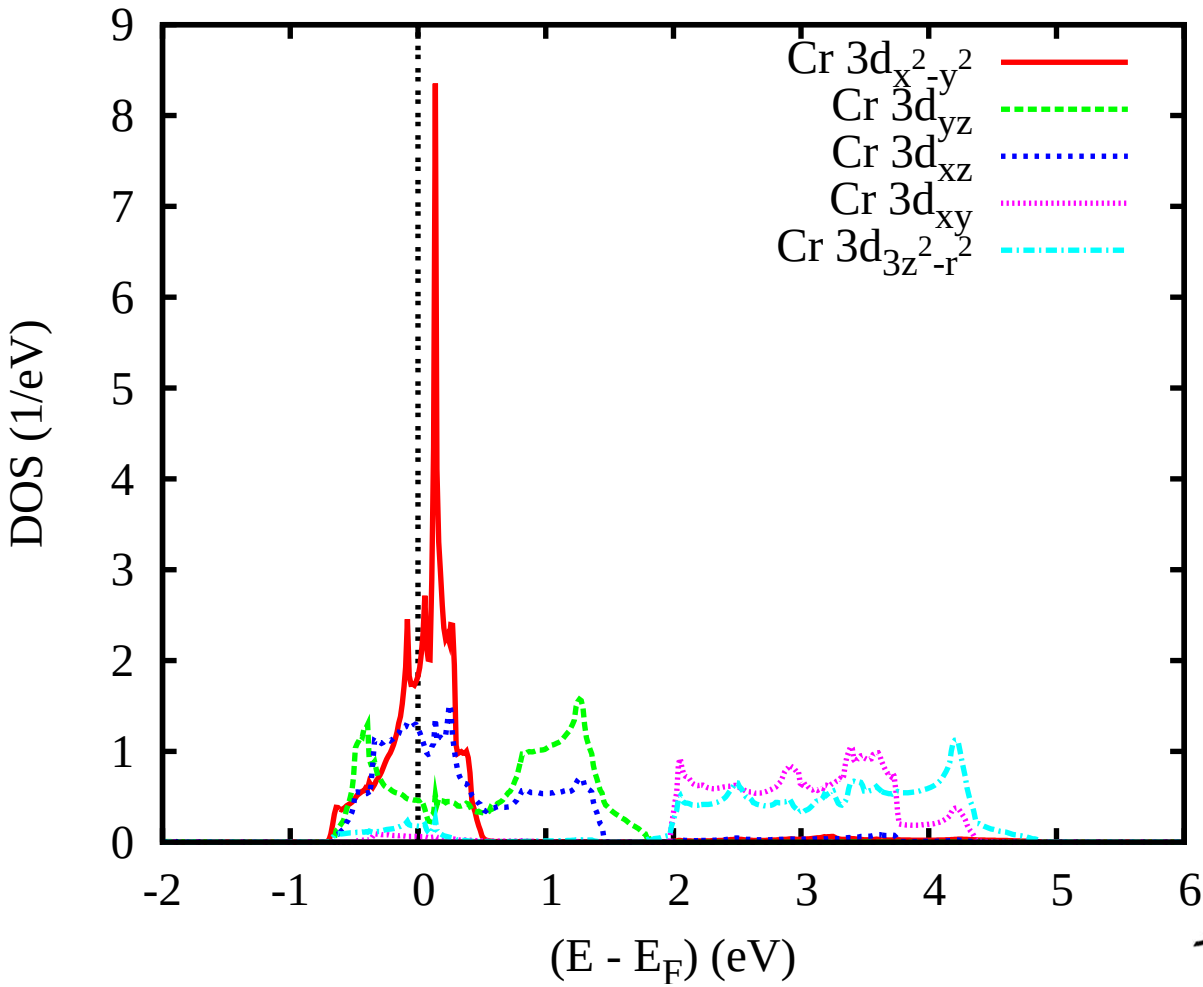
Running the Plot Programs IV

Partial Densities of States: pldos.x/pldos.run



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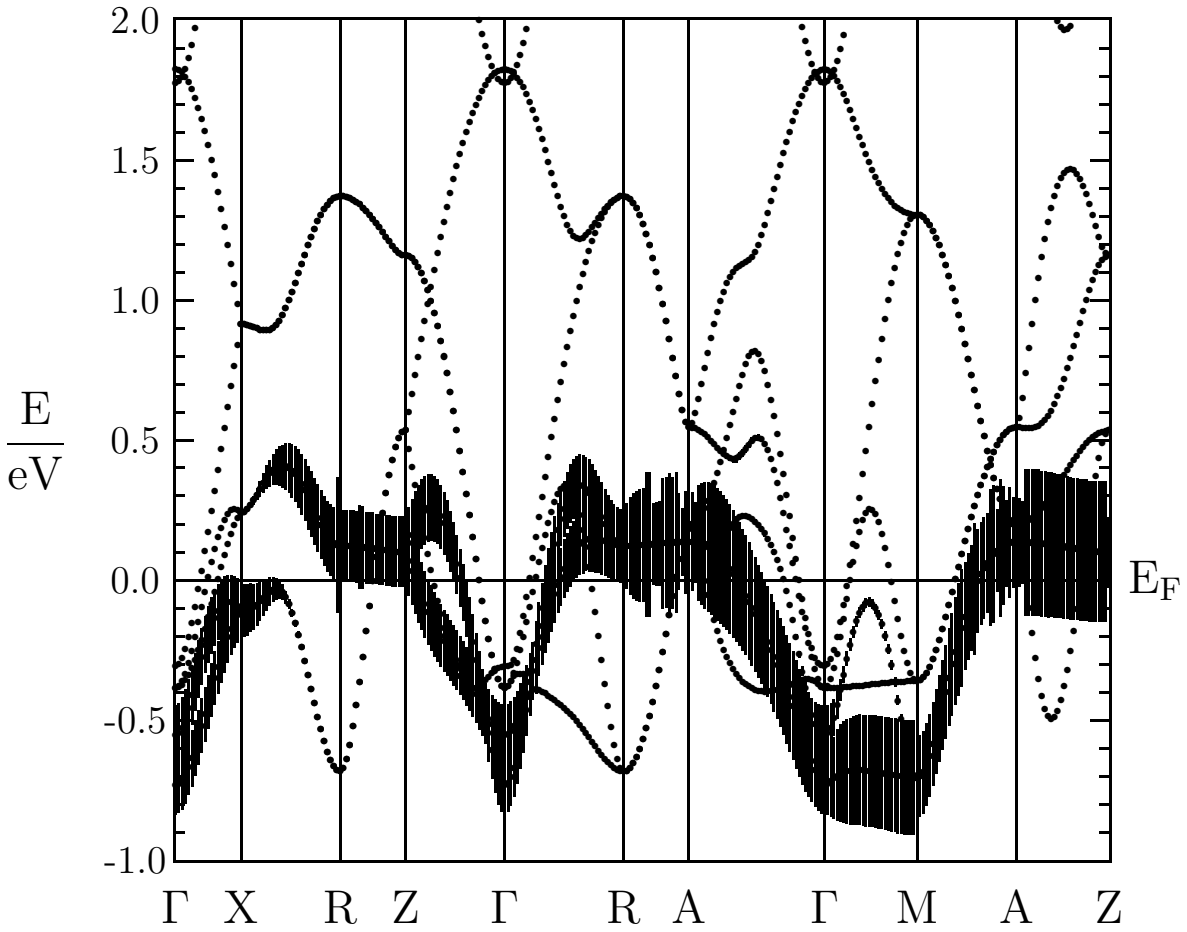
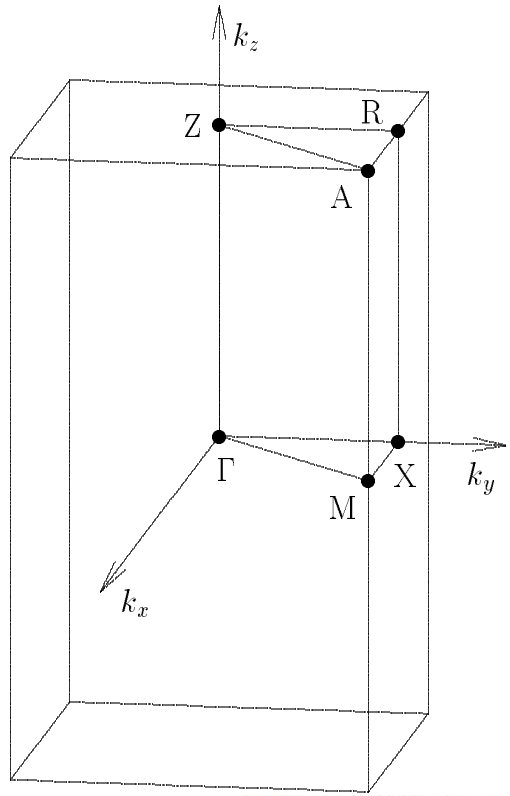
Running the Plot Programs V

Weighted Band Structure: plbnd.x/plbnd.run





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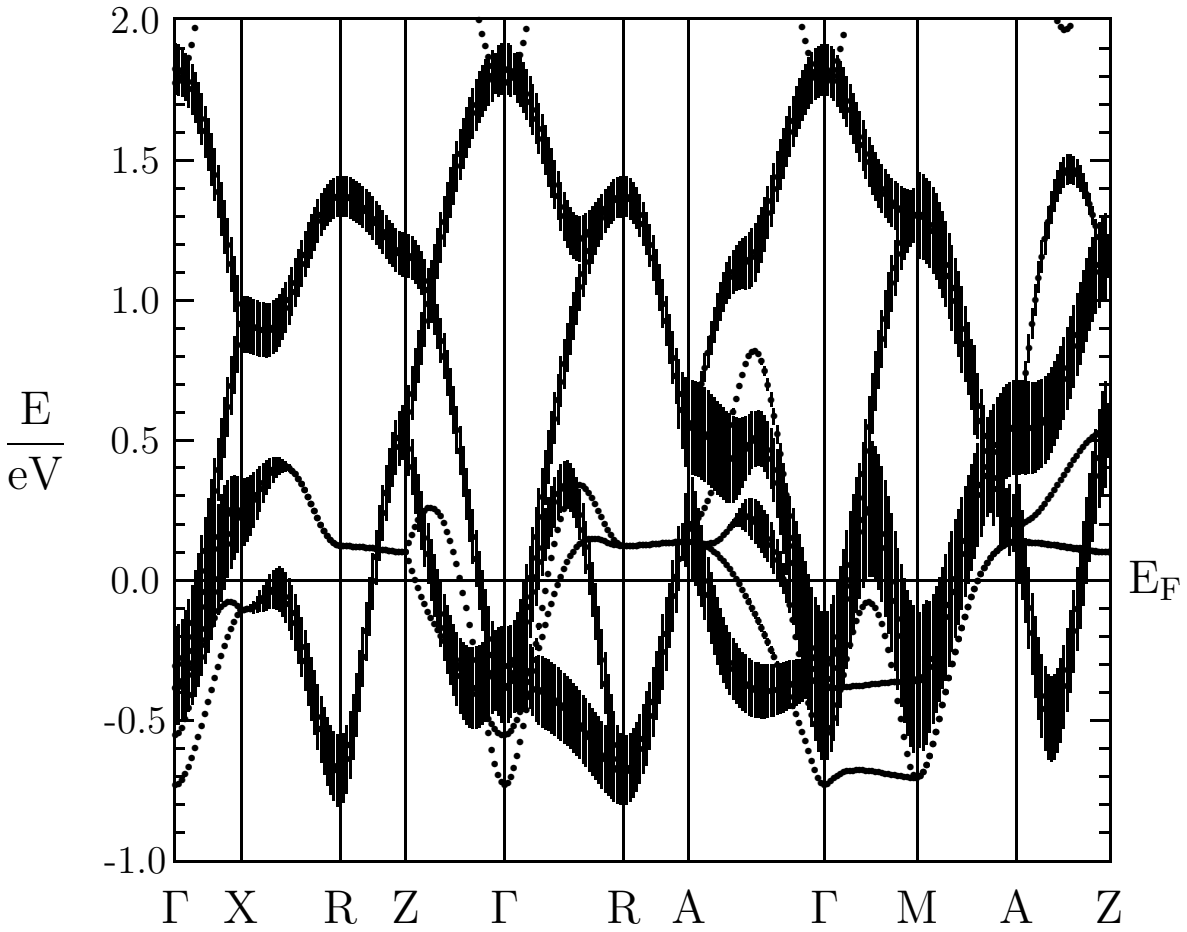
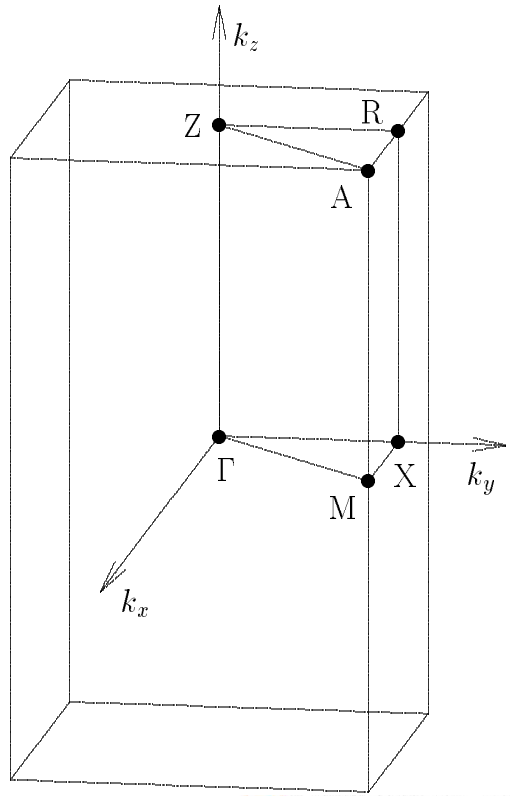
Running the Plot Programs V

Weighted Band Structure: plbnd.x/plbnd.run





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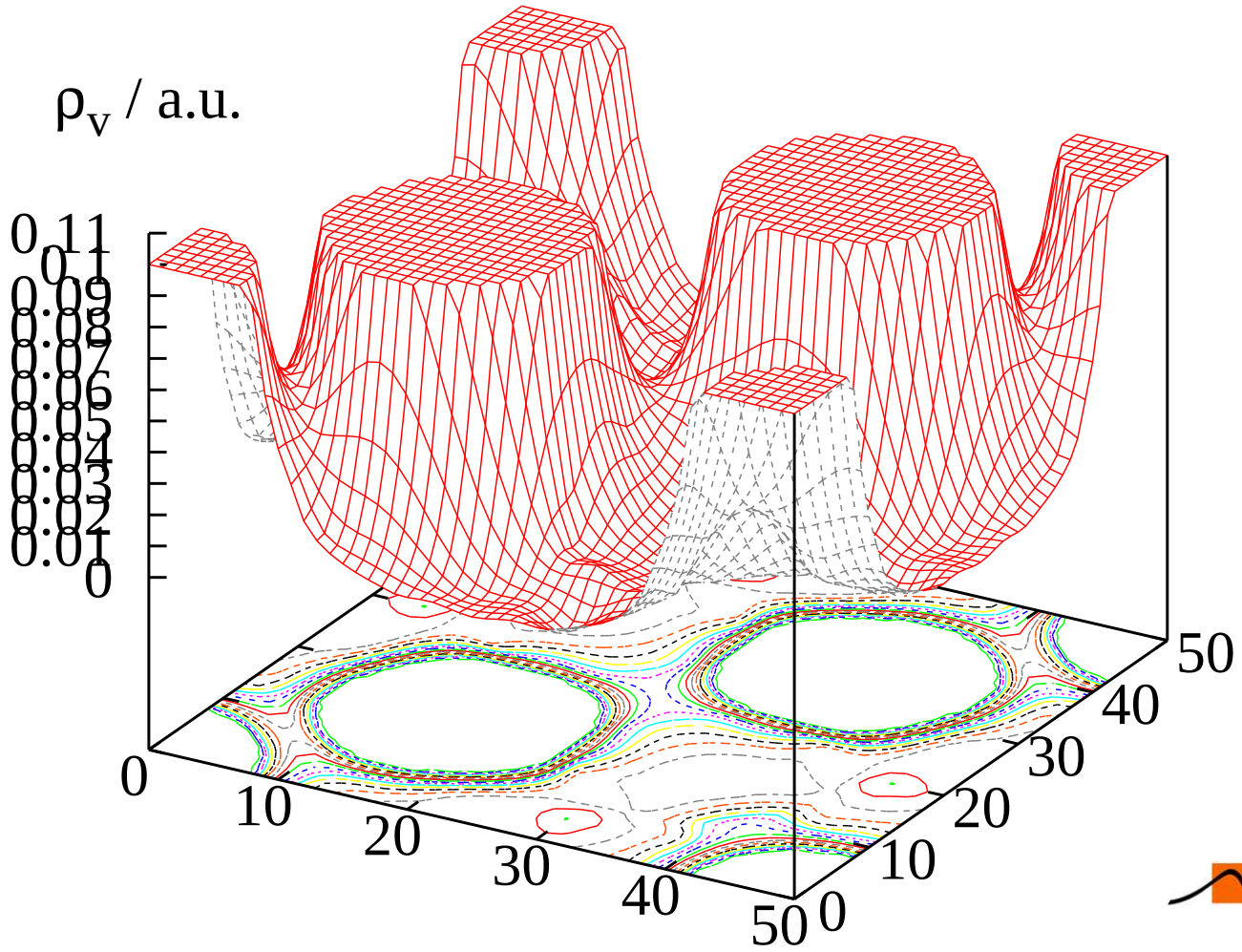
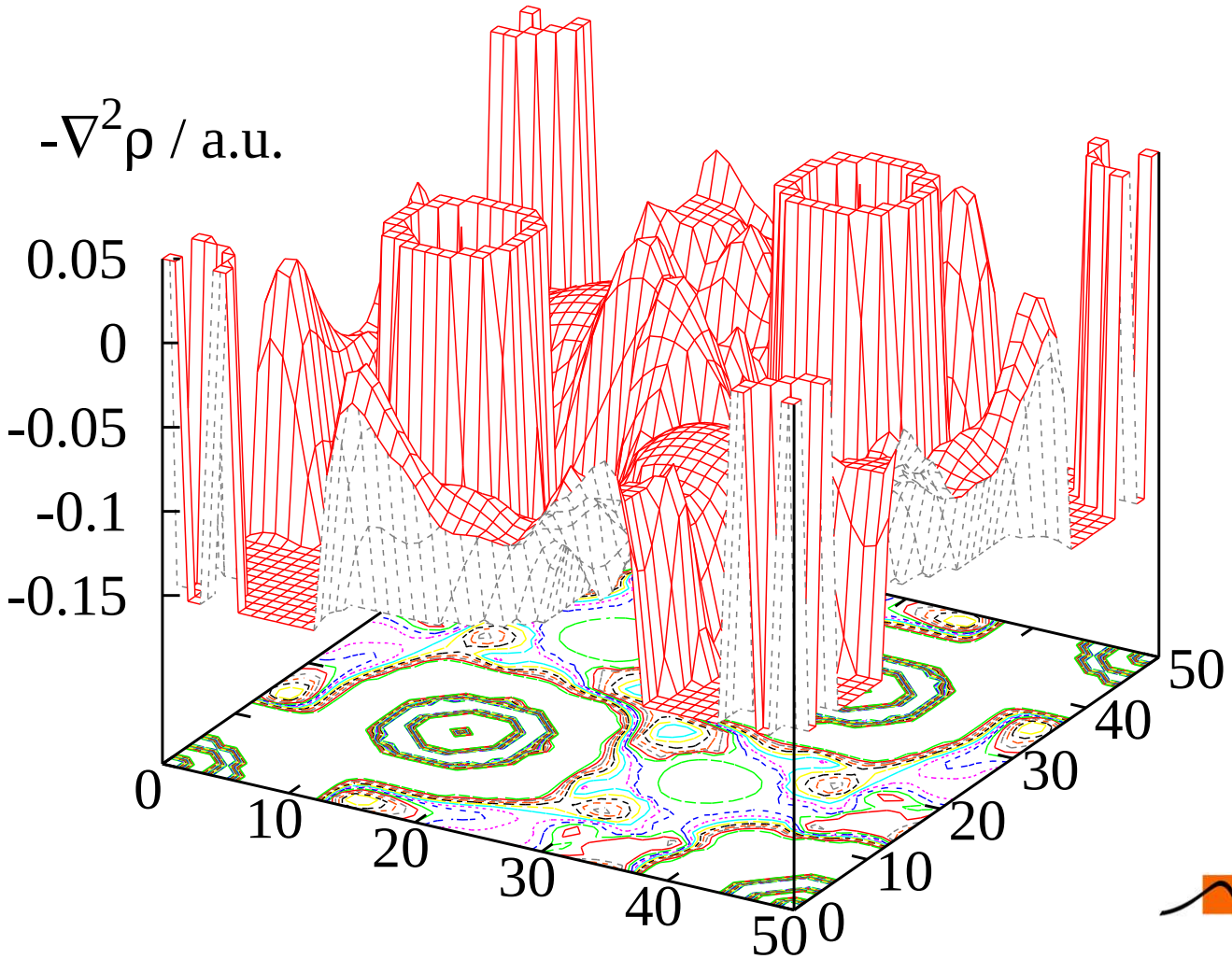
Running the Plot Programs VI

Valence Electron Density: plrho.x/plrho.run



Running the Plot Programs VII

Laplacian of Electron Density: plrho.x/plrho.run



Spin-Polarized Ferromagnetic Calculations

Additions to the CTRL File

Category OPTIONS

```
OPTIONS REL=T NSPIN=2 OVLCHK=T
```

Category CLASS

```
CLASS   ATOM=CR Z=24 R=2.16612899 LMXL=2 CONF=4 4 3 4
        QVAL= 1.0 0.0 5.0 0.0 MVAL= 0.0 0.0 2.0 0.0
        ATOM=O  Z= 8 R=1.87483912 LMXL=1 CONF=2 2 3
        QVAL= 2.0 4.0 0.0     MVAL= 0.0 0.0 0.0
        ATOM=E1 Z= 0 R=1.65252923 LMXL=1 CONF=1 2 3
        QVAL= 0.0 0.0 0.0     MVAL= 0.0 0.0 0.0
        ATOM=E2 Z= 0 R=1.76771917 LMXL=1 CONF=1 2 3
        QVAL= 0.0 0.0 0.0     MVAL= 0.0 0.0 0.0
        ATOM=E3 Z= 0 R=0.85735960 LMXL=0 CONF=1 2
        QVAL= 0.0 0.0         MVAL= 0.0 0.0 0.0
```

Running the Main Programs

Spin-Polarized Ferromagnetic Calculations

Complete set of calculations: mnall.x

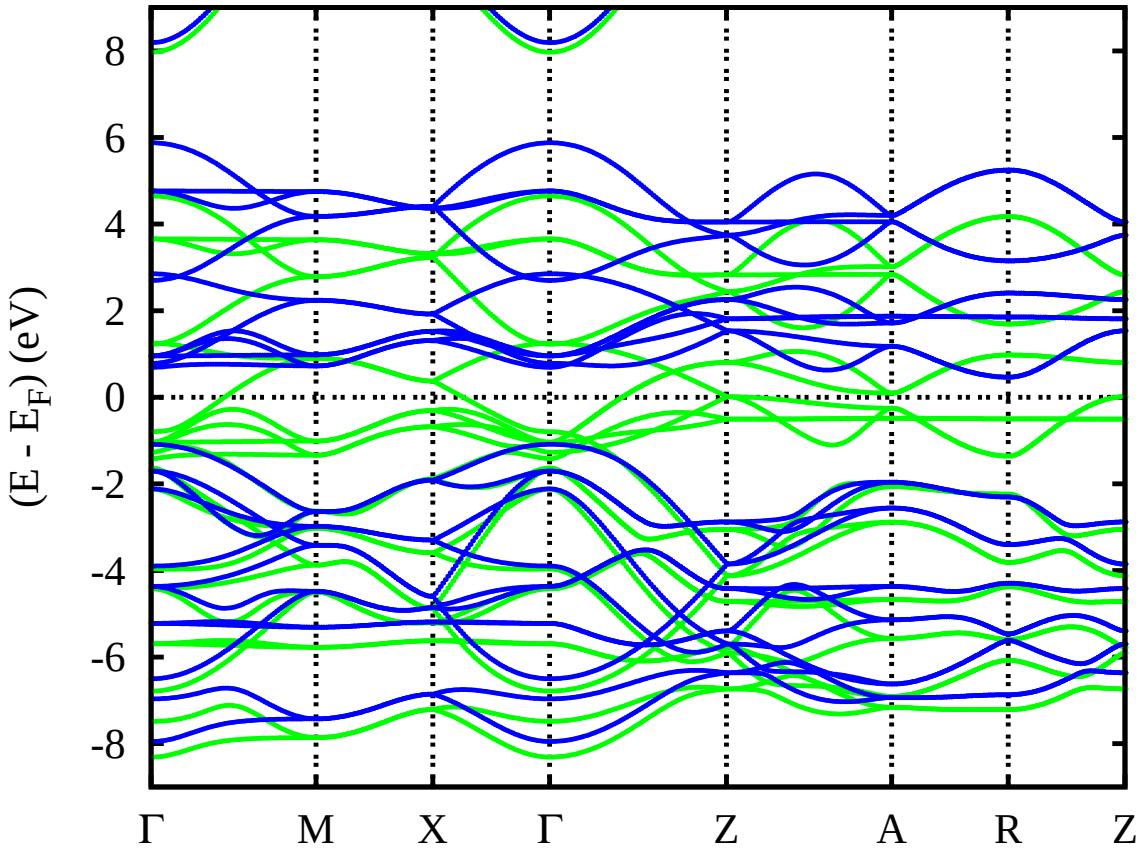
scf-cycle + band structure + DOS, COOP, Fermi surface

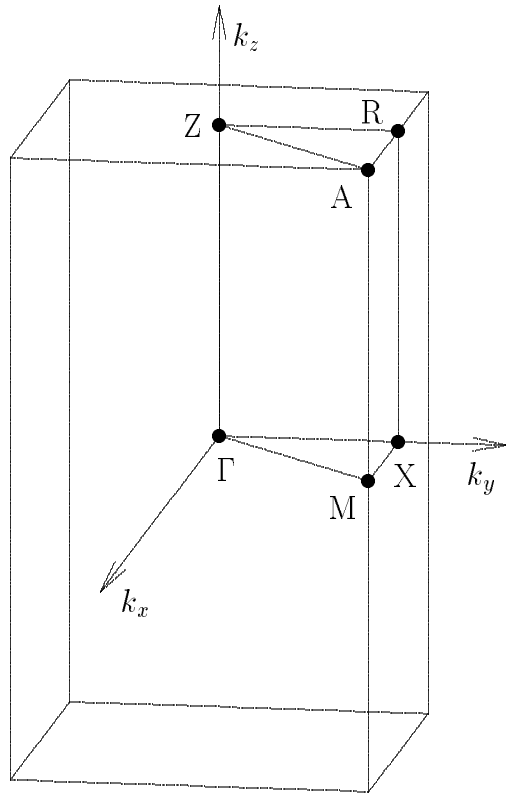
Summary Generated by Shell Script monic

```
ASW-2.3, program MNSCF started on asterix at Fri, 19 Jan 2007, 19:16:52.
Calculation converged after  18 iteration(s).
                     Start of Iteration   18
    24 irreducible k-points generated from     175 (  5,  5,  7).
           Fermi energy - MTZ =     0.754887 Ryd
The system is a half-metallic ferromagnet:
            Indirect band gap =     0.118091 Ryd =     1.606710 eV
           DOS at Fermi energy:    17.123320 1/Ryd
           Gamma * (f.u./cell):     2.966565 mJ/(mole*K**2)
Magnetic moment of unit cell    =     4.000000
Mean-square residual:                   0.599969D-23
Total free atom energies     :  -4790.190932 Ryd
Total variational energy     :  -4794.139707 Ryd
Cohesive energy              :     3.948775 Ryd
 qdiff =       0.00000000  <        0.00000001
 ediff =       0.00000000  <        0.00000001
ASW-2.3, program MNSCF ended on asterix at Fri, 19 Jan 2007, 19:28:39.
```

Running the Plot Programs I

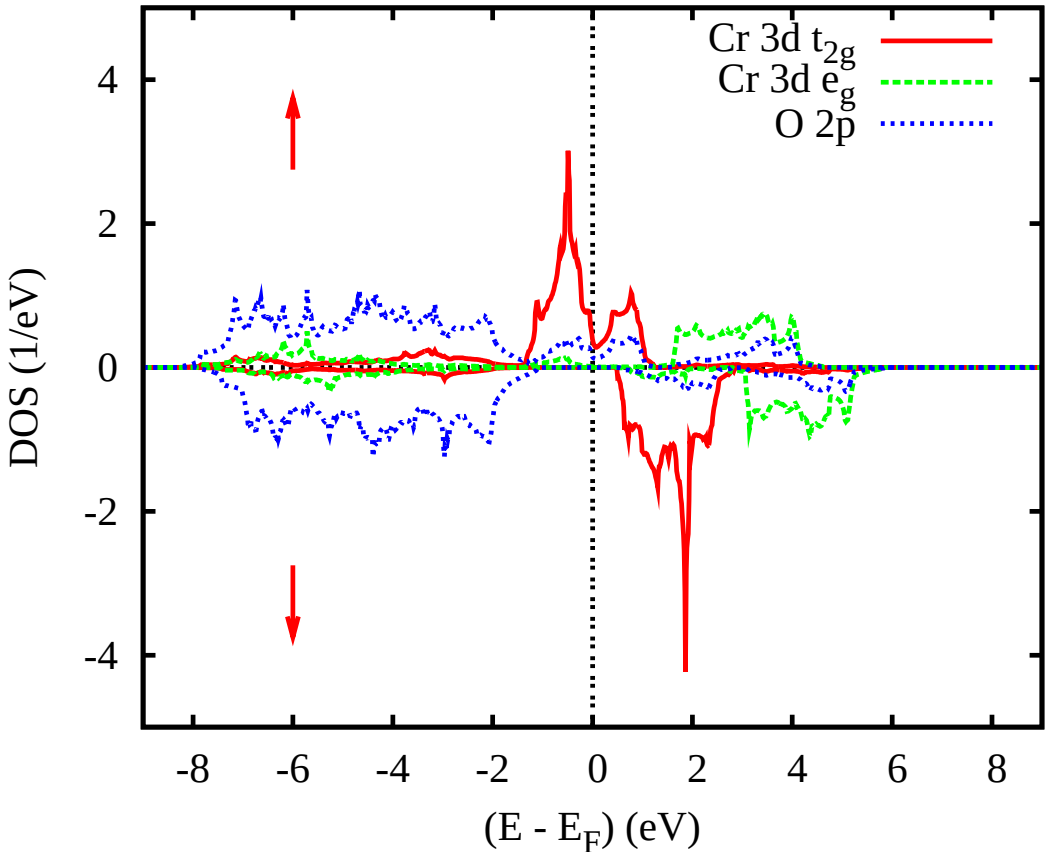
Band Structure: plbnd.x/plbnd.run





Running the Plot Programs II

Partial Densities of States: pldos.x/pldos.run



Crystal field splitting

Cr 3*d* in octahedron: t_{2g} and e_g states

with rotation
R8(-1,-1,0)
*R4(1,-1,0)

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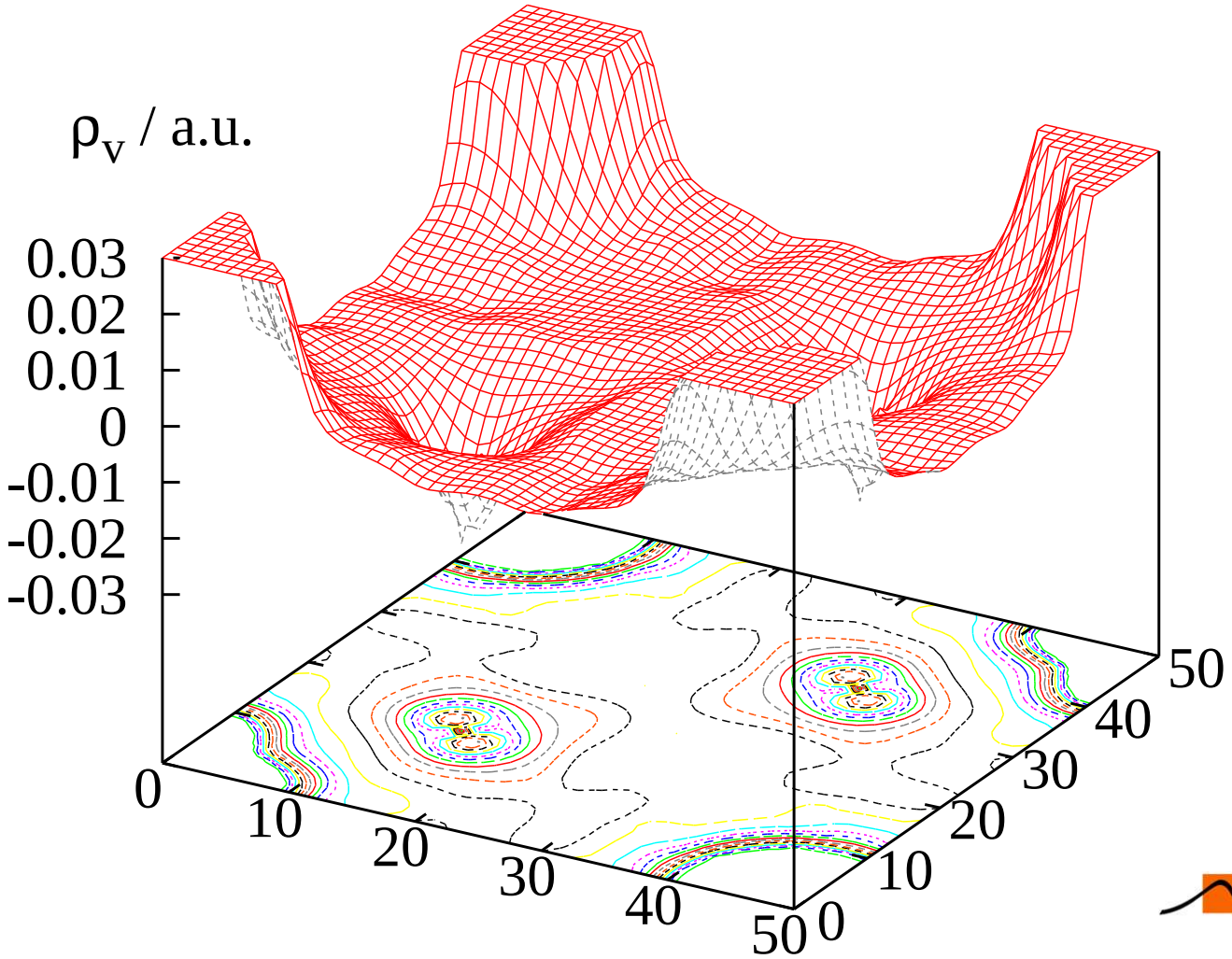
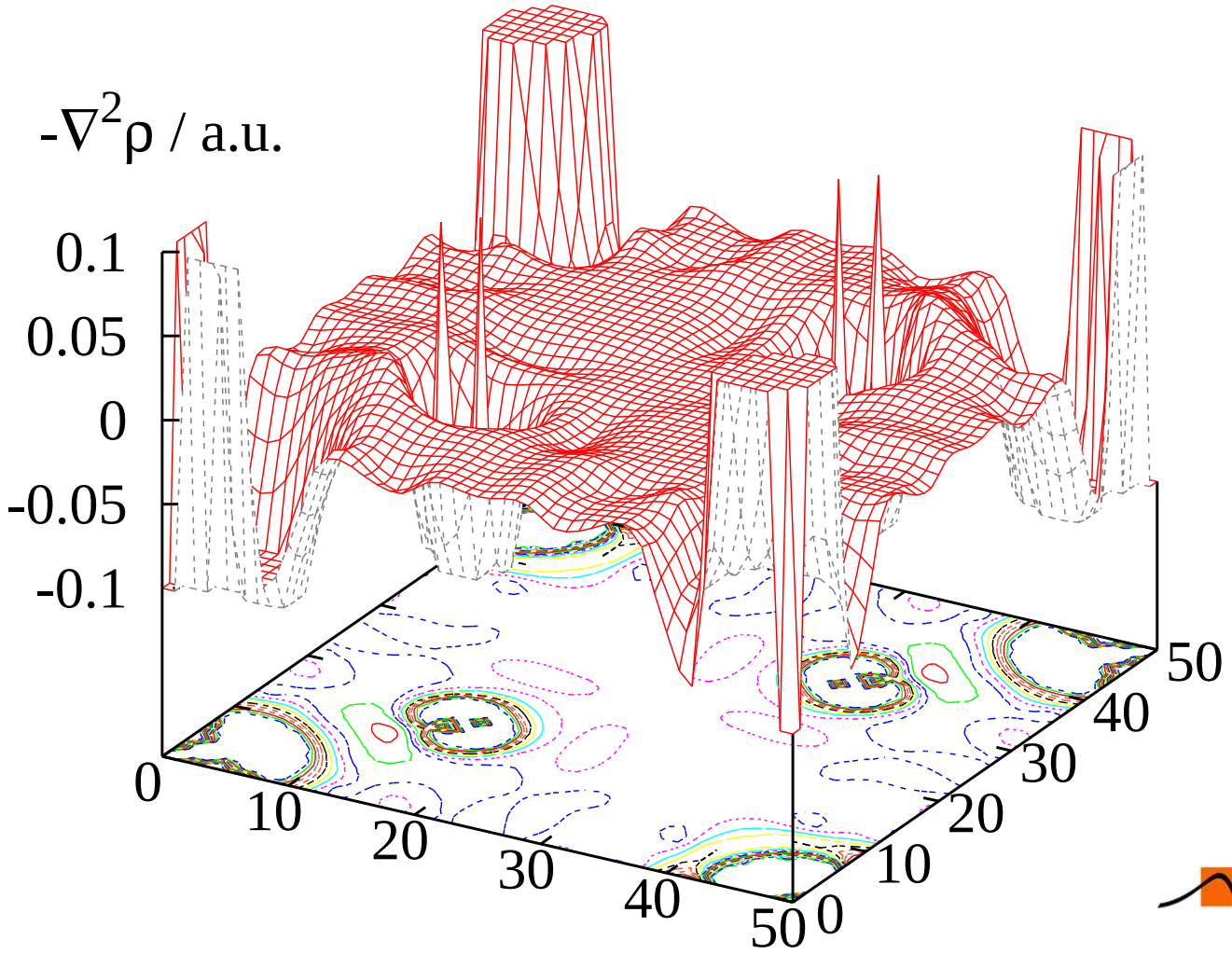
Running the Plot Programs III

Valence Electron Spin Density: plrho.x/plrho.run



Running the Plot Programs IV

Laplacian of Electron Spin Density: plrho.x/plrho.run



Spin-Polarized Antiferromagnetic Calculations

Additions to the CTRL File

Category OPTIONS

```
OPTIONS REL=T NSPIN=2 AFSYM=T OVLCHK=T
```

Category SITE

```
SITE    CARTP=F
        ATOM=CR POS= 0.000000  0.000000  0.000000 SPIN=UP
        ATOM=CR POS= 0.500000  0.500000  0.500000 SPIN=DN
        ATOM=O  POS= 0.302400  0.302400  0.000000 SPIN=UP
        ATOM=O  POS=-0.302400 -0.302400  0.000000 SPIN=UP
        ATOM=O  POS=-0.197600  0.197600  0.500000 SPIN=DN
        ATOM=O  POS= 0.197600 -0.197600  0.500000 SPIN=DN
        ATOM=E1 POS= 0.500000  0.000000 -0.250000 SPIN=DN
        ATOM=E1 POS= 0.500000  0.000000  0.250000 SPIN=UP
        ATOM=E1 POS= 0.000000 -0.500000 -0.250000 SPIN=DN
        ATOM=E1 POS= 0.000000 -0.500000  0.250000 SPIN=UP
...
```

Running the Main Programs
Spin-Polarized Antiferromagnetic Calculations

Complete set of calculations: mnall.x

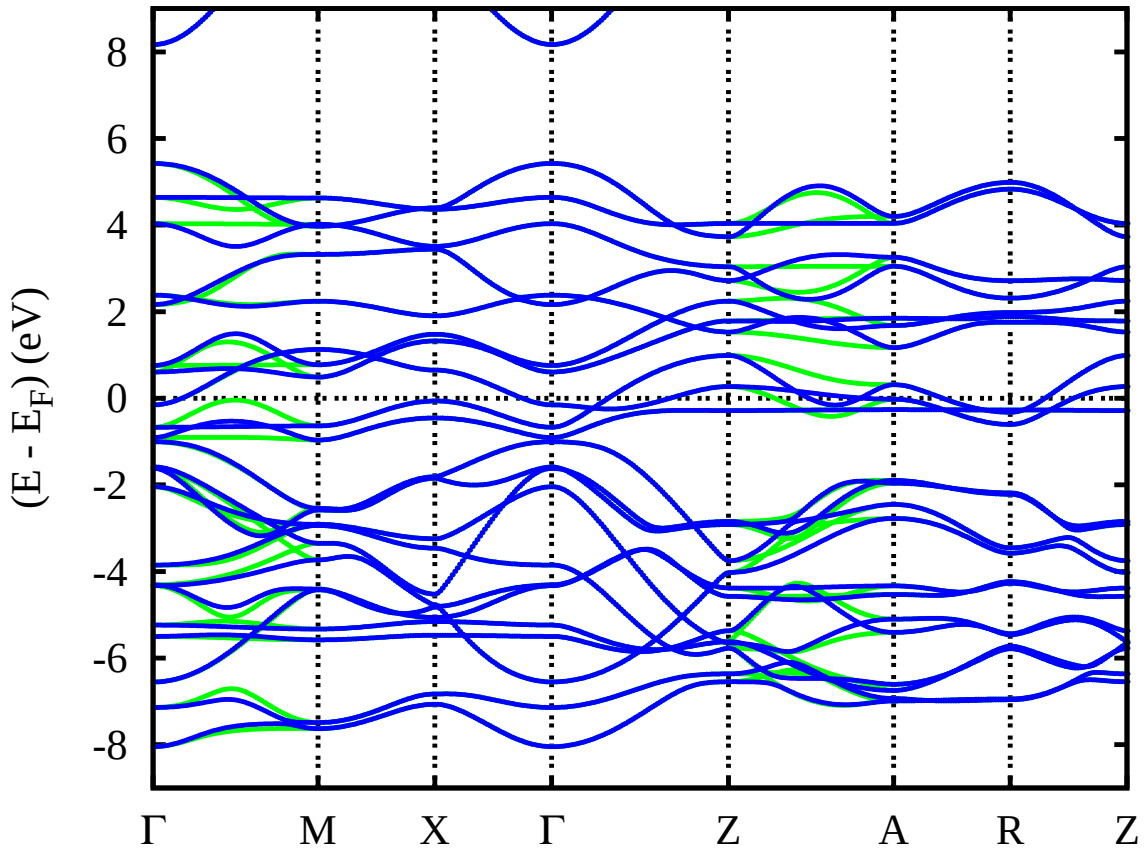
scf-cycle + band structure + DOS, COOP, Fermi surface

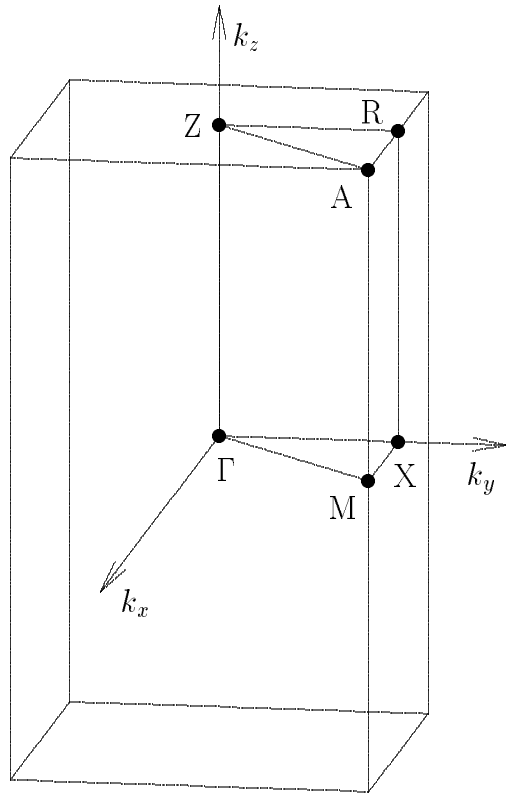
Summary Generated by Shell Script monic

```
ASW-2.3, program MNSCF started on asterix at Tue, 30 Jan 2007, 22:04:56.
Calculation converged after  25 iteration(s).
                     Start of Iteration   25
    42 irreducible k-points generated from     175 (  5,  5,  7).
           Fermi energy - MTZ =     0.747316 Ryd
The system is a magnetic metal and could still be a half-metallic ferromagnet:
           DOS at Fermi energy:    38.926427 1/Ryd
           Gamma * (f.u./cell):     6.743889 mJ/(mole*K**2)
Magnetic moment of UP atoms     =     1.707078
Magnetic moment of unit cell    =     0.000000
Mean-square residual:                   0.574144D-22
Total free atom energies     :  -4790.190932 Ryd
Total variational energy     :  -4794.116546 Ryd
Cohesive energy              :     3.925613 Ryd
 qdiff =       0.00000000  <        0.00000001
 ediff =       0.00000001  <        0.00000001
ASW-2.3, program MNSCF ended on asterix at Tue, 30 Jan 2007, 22:27:54.
```

Running the Plot Programs I

Band Structure: plbnd.x/plbnd.run





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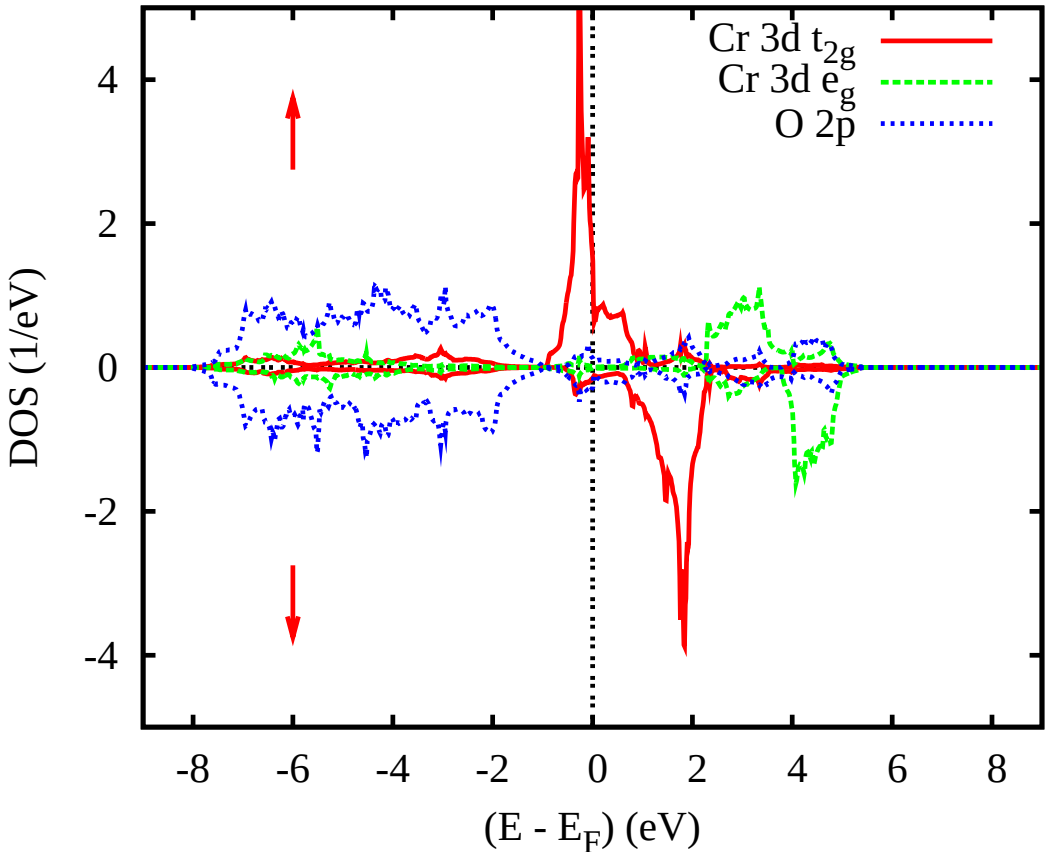
Running the Plot Programs II

Partial Densities of States: pldos.x/pldos.run



Crystal field splitting

Cr 3*d* in octahedron: t_{2g} and e_g states

with rotation
R8(-1,-1,0)
*R4(1,-1,0)

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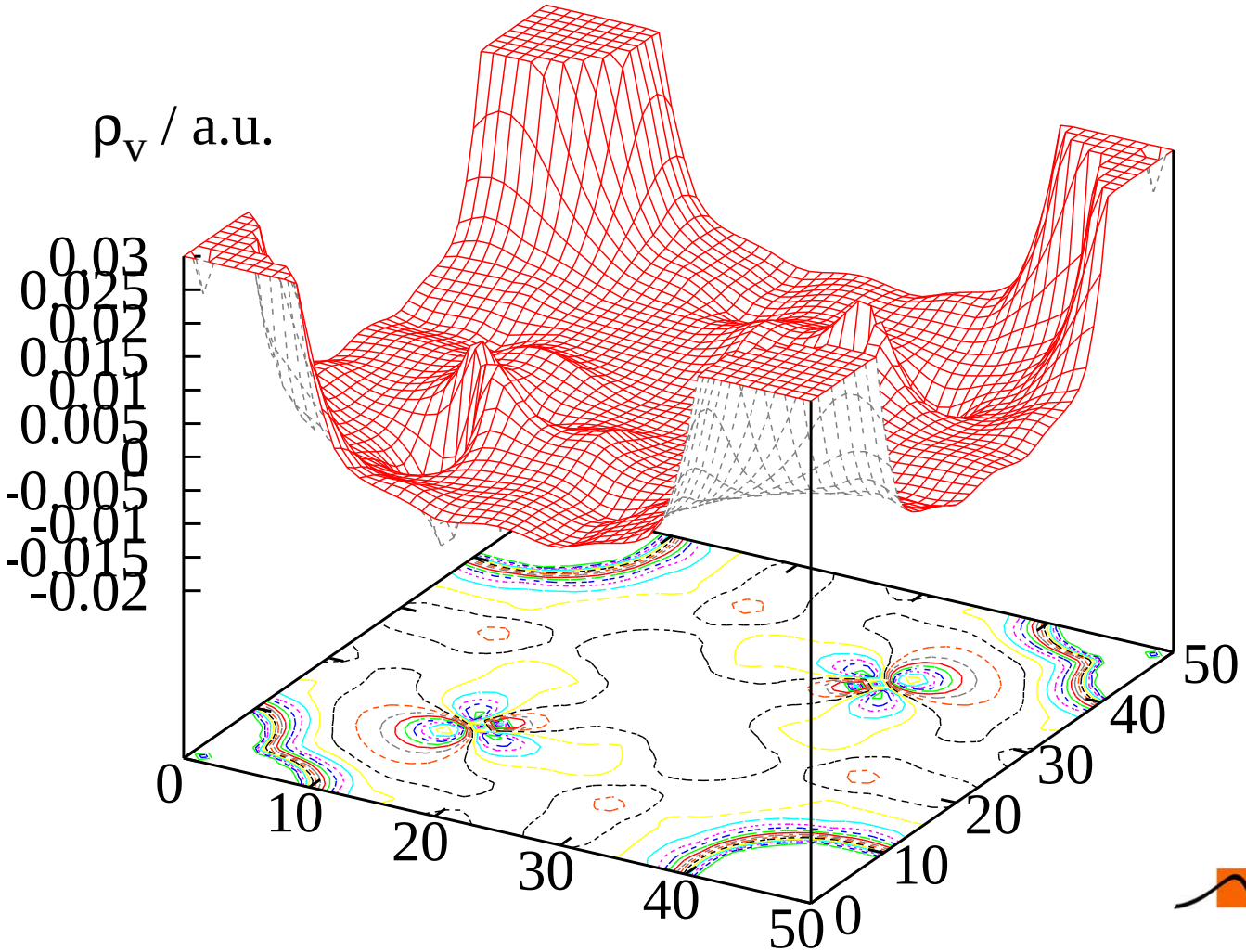
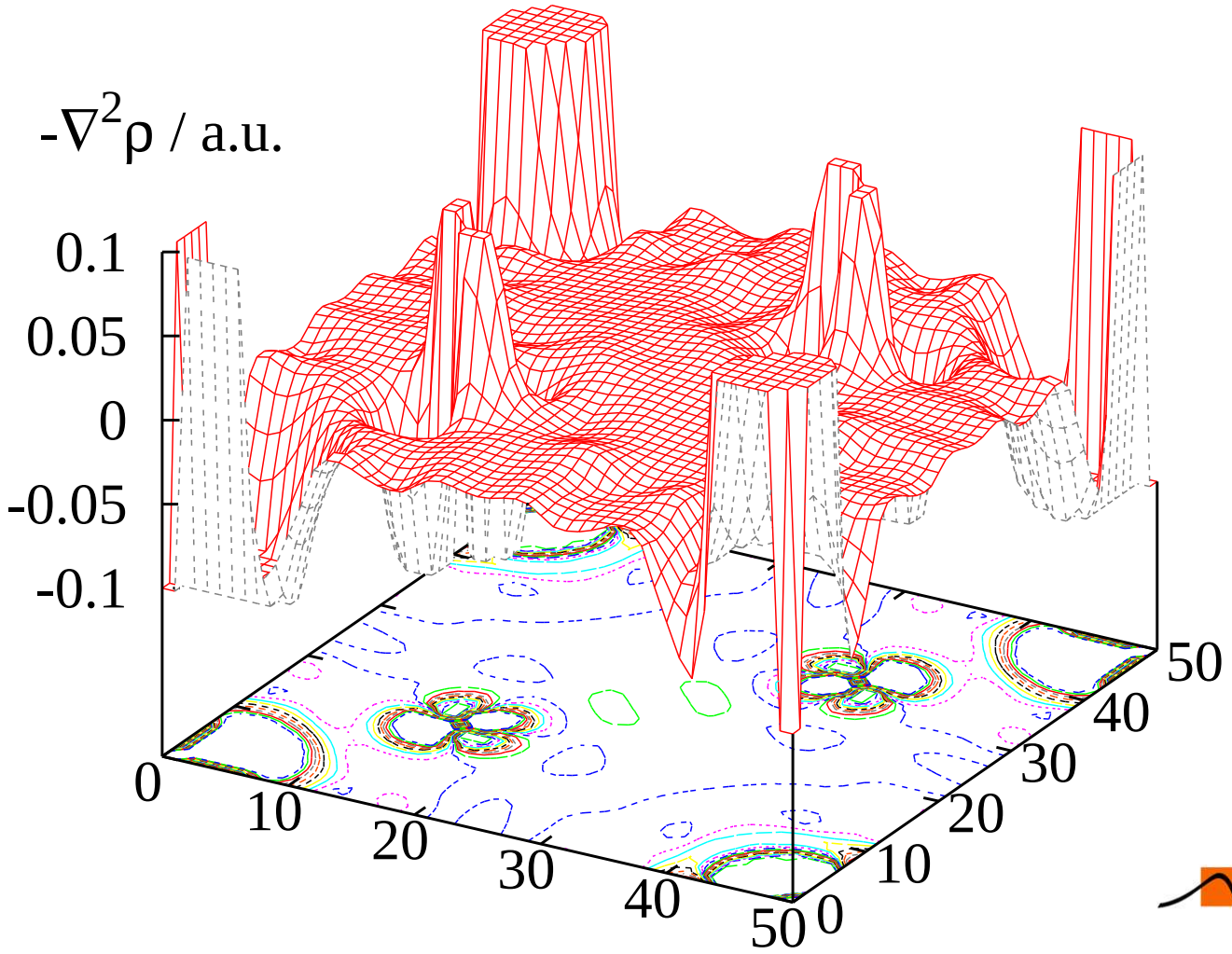
Running the Plot Programs III

Valence Electron Spin Density: plrho.x/plrho.run



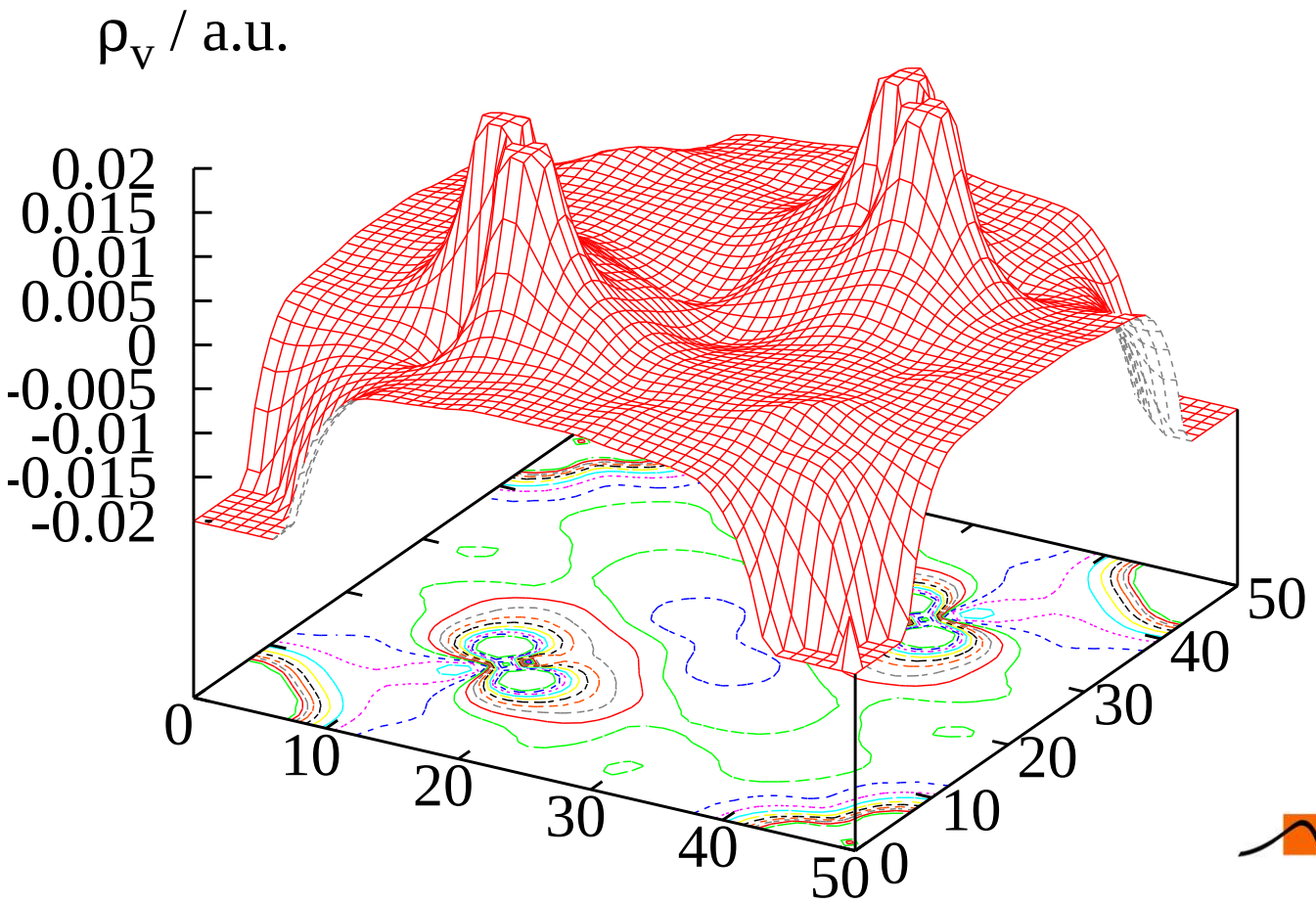
Running the Plot Programs IV

Laplacian of Electron Spin Density: plrho.x/plrho.run



Running the Plot Programs V

Valence Electron Spin Density: plrho.x/plrho.run



Summary

Sphere Geometry Optimization (SGO)

- sphere packing (mnpac.run)

Complete set of calculations: mnall.x

- self-consistent field calculation
- band structure, DOS, COOP, FS

Analyze results

- check output (use monic or edit)
- use rotated reference frames for plotting weighted band structures and partial DOS

Further Reading I

V. Eyert
The Augmented Spherical Wave Method — An Extended User Guide.