Running the LMTO code

A quick tutorial

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Outline

- LDA calculation
- Estimation of U and J
- LDA+U calculation

Technical details

- Realization of DFT method: Local Density Approximation in Tight-Binding Linearized Muffin-Tin formalism (TB-LMTO)
- Manuals for the TB-LMTO can be found in tb/OTHER/doc/
- Tested with **ifort** and **g95** compilers
- Configure makefile and copy the binaries to your local /bin
- To get the code ask tutor

What do we need to know to get started?

- Crystal structure:
  - Lattice constants
  - Crystal symmetry
  - Translation vectors
  - Atomic positions
- Information about elements:
  - Atomic number
  - Configuration of valent shells
  - Initial guess of charge distribution

What can we get?

- Total energy
- Density of states
- Charge and spin distributions
- Fermi surface
- Band structure along directions in k-space between high symmetry points
- Forces
- ...

CoO

- CoO periclase (rock salt) structure;
  - Co has octahedral coordination of O;
  - t_{2g} and e_g are separated in energy;
  - t_{2g} and e_g are not hybridized;
- CoO is a d^7 system;
- CoO is an antiferromagnetic charge-transfer insulator ($T_N = 291K$);

Crystal structure parameters of CoO

Space group	$Fm\bar{3}m$ (Number 225)
Lattice constant	4.2615 atomic units
Atomic coordinates:	Co (0, 0, 0)
	O (0.5, 0.5, 0.5)

Part I

Calculation of a bandstructure within LDA

Production of CTRL file

- make INIT file: change to your working directory and type *lm47.run lminit*

```
QUERY : Spacegroup symbol or number  225

 Space group: Fm-3m      No.:225
 Crystal system: cubic
 Generators: I R4X R3D
QUERY : atomic-units? (else Angstrom)(DEFAULT=T) F

  Now enter lattice parameters
QUERY : A :lattice parameter (in Angstrom)      4.2615

CTRLUC:              PLAT                ALAT=    8.05307
       0.00000    0.50000    0.50000
       0.50000    0.00000    0.50000
       0.50000    0.50000    0.00000

QUERY : Label or nuclear charge   Co
QUERY : X = position of Co  (DEFAULT=0. 0. 0.) 0.0 0.0 0.0
QUERY : Label or nuclear charge   O
QUERY : X = position of O   (DEFAULT=0. 0. 0.) 0.5 0.5 0.5
QUERY : Label or nuclear charge   q
```

Production of CTRL file

- determine atomic sphere radius:
  user@somehost > *lm47.run lmhart*
- check atomic sphere overlap:
  user@somehost > *lm47.run lmovl*
- try to insert empty spheres (and again check atomic sphere overlap):
  user@somehost > *lm47.run lmes*
  user@somehost > *lm47.runl movl*
- complete CTRL file:
  set VERBOS parameter(CTRL file 3rd line) to 50
  user@somehost > *lm47.run lmctl*

Important categories and tokens of CTRL file

```
IO          VERBOS=50 OUTPUT=LOUT ERR=LERR
SYMGRP      NGEN=3 GENGRP=I R4X R3D
            SPCGRP=Fm-3m USESYM=F
STRUC       ALAT=8.0530711
            PLAT=0.0 0.5 0.5
                 0.5 0.0 0.5
                 0.5 0.5 0.0 FIXLAT=T
OPTIONS     NSPIN=1 REL=T CCOR=T NONLOC=F NRXC=1 NRMIX=2 CORDRD=F
            NITATOM=30 CHARGE=F FATBAND=F AFM=F SEWALD=F FS=F
            CARTESIAN=T WRIBAS=F Q=---- LOCALCS=F GAMMA=F Zero_Ppar=F
CLASS       ATOM=Co Z=27 R=2.57891492 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1
            IDMOD=0 0 0 RHO_print=0 0 0
            ATOM=O  Z= 8 R=2.03070701 LMX=2 CONF=3 2 3 4 IDXDN=2 1 2
            IDMOD=0 0 0 RHO_print=0 0 0
SITE        ATOM=Co POS= 0.00  0.00  0.00
            ATOM=O  POS= 0.50  0.50  0.50
            ATOM=E  POS= 0.25  0.25  0.25
            ATOM=E  POS=-0.25 -0.25 -0.25
```

Important categories and tokens of CTRL file

```
START     NIT=30 BROY=T WC=-1 NMIX=1 BETA=0.5
          FREE=F CNVG=0.00001 CNVGET=0.00001 BEGMOM=T CNTROL=T
          EFERMI=-0.25 VMTZ=-0.75
          ATOM=Co  P=4.66 4.41 3.83
                   Q=0.6 0.0 0.0
                     0.8 0.0 0.0
                     7.6 0.0 0.0
              enu   =-0.452 -0.282 -0.194
              c     =-0.267  0.830 -0.141
              sqrdel=0.514 0.642 0.236
              p     =0.033 0.019 1.390
              gamma = 0.558  0.252 -0.003
SCELL     PLAT=0.0 0.5 0.5
               0.5 0.0 0.5
               0.5 0.5 0.0 EQUIV=T
UCORREC   Ucorr=F unitsEV=T DOSp=F Classes=1 N_avr=F LSDA+U=T
          CLASS=Co L=2 Uvalue=0 Jvalue=0
          MixVCL=1 add_Hole=0 U_on_pO=F
FANTOMS   Constrn=F Leip=F HMLT=F Sabbath=F
```

Changes in CTRL before start of self-consistency loop

```
UCORREC   Ucorr=T unitsEV=T DOSp=F Classes=1 N_avr=F LSDA+U=T
          CLASS=Co L=2 Uvalue=0 Jvalue=0
```

Keep INIT **and** CTRL **files** (cp CTRL CTRL.start)
and remove other files from working directory.

Start of self-consistency loop:

user@somehost > lm47.run lm &

Trace the process of self-consistency

- how many iterations are finished already:
  grep OF LOUT
- value of the Fermi energy:
  grep 'S: F' LOUT
- density of states at the Fermi level:
  grep Den LOUT
- difference in total energy:
  grep DETOT LOUT
- when the calculation is self consistent?

```
Jolly good show!  You converged to  DETOT=0.00000100
```

Information obtained from LDA calculation

- Density of states at the Fermi energy
  grep Den LOUT

```
BANDWT: Density of states at E_f:   N(E_f) =   40.432768
```

- total energy of the system is
  grep OF LOUT

```
ITER  1 OUT OF 30:   MAG MOM=  0.00000000   ETOT=   -2933.01524920
```

- occupancy of 3d-orbital of Co
  grep -5 maj LOUT

```
          ========== LSDA+U calculation ==========
 U=0.00000 and J=0.00000 for d orbitals of Co
 OCCUPATIONS MATRIX :
  ----> majority spin      diagonal occupancy   7.59865 <----
  1.90619756 -0.00000000  0.00000000  0.00000000  0.00000000
 -0.00000000  1.90619756 -0.00000000  0.00000000 -0.00000000
  0.00000000 -0.00000000  0.94002958 -0.00000000  0.00000000
  0.00000000  0.00000000 -0.00000000  1.90619756  0.00000000
  0.00000000 -0.00000000  0.00000000  0.00000000  0.94002958
```

Calculation of bands (spaghetti)

- edit the CTRL file

```
OPTIONS   NSPIN=1 REL=T CCOR=T NONLOC=F NRXC=1 NRMIX=2 CORDRD=F
          NITATOM=30 CHARGE=F FATBAND=T AFM=F SEWALD=F FS=F
          CARTESIAN=T WRIBAS=F Q=---- LOCALCS=F GAMMA=F Zero_Ppar=F
```

- information about symmetry lines is in category SYML

```
SYML      NQ=35 Q1=0.50 0.50 0.50 LAB1=L
            Q2=0.00 0.00 0.00 LAB2=G
          NQ=40 Q1=0.00 0.00 0.00 LAB1=G
            Q2=0.00 1.00 0.00 LAB2=X
          NQ=20 Q1=0.00 1.00 0.00 LAB1=X
            Q2=0.50 1.00 0.00 LAB2=W
          NQ=30 Q1=0.50 1.00 0.00 LAB1=W
            Q2=0.50 0.50 0.50 LAB2=L
          NQ=25 Q1=0.50 0.50 0.50 LAB1=L
            Q2=0.00 0.75 0.75 LAB2=K
          NQ=45 Q1=0.00 0.75 0.75 LAB1=K
            Q2=0.00 0.00 0.00 LAB2=G
```

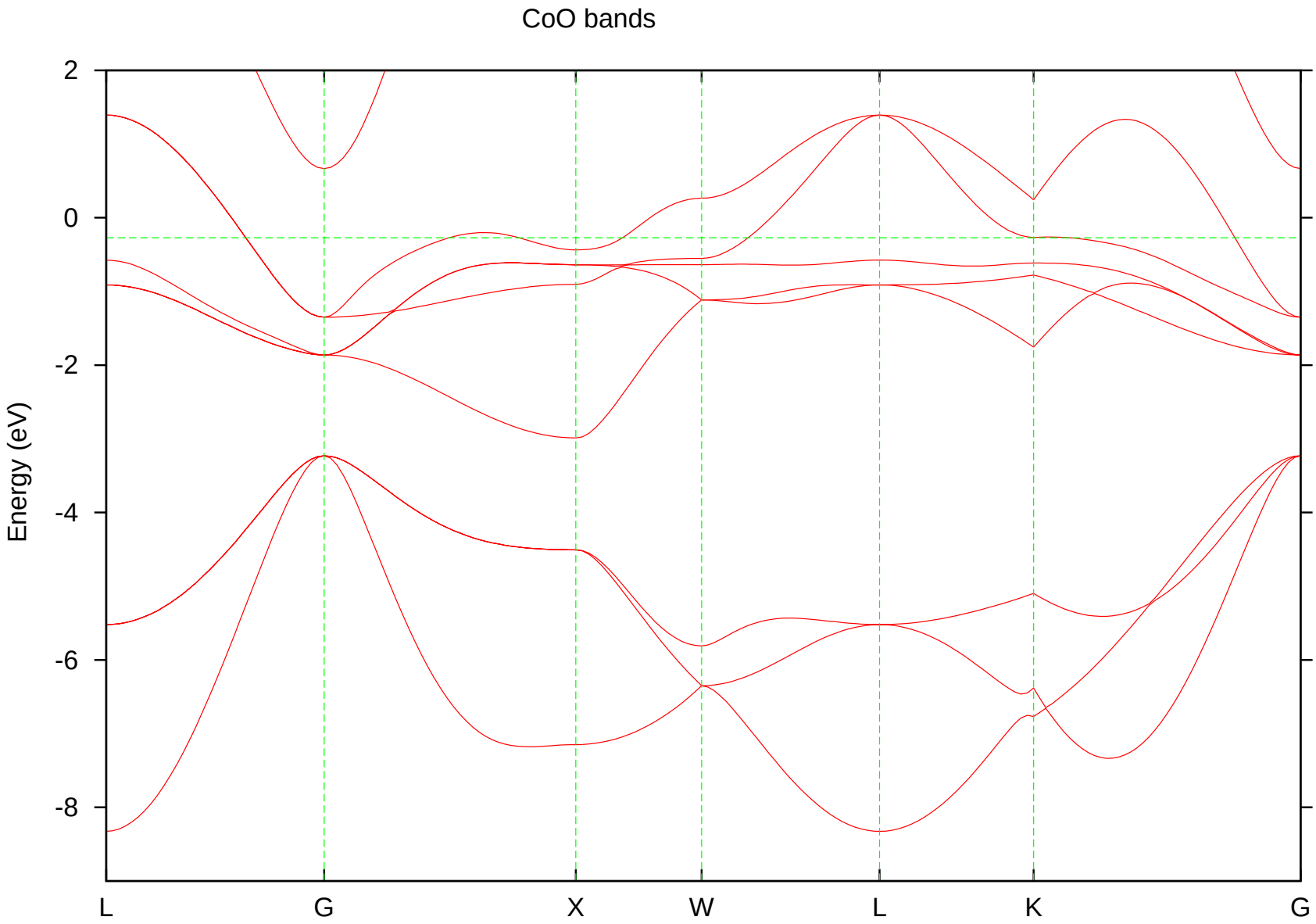
- execute the command

  user@somehost > lm47.run lmbnd

- run gnubnd.run command to prepare files for plotting the bands
  user@somehost > *gnubnd.run*
  (it is interactive) and answer some questions:

```
 enter title
CoO bands
  energies in Rydberg (f) or eV (t) ? (default is Rydberg)
t
  energies relative to EF (t)? (default is f)
f
  landscape plot (t) ? (default t)
t
  energies connected by lines (t)? (default t)
t
  show E_nu's ? (default t)
f
  plot orbital character(t)? (default f)
f
 Bands= 14 Fermi Energy= -0.2724 Lattice const.= 8.053 Spins= 1
 ebot=  -8.325   etop=  40.089   efermi= -0.272   nkp= 195   nline= 6
 default emin and emax =   -9.000  41.000
 enter emin, emax
-9 2
```

- visualize the band structure (using gnuplot)
  user@somehost $>$ *gnuplot* $<$ *BNDS.GNU*
- now you have the file *bnds.ps*
- View it!


CoO bands
Energy (eV)
2
0
-2
-4
-6
-8
L
G
X
W
L
K
G

- Rename this file, for example : *mv bnds.ps all.bnds.ps*

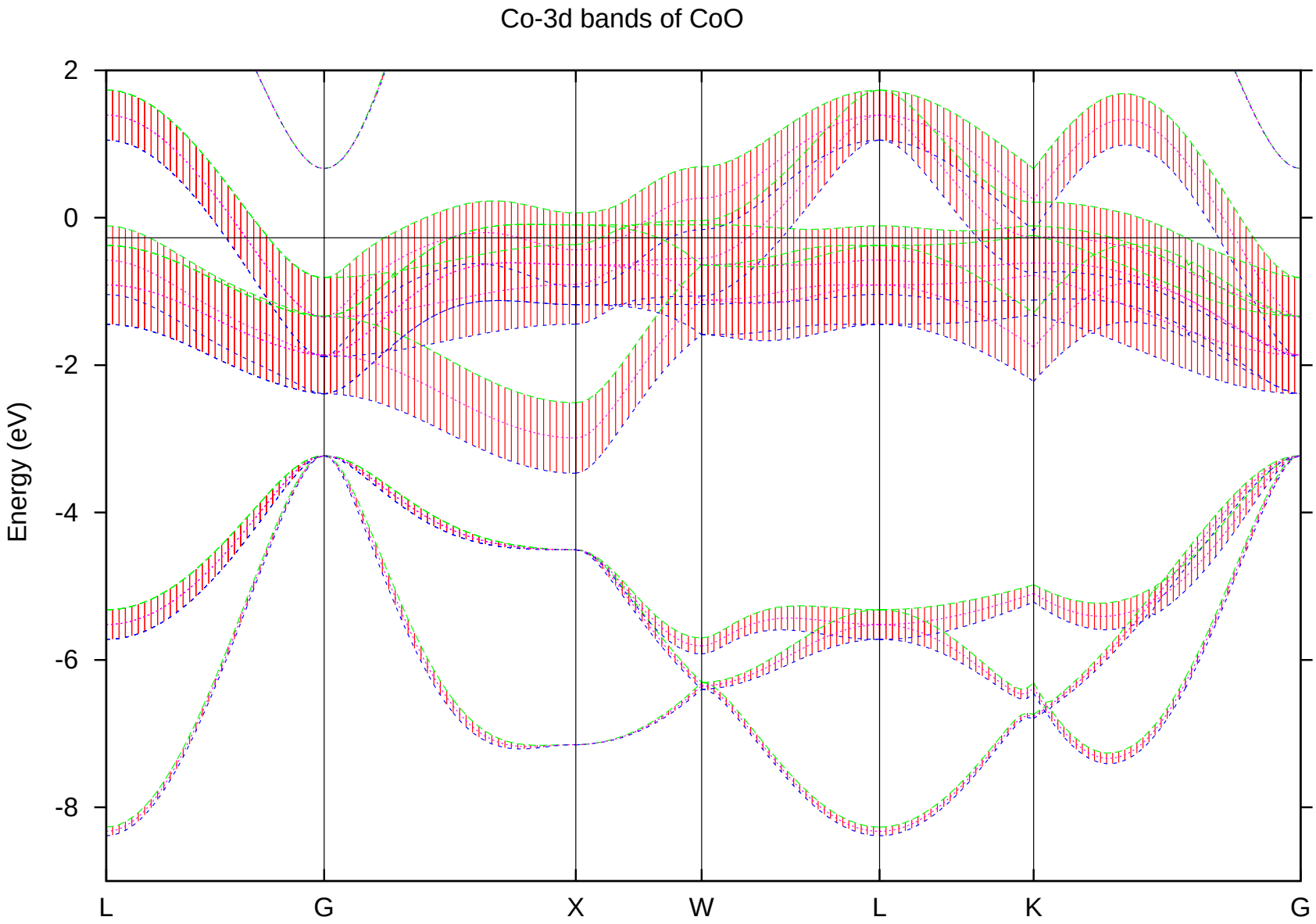
How to determine contributions from different states to the band structure? Let us plot orbital projected bands or "fat bands" for the Co *d* states.

- run *gnubnd.run* command again and answer some questions:

```
 enter title
Co-3d bands of CoO
  energies in Rydberg (f) or eV (t) ? (default is Rydberg)
t
  energies relative to EF (t)? (default is f)
f
  landscape plot (t) ? (default t)
t
  energies connected by lines (t)? (default t)
t
  show E_nu's ? (default t)
f
  plot orbital character(t)? (default f)
t
  Change coordinate system? If so enter Euler angles:
  alpha, beta, gamma(units of Pi). If nochange: enter '/'
/
  no coordinate transformation!
  Do you want to make a compound orbital? (default f)
f
  Enter orbital character to be plotted as "fatbands"

 First select classes from: Co   O    E

Co
```

```
 For each selected atom specify orbital number from list
 NB! Orbitals are in the new coordinate system!

 s  y  z  x  xy  yz  3z^2-1 xz  x^2-y^2 y(3x^2-y^2) xyz
 1  2  3  4   5   6     7    8     9         10      11
 y(5z^2-1) z(5z^2-3) x(5z^2-1) z(x^2-y^2) x(3y^2-x^2)
     12        13        14        15          16
Co  number  1 enter number(s) followed by "/":
5 6 7 8 9 /
 Bands= 14 Fermi Energy= -0.2724 Lattice const.= 8.053 Spins= 1
 ebot=  -8.325   etop=  40.089   efermi= -0.272   nkp= 195   nline= 6
 default emin and emax =   -9.000  41.000
 enter emin, emax
-9 2
 max. width 0.550000
```

- visualize the bands with gnuplot
  user@somehost > *gnuplot* < *BNDS.GNU*
- View bnds.ps file. The more fat is the band – the larger is contribution of Co 3d states

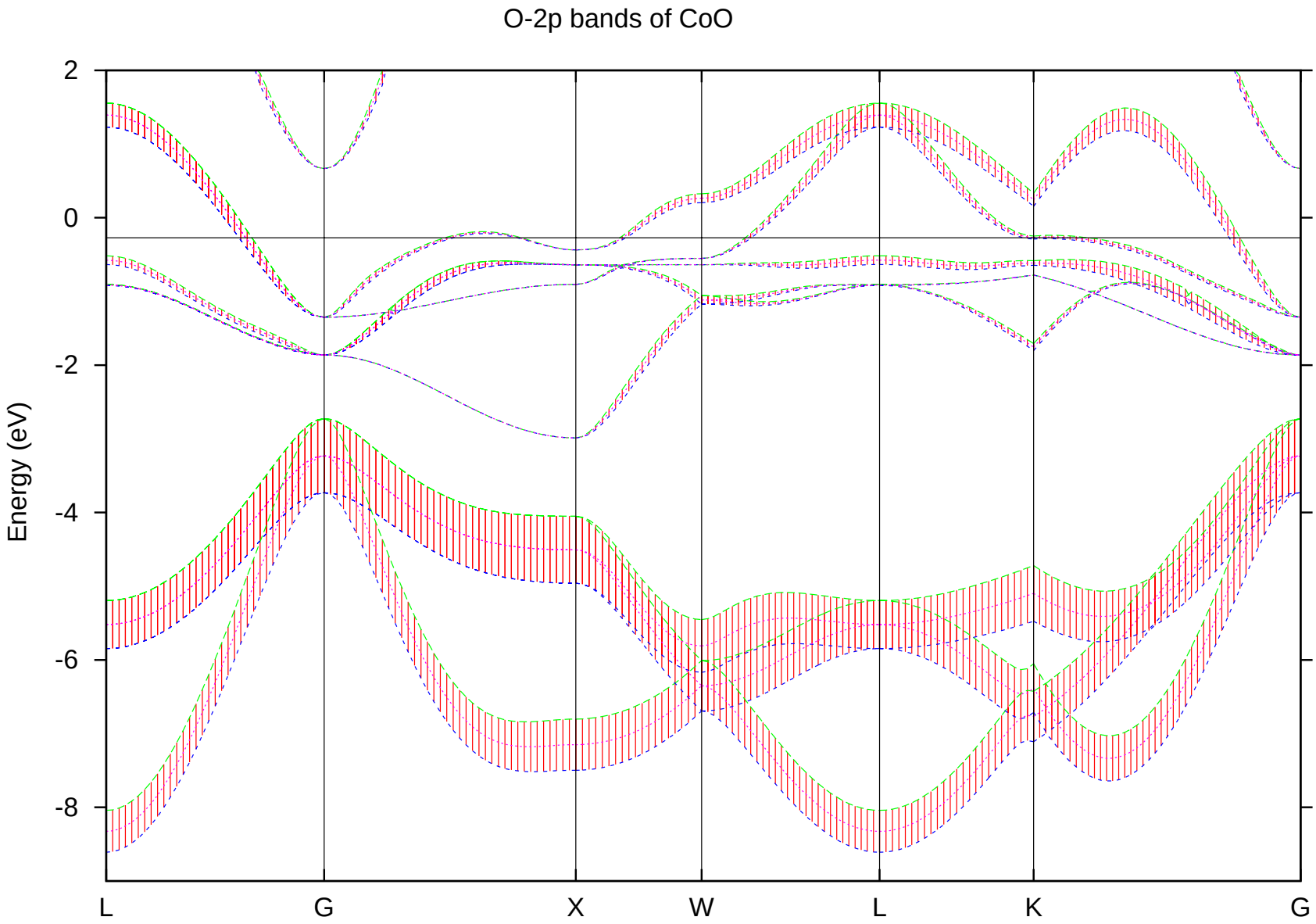

Co-3d bands of CoO
Energy (eV)
2
0
-2
-4
-6
-8
L
G
X
W
L
K
G

- Now lets do same analysis for the O-2p contributions...

```
 enter title
O-2p bands of CoO
  energies in Rydberg (f) or eV (t) ? (default is Rydberg)
t
  energies relative to EF (t)? (default is f)
f
  landscape plot (t) ? (default t)
t
  energies connected by lines (t)? (default t)
t
  show E_nu's ? (default t)
f
  plot orbital character(t)? (default f)
t
  Change coordinate system? If so enter Euler angles:
  alpha, beta, gamma(units of Pi). If nochange: enter '/'
/
  no coordinate transformation!
  Do you want to make a compound orbital? (default f)
f
```

```
 Enter orbital character to be plotted as "fatbands"

 First select classes from: Co   O    E

O

 For each selected atom specify orbital number from list
 NB! Orbitals are in the new coordinate system!

 s  y  z  x  xy  yz  3z^2-1 xz  x^2-y^2 y(3x^2-y^2) xyz
 1  2  3  4   5   6     7    8     9         10      11
 y(5z^2-1) z(5z^2-3) x(5z^2-1) z(x^2-y^2) x(3y^2-x^2)
     12        13        14        15          16
O   number  1 enter number(s) followed by "/":
2 3 4 /
 Bands= 14 Fermi Energy= -0.2724 Lattice const.= 8.053 Spins= 1
 ebot=  -8.325   etop=  40.089   efermi= -0.272   nkp= 195   nline= 6
 default emin and emax =   -9.000  41.000
 enter emin, emax
-9 2
 max. width 0.550000
```

- ...and plot the bands


O-2p bands of CoO
Energy (eV)
2
0
-2
-4
-6
-8
L
G
X
W
L
K
G

Calculation of density of states (DOS)

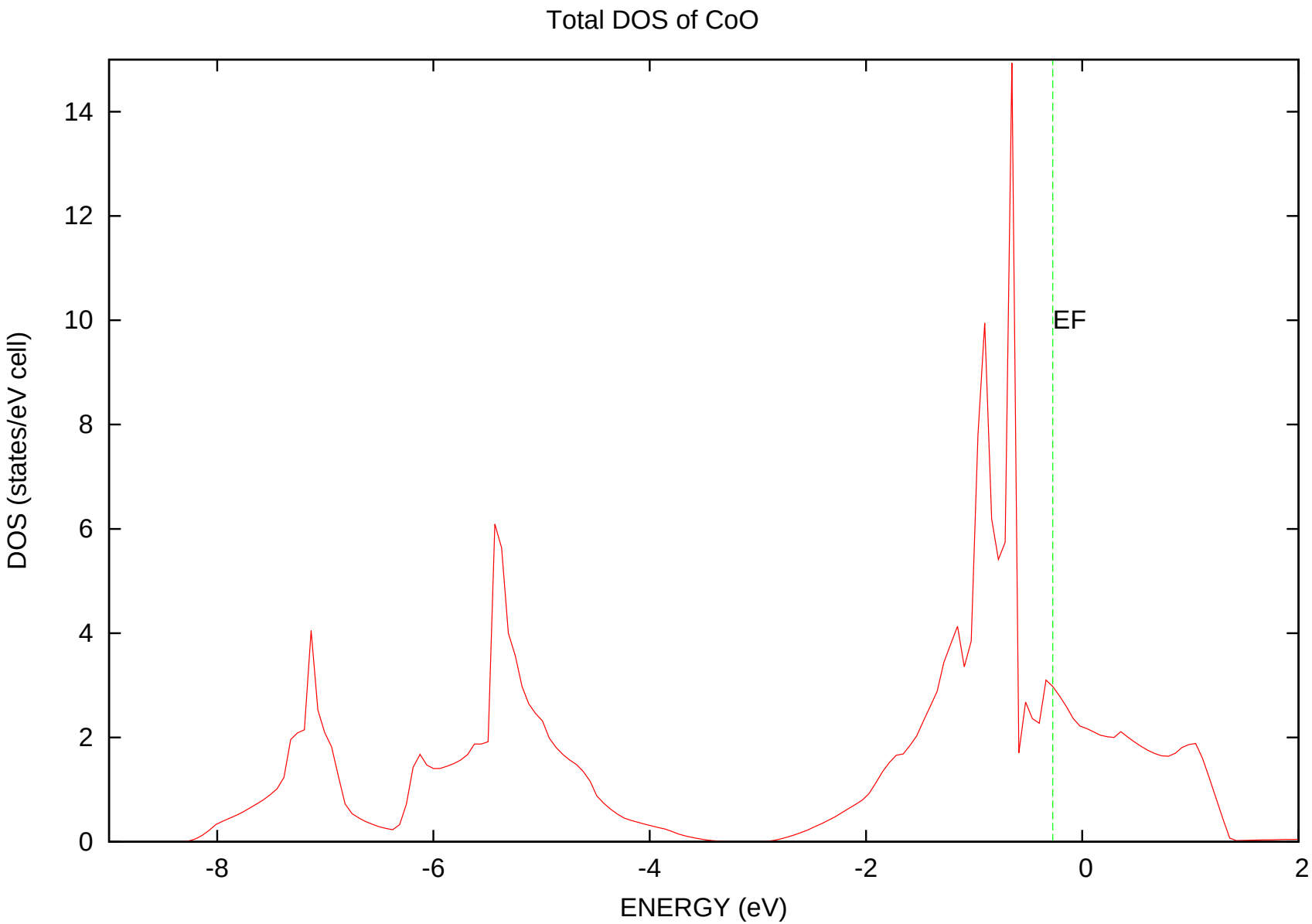
- edit the CTRL file

```
UCORREC   Ucorr=T unitsEV=T DOSp=T  Classes=1 dblUset=F LSDA+U=T
          CLASS=Co L=2 Uvalue=0 Jvalue=0
```

- execute the command
  user@somehost > lm47.run lmdos
- run the command to prepare files for plotting the total DOS
  user@somehost > gnudos.run
  and answer some questions...

```
  Differential (f, default) or integer (t) DOS ?
f
 energies in Rydberg (f) or eV (t)? (default is Rydberg)
t
 energies relative to EF (t)? (default is f)
f
 emin,emax= -9.5226 40.8188, nopts= 801, nd=   9   efermi= -0.2724

 classes are: Co   O    E
 l's     are: s  p  d

 Enter class1-l1, class2-l2, ... to be added to DOS.
 Examples:   all (default)   s   p   Co-d  E-s
/

 Take: Co-s    Co-p    Co-d    O-s     O-p     O-d     E-s     E-p
       E-d

 Now enter weights for partial DOS (default = 1.0, 1.0, ...)
 A weight of 1.0 for each partial DOS gives the correct total DOS.
/

 emin   , emax    =  -9.523  40.819
 if desired, enter new emin, emax, / for default
-9 2
```

- and plot the result:

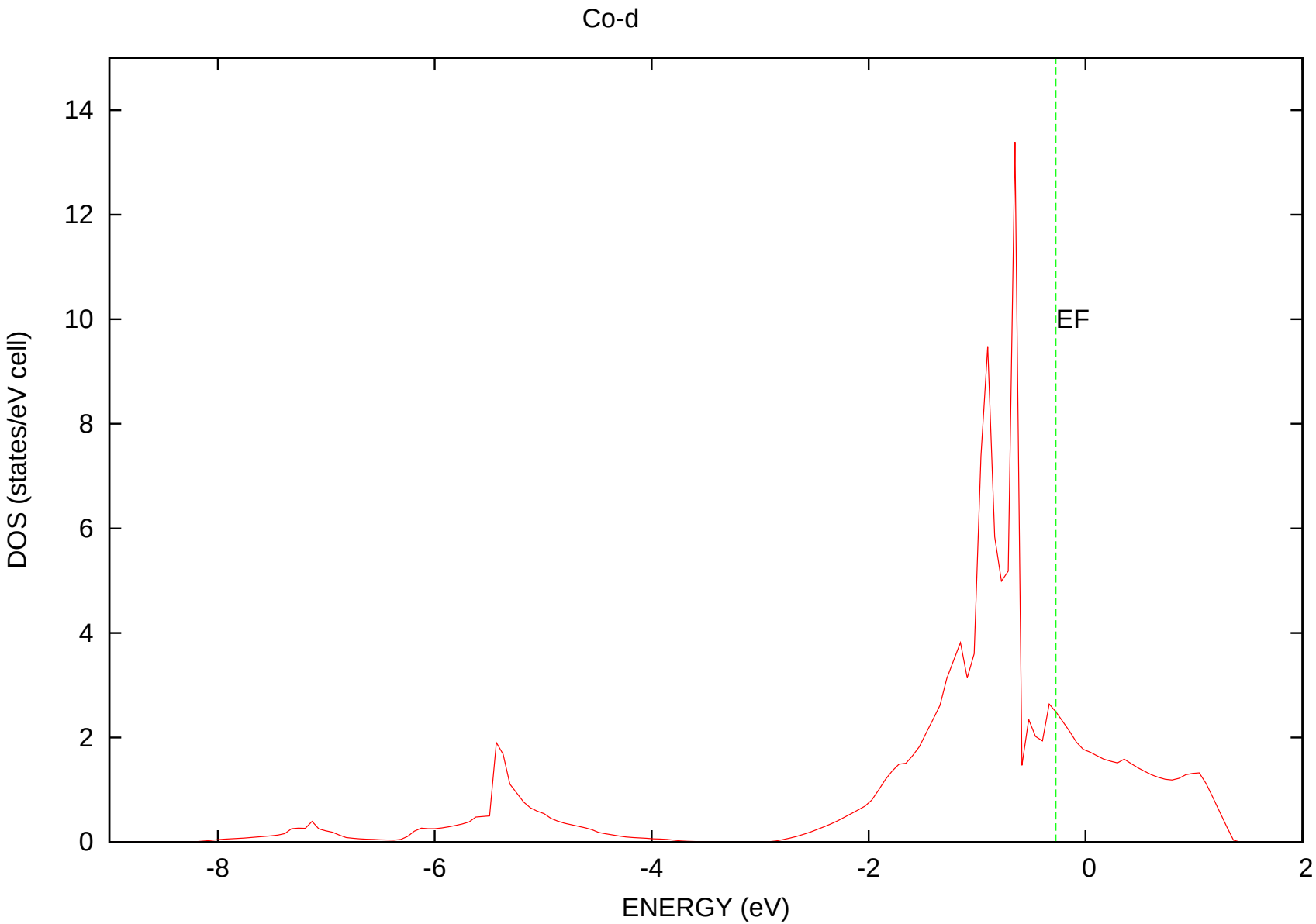


- Rename the file dos.ps *mv dos.ps total.dos.ps*

How to plot *l*-projected densities of states (partial DOS)?
Let us plot partial DOS for Co *d* states.

- run again the command to prepare files for plotting the DOS
  user@somehost $>$ *gnudos.run*
  and answer some questions(part of the dialog is skipped):

```
 energies relative to EF (t)? (default is f)
f
 emin,emax= -9.5226 40.8188, nopts= 801, nd=   9   efermi= -0.2724

 classes are: Co   O    E
 l's     are: s  p  d

 Enter class1-l1, class2-l2, ... to be added to DOS.
 Examples:   all (default)   s   p   Co-d  E-s
Co-d

 Take: Co-d

 Now enter weights for partial DOS (default = 1.0, 1.0, ...)
 A weight of 1.0 for each partial DOS gives the correct total DOS.
/

 emin   , emax    =  -9.523  40.819
 if desired, enter new emin, emax, / for default
-9 2

 dosmin, dosmax =.0   13.392
 if desired, enter new dosmin, dosmax, / for default
/
```

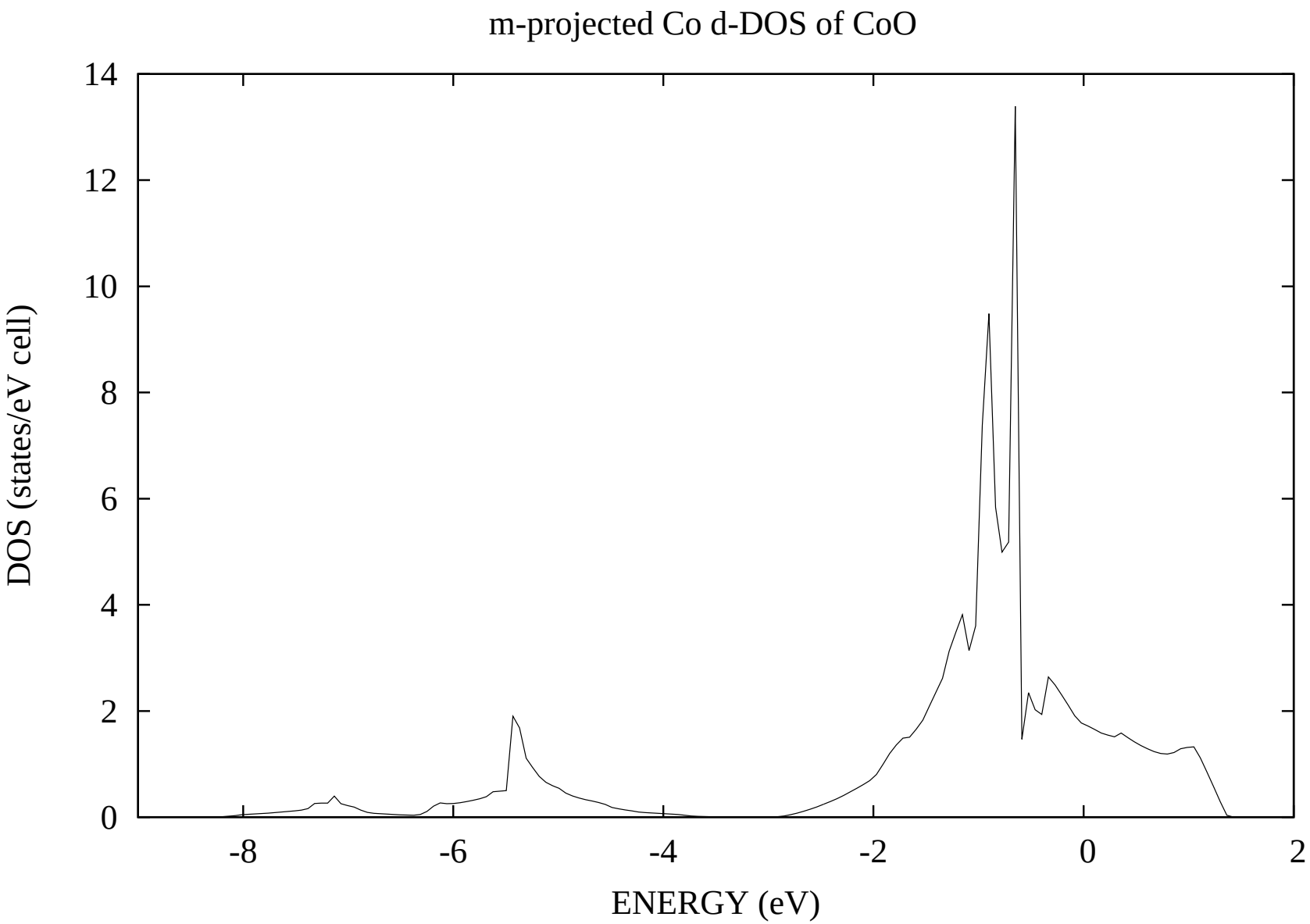

Co-d
DOS (states/eV cell)
ENERGY (eV)
EF
0
2
4
6
8
10
12
14
-8
-6
-4
-2
0
2

How to plot m projected densities of states for Co (DOS for xy, yz, $3z^2 - r^2$, zx, $x^2 - y^2$ orbitals)?

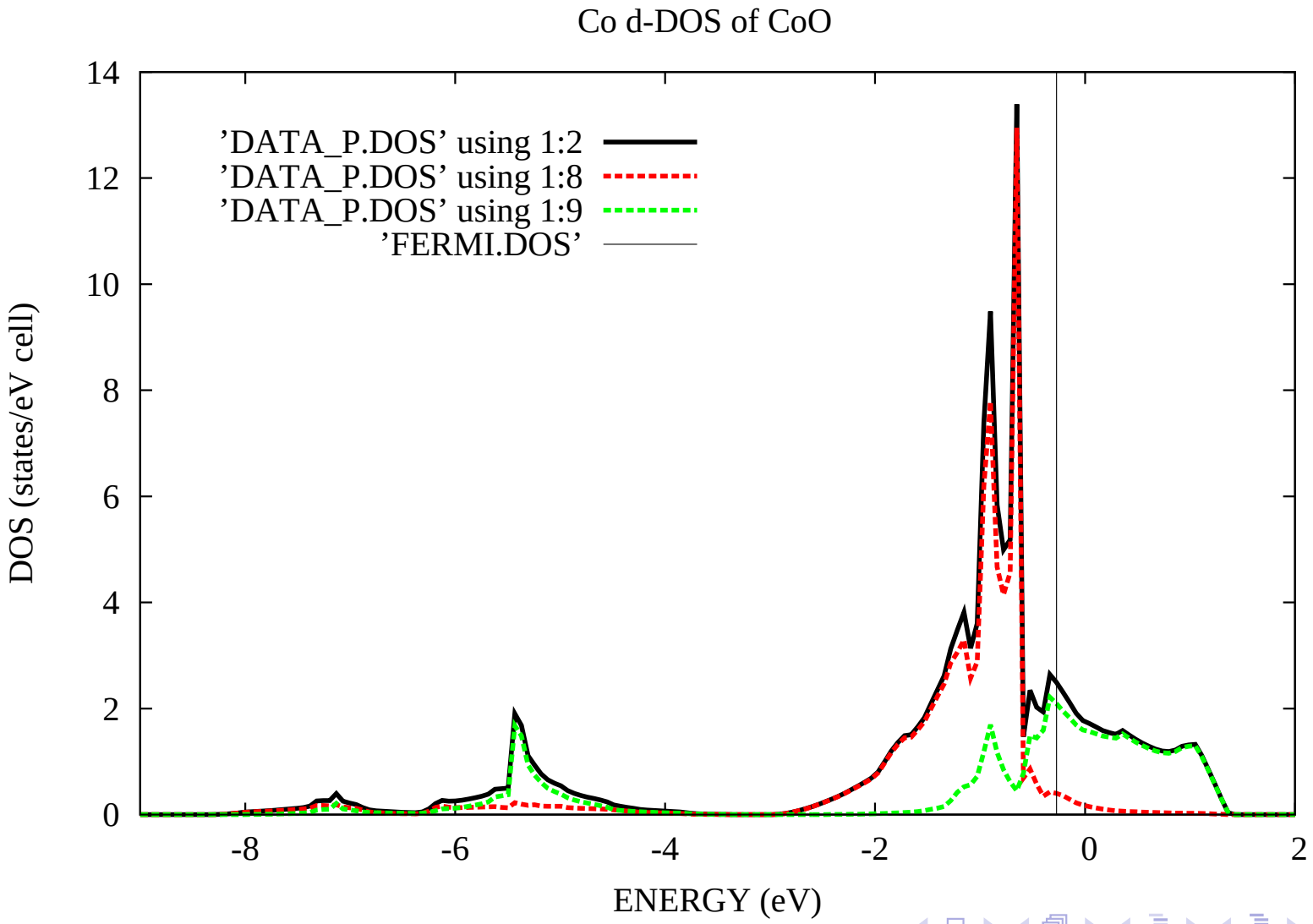
- run the other command to prepare files for plotting the DOS
  gnudosp.run
  and answer some questions(part of the dialog is skipped):

```
 energies relative to EF (t)? (default is f)
f
 Atom number?
1
 emin,emax= -9.5226 40.8188, nopts= 801    efermi= -0.2724
 Do you need rotation? (default is (f))
f

 Enter title
m-projected Co d-DOS of CoO
 Print DOS file in matrix form? (default - f)
f
```

- visualize the result using gnuplot: *gnuplot DOSP.GNU*



- orbitally resolved densities of states for Co atom are in `\DATA_P.DOS` file. The columns contain Energy, Total Co-d, xy, yz, $3z^2 - r^2$, zx, $x^2 - y^2$, t_{2g}, e_g orbitals, respectively



Part II

Calculation of U and J parameters

Calculation of on-site Coulomb interaction parameter U with the use of *constrain* method

- $U = \delta\epsilon_{3d}/\delta n_{3d}$,
  where ϵ_{3d} is the energy of $3d$ band
  and n_{3d} is the occupancy of $3d$ shell
- ϵ_{3d} corresponds to c parameter (center of gravity of the occupied band) of the LMTO method

see also *Pickett W.E., Erwin S.C. and Ethridge E.C.* Reformulation of the LDA + U method for a local-orbital basis // Phys. Rev. B. 1998. V. 58. N 3. P. 1201–1209.

Step 1.

- Take the CTRL file from converged LDA calculation
- Make supercell of CoO which contains four Co atoms. Open the CTRL file and edit SCELL category:

```
SCELL     PLAT=1  0  0
               0  1  0
               0  0  1 EQUIV=T
```

- run the command to produce supercell
  user@somehost > lm47.run lmscell
- View new CTRL file! Now it containes four initial cells
  Note: there are still 2 classes of atoms: Co and O.

Step 2.

- Make two Co atoms non-equivalent:

```
CLASS     ATOM=Co1 Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1      <-
          IDMOD=0 0 0 RHO_print=0 0 0
          ATOM=Co2 Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1      <-
          IDMOD=0 0 0 RHO_print=0 0 0
          ATOM=O  Z= 8 R=2.03007195 LMX=2 CONF=3 2 3 4 IDXDN=2 1 2
          IDMOD=0 0 0 RHO_print=0 0 0
          ATOM=E  Z= 0 R=1.41271966 LMX=1 CONF=1 2 3 4 IDXDN=1 2
          IDMOD=0 0 RHO_print=0 0
SITE      ATOM=Co1 POS= 0.00  0.00  0.00                                 <-
          ATOM=Co2 POS= 0.50  0.50  0.00                                 <-
          ATOM=Co2 POS= 0.50 -0.00  0.50                                 <-
          ATOM=Co2 POS= 0.00  0.50  0.50                                 <-
          ...
```

- and delete all lines starting from SCALE category

- run the command to produce new CTRL file
  user@somehost > lm47.run lmctl
- View the CTRL file! Now It contains two classes of Co
- All the O atoms we will consider as belonging to the same class. This assumption will stabilize the procedure of self-consistency.
- Edit the CTRL file again. Be accurate!
- Edit SYMGRP category:

```
SYMGRP     NGEN=3 GENGRP=I R4X R3D
           SPCGRP=Pm-3m USESYM=T
```

- Change CLASS category:

```
CLASS     ATOM=Co1 Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1
          IDMOD=0 0 2 RHO_print=0 0 0                                  <-
          ATOM=Co2 Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1
          IDMOD=0 0 2 RHO_print=0 0 0                                  <-
          ATOM=O   Z= 8 R=2.03007195 LMX=2 CONF=3 2 3 4 IDXDN=2 1 2
          IDMOD=0 0 0 RHO_print=0 0 0
          ATOM=E   Z= 0 R=1.41271966 LMX=1 CONF=1 2 3 4 IDXDN=1 2
          IDMOD=0 0 RHO_print=0 0
          ATOM=O1  Z= 8 R=2.03007195 LMX=2 CONF=3 2 3 4 IDXDN=2 1 2
          IDMOD=0 0 0 RHO_print=0 0 0
```

- Change START directory and keep only first three lines

```
START     NIT=50 BROY=F WC=-1 NMIX=0 BETA=0.01
          FREE=F CNVG=0.00001 CNVGET=0.00001 BEGMOM=T CNTROL=T
          EFERMI=-0.0191586 VMTZ=-0.6712252
```

- Edit UCORREC and FANTOMS categories

```
UCORREC   Ucorr=T unitsEV=T DOSp=F Classes=2 N_avr=F LSDA+U=T
          CLASS=Co1 L=2 Uvalue=0 Jvalue=0
          CLASS=Co2 L=2 Uvalue=0 Jvalue=0
          MixVCL=1 add_Hole=0 U_on_pO=F
FANTOMS   Constrn=T Leip=F HMLT=F Sabbath=F
```

- Complete the CTRL file

  user@somehost > lm47.run lmctl

- Now we want to enforce a difference in occupancy of the Co 3*d* states. Edit the CPOC file in the working directory so that it looks like this:

```
POTCOR:     Hubbard correction  0.000000000000D+00
Co1 :
L=2:
 -0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000 -0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000 -0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000 -0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000 -0.100000000000
  double counting energy 0.000000000000D+00
 -------------------------------------------------
Co2 :
L=2:
  0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  0.100000000000
  double counting energy  0.000000000000D+00
 -------------------------------------------------
  0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  0.100000000000
  double counting energy  0.000000000000D+00
 -------------------------------------------------
  0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  0.100000000000
  double counting energy  0.000000000000D+00
 -------------------------------------------------
```

- Start self-consistency process
  user@somehost > lm47.run lm

- If self-consistency is not reached after NIT iterations, set BEGMOM=F in the CTRL file and re-run lm command

```
FREE=F CNVG=0.00001 CNVGET=0.00001 BEGMOM=F CNTROL=T
```

- Take information obout the Co-3*d* occupations and energies from the CTRL file:

```
ATOM=Co1 P=4.59403291 4.30946740 3.89758362
     Q= 0.31720885 -0.01265951  0.01045560
        0.41085358 -0.01289696  0.00523537
        7.77135744 -0.16171997  0.12034854
   enu   =-0.43667920 -0.40272434  0.01141031
   c     =-0.13286303  0.97122077  0.01141067
   sqrdel=-0.50692113  0.64424814  0.23362663
   p     =0.03308971 0.01850979 1.53406627
   gamma = 0.5613183  0.2586050 -0.0146474
ATOM=Co2 P=4.63462771 4.33167747 3.89758362
     Q= 0.35097538 -0.01443908  0.01154048
        0.44317633 -0.01329211  0.00494702
        7.46800177 -0.13639201  0.11664946
   enu   =-0.45356273 -0.41468550 -0.16388059
   c     =-0.22228933  0.87212940 -0.16388027
   sqrdel=-0.50235259  0.63684762  0.22186230
   p     =0.03570924 0.01953683 1.62240954
   gamma = 0.55882812  0.25617514 -0.00895143
```

- Now let's calculate the local coulomb potential, taking into account that:
  Co1: ϵ_{3d}=0.011 Ry, n_{3d}=7.771
  Co2: ϵ_{3d}=-0.164 Ry, n_{3d}=7.468

$$\underline{U = \frac{\delta\epsilon}{\delta n} = \frac{0.175}{0.303} = \mathbf{0.578}\ Ry = \mathbf{7.855}\ eV}$$

Calculation of intraatomic exchange interaction parameter J with the use of *constrain* method

- $J = |\delta\epsilon_{3d}^{\uparrow\downarrow}/\delta n_{3d}^{\uparrow\downarrow}|$,

  where $\delta\epsilon_{3d}^{\uparrow\downarrow}$ is the energy difference of majority and minority c parameters (centers of gravity) for $3d$ bands: $\delta\epsilon_{3d}^{\uparrow\downarrow} = \epsilon_{3d}^{\uparrow} - \epsilon_{3d}^{\downarrow}$

  and $\delta n_{3d}^{\uparrow\downarrow}$ is the difference in occupancy between majority and minority bands: $\delta n_{3d}^{\uparrow\downarrow} = n_{3d}^{\uparrow} - n_{3d}^{\downarrow}$

- Take the CTRL file from converged LDA calculation
- Edit CTRL file:
  - in category IO set VERBOS=50
  - in category OPTIONS set NSPIN=2
  - in category PHANTOM set Constrn=T
- Edit CLASS category

```
CLASS     ATOM=Co Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1
          IDMOD=0 0 2 RHO_print=0 0 0
```

- Set Ucorr=T (category UCORREC)
- Erase all lines in START category except the first three and change the following tokens and parameters:

```
START       NIT=50 BROY=F WC=-1 NMIX=0 BETA=0.01
```

- complete the CTRL file
  user@somehost > lm47.run lmctl

- Enforce the energy difference of the Co-3*d* states by changing diagonal elements in the CPOC file:

```
POTCOR:     Hubbard correction  0.000000000000D+00
Co  :
L=2:
  -.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  -.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  -.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  -.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  -.100000000000
  double counting energy  0.000000000000D+00
  0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  0.100000000000
  double counting energy  0.000000000000D+00
 -----------------------------------------------
```

- start self-consistency cycle
  user@somehost > lm47.run lm

- If self-consistency is not reached after NIT iterations, set BEGMOM=F in the CTRL file and re-run lm command
- After self-consistency cycle is finished extract the Co-3d occupations and c-parameters from the CTRL file:

```
ATOM=Co  P=4.66735709 4.35922298 3.89758362
           4.63859420 4.34355043 3.89758362
         Q= 0.19823045 -0.00453332  0.00795638
            0.25593771 -0.00222151  0.00910358
            4.97008829  0.08880200  0.07352792
            0.17641215 -0.00642166  0.00449599
            0.23373375 -0.00677706  0.00286026
            2.36087373 -0.14808511  0.06042935
      enu   =-0.40708807 -0.34743219 -0.25661916
            -0.41101015 -0.34841174 -0.07511793
      c     =-0.23620573  0.84901196 -0.25661886
            -0.18522640  0.90831806 -0.07511757
```

- Compute J:

$$J = \frac{\epsilon_{3d}^{\uparrow} - \epsilon_{3d}^{\downarrow}}{n_{3d}^{\uparrow} - n_{3d}^{\downarrow}} = \frac{0.257 - 0.075}{4.970 - 2.361} = \mathbf{0.0698}\ Ry = \mathbf{0.949}\ eV$$

Part III

Calculation of a bandstructure within LDA+U

- Take the CTRL file from the converged LDA calculation
- Edit SYMGRP category:

```
SYMGRP    NGEN=3 GENGRP=I R4X R3D
          SPCGRP=Pm-3m USESYM=T
```

- Change CLASS and OPTIONS categories:

```
OPTIONS   NSPIN=2 REL=T CCOR=T NONLOC=F NRXC=1 NRMIX=2 CORDRD=F
          NITATOM=30 CHARGE=F FATBAND=F AFM=F SEWALD=F FS=F
          CARTESIAN=T WRIBAS=F Q=---- LOCALCS=F GAMMA=T Zero_Ppar=F

CLASS     ATOM=Co Z=27 R=2.57790832 LMX=2 CONF=4 4 3 4 IDXDN=1 1 1
          IDMOD=0 0 2 RHO_print=0 0 0
```

- Erase all lines in START category except the first three and change the following tokens and parameters:

```
START     NIT=50 BROY=F WC=-1 NMIX=0 BETA=0.01
```

- Enter the calculated values of U and J parameters to UCORREC category:

```
UCORREC   Ucorr=T unitsEV=T DOSp=F Classes=1 N_avr=F LSDA+U=F
          CLASS=Co L=2 Uvalue=7.86 Jvalue=0.95
```

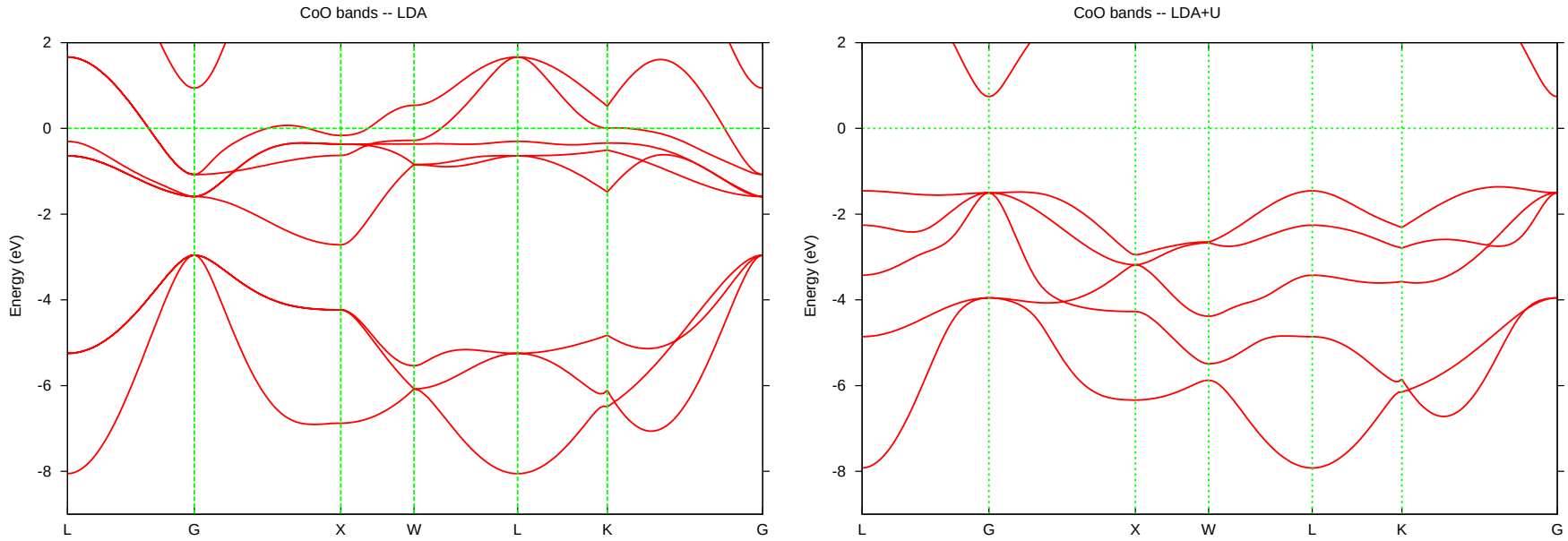
- Complete the CTRL file using lmctl command
  user@somehost > lm47.run lmctl
- Edit the POCO file inserting initial energy difference between spin-up and spin-down:

```
POTCOR:     Hubbard correction  0.000000000000D+00
Co  :
L=2:
  0.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  0.100000000000
  double counting energy  0.000000000000D+00
  -.100000000000  0.000000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  -.100000000000  0.000000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  -.100000000000  0.000000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  -.100000000000  0.000000000000
  0.000000000000  0.000000000000  0.000000000000  0.000000000000  -.100000000000
  double counting energy  0.000000000000D+00
 ------------------------------------------------
```

- run the self-consistency cycle
  user@somehost > lm47.run lm

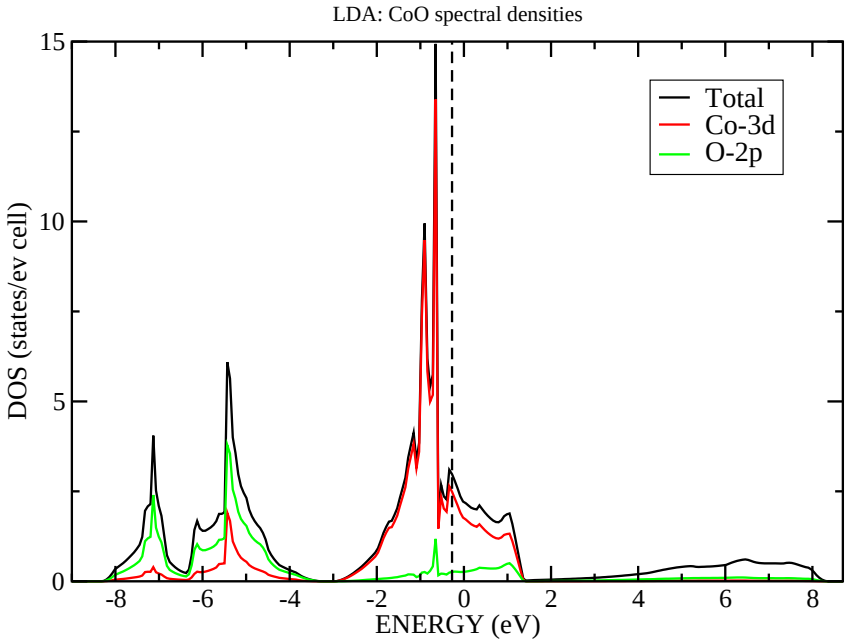
- By complete analogy with conducted LDA calculation one can get:
  - Total density of states
  - Element-resolved and orbitally resolved densities of states
  - Total band structure, its element and orbital contributions
- Next several slides demonstrate listed characteristics and properties for the case of CoO

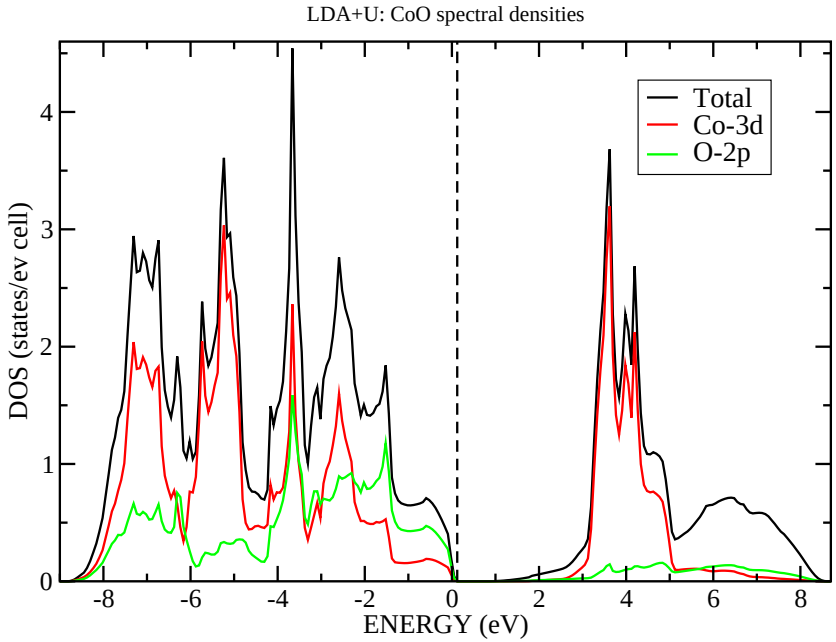
CoO: LDA vs LDA+U – band structure



- Qualitative improvement of LDA results
- The gap of experimentally observed magnitude

CoO: LDA vs LDA+U – spectral densities





- Qualitative improvement of LDA results
- The gap of experimentally observed magnitude