Package 2Doptimize

This package performs a convenient 2-Dimensional structure optimization (Volume and c/a) for hexagonal or tetragonal spacegroups.

If you want to use this package please follow the following steps.

FOR USING

1- Make struct file.
2- Do initialization (run "instgen_lapw" and "init_lapw" in Terminal).
3- If you want to do Spin-Orbit calculations run "initso_lapw" in Terminal.
4- If you want to do LDA+U calculations make "case.inso" and “case.inorb” files in your present work directory.
5- call “**set2D_lapw**” in Terminal (type **set2D_lapw**).

```
[root@localhost Mg]# set2D
```

This program generates a set of structures (by using “**setup2D**” program) and a job-file (**2Doptimize.job**). Moreover you have to specify the “order of fit” (stored in “**.fordfitcoa**” file) and the changes in volume and c/a.

```
########################################
# set2D_lapw prepares 2D-optimization #
#     C(2008) by Morteza Jamal        #
#  it creates    2Doptimize.job       #
#  which must be executed             #
#  and can be analyzed by             #
#             ana2D_lapw              #
########################################
        (C) 2008 by Morteza Jamal
 ****************************************
 ** Setup for EOS calculations(2D-case)**
 ****************************************

 Please enter order of fit for c/a rations (3,4,5).
```

In the following examples, we select order of fit **5**

```
########################################
# set2D_lapw prepares 2D-optimization  #
#     C(2008) by Morteza Jamal         #
#  it creates    2Doptimize.job        #
#  which must be executed               #
#  and can be analyzed by               #
#             ana2D_lapw                #
########################################
        (C) 2008 by Morteza Jamal
 ****************************************
 ** Setup for EOS calculations(2D-case)**
 ****************************************

 Please enter order of fit for c/a rations (3,4,5).
5
 ****************************************
 **************Please note*****************
 For the first run the number of volumes and c/a
 changes must to be at least the order of the fit
 ****************************************

 *******Start for volume changes*******

 Do you want to use default parameters ?(y/n)
      (-10%,-5%,0,5%,10%)
```

And default parameters for volume and c/a changes

```
 ****************************************
 **************Please note*****************
 For the first run the number of volumes and c/a
 changes must to be at least the order of the fit
 ****************************************

 *******Start for volume changes*******

 Do you want to use default parameters ?(y/n)
      (-10%,-5%,0,5%,10%)
y

 ******* Start for c/a changes*******

 Do you want to use default parameters ?(y/n)
      (-4%,-2%,0,2%,4%)
y
          25 2D_Vxx_COAxx.struct files generated

 Now 2Doptimize.job is ready

 Please modify running command in "2Doptimize.job"
 according to your needs and then run 2Doptimize.job
```

Note 1: number of volume and c/a changes must be equal or greater than “order of fit”.

6- Edit “**2Doptimize.job**” file with '*gedit*' or ' *vi* ' in Terminal Environment and modify it according to your needs. For example, use "runsp_lapw" for Spin-Polarized (SP) system or even "min_lapw" or specify different convergence parameters.

```
# if you have a previous optimize-run:
 #    cp  $i.clmsum Be.clmsum
 #    cp  $i.clmup Be.clmup
 #    cp  $i.clmdn Be.clmdn
 # if you want to start with dstart:
 #    x dstart   # -c
 #    x dstart -up  # -c
 #    x dstart -dn  # -c
 # recommended option: use charge extrapolation
 clmextrapol_lapw                    (Convert to #clmextrapol_lapw for SP case)
 if (-e Be.clmup  && \
  ! -z Be.clmup  ) then
     clmextrapol_lapw -up
     clmextrapol_lapw -dn
 endif

 run_lapw -ec 0.0001   # -in1new 3 -in1orig
 #    runsp_lapw -ec 0.0001
 #    min -I -j "run_lapw -I -fc 1.0 -i 40 "

     set stat = $status
     if ($stat) then
        echo "ERROR status in" $i
        exit 1
     endif
 save_lapw  ${i}$savename
 #    save_lapw  -f -d XXX $i
```

For SO and LDA+U calculations
It’s better do it step by step i.e:

```
runsp_lapw -ec 0.0001 -in1new 2
save scfsimple
runsp_lapw –ec 0.0001 –so
save scfso
runsp_lapw –ec 0.0001 –so -orb
```

7- Now run **2Doptimize.job** in Terminal Environment (type **2Doptimize.job**). It will take time.

Note 2: When you want to rerun **2Doptimize.job** with modifications in (RKmax, k-mesh, XC-potentials) choose "answscf=no" in **2Doptimize.job** file and a new "savename" (eg. "_use_pbe_rk8").

```
#!/bin/csh -f
 #
 #Modify this script according to your needs
 unalias rm
 #
 # to reuse previous scf runs (without a new scf run) set answscf=y
 # and use the same "savename".
 # When you make modifications (RKmax, k-mesh, XC-potentials) choose
 # answscf=no and a new savename (eg. "_pbe_rk8_1000k").
 set answscf=y
 set savename=
 #
```

8- Run "**ana2D_lapw**" in Terminal Environment (type **ana2D_lapw**) and answer to questions.
"**ana2D_lapw"** will analyze the results. It uses a set of **case.Vconst*** files (produced by **2Doptimize.job** and stored also in subdirectory **Vconst**) and the **numbvcoa** file.
You can see results for

- energy vs. c/a for each volume,
- energy vs. volume (with optimized c/a) and
- c/a vs. volume.

Optionally you can specify more cases by rerunning **set2D lapw**. Specify also your **''old'' volume and c/a points again** (or leave them out on purpose in case they were very bad eg. very far from the minimum). The old results will then be taken automatically into account without recalculation (unless you modify **2Doptimize.job** i.e: set answscf=no).

At the end, you can see the results for lattice parameters, bulk modules, ...
Moreover the results of Volume-optimized, bulk modules, ... save in "**case.outputeos**" file.

Suppose you would like to change order of fit and check the sensitivity of the results with the fitting. Edit "**.fordfitcoa**" file with '*gedit*' or ' *vi* ' in Terminal Environment and type in it order of fit and then save it and then rerun "**ana2D_lapw**" (don't forget to attention to note 1).

_____
EXAMPLE

Calculation 2-Dimensional of Equation Of State for hexagonal Mg

```
Mg
H   LATTICE,NONEQUIV.ATOMS:  1 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  6.066023  6.066023  9.851222 90.000000 90.000000120.000000
ATOM  -1: X=0.33333334 Y=0.66666666 Z=0.75000000
          MULT= 2          ISPLIT= 4
```

```
      -1: X=0.66666666 Y=0.33333334 Z=0.25000000
Mg1        NPT=  781  R0=0.00010000 RMT=    2.3000   Z: 12.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
```

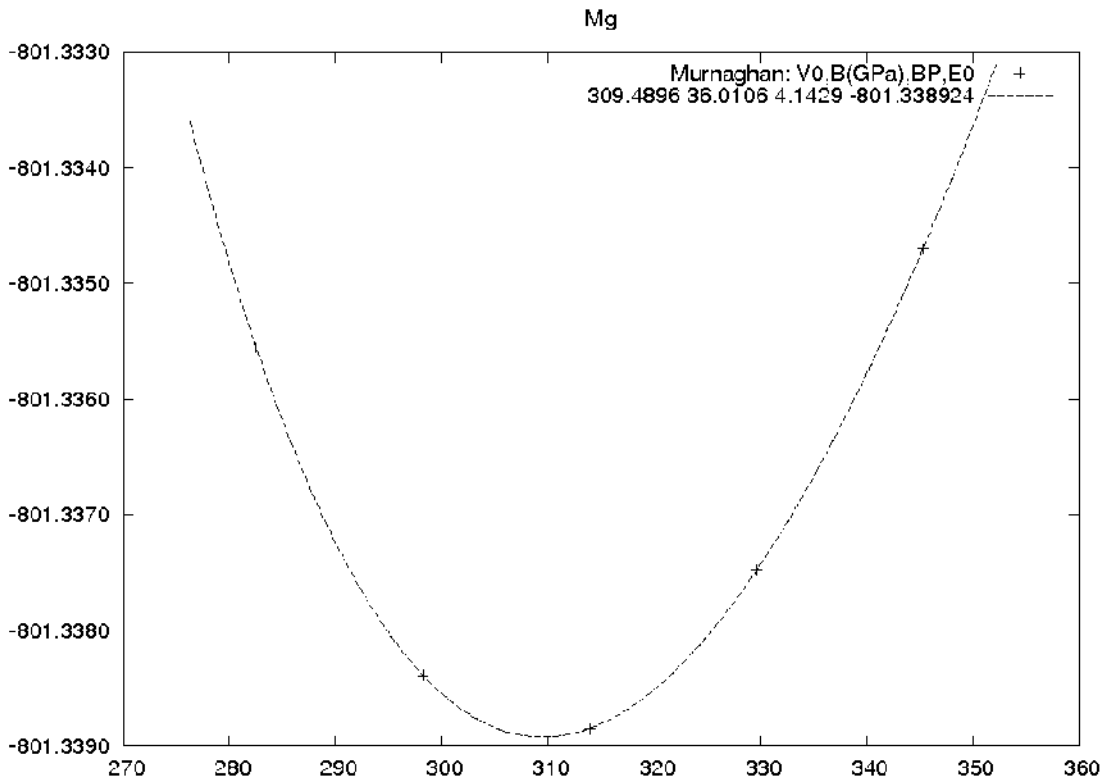
Select R_Kmax = 8 , L_max = 9 , XC = pbe, and nkpoint = 3000
Select order of fit 5 and default parameters for volume and c/a changes.
Since **Mg** is not spin-polarized system, it is not necessary to modify **2Doptimize.job** file and you can run it.
After running **2Doptimize.job** file and **ana2D_lapw**, you will find the below values in Terminal and **Mg.outputeos** file.

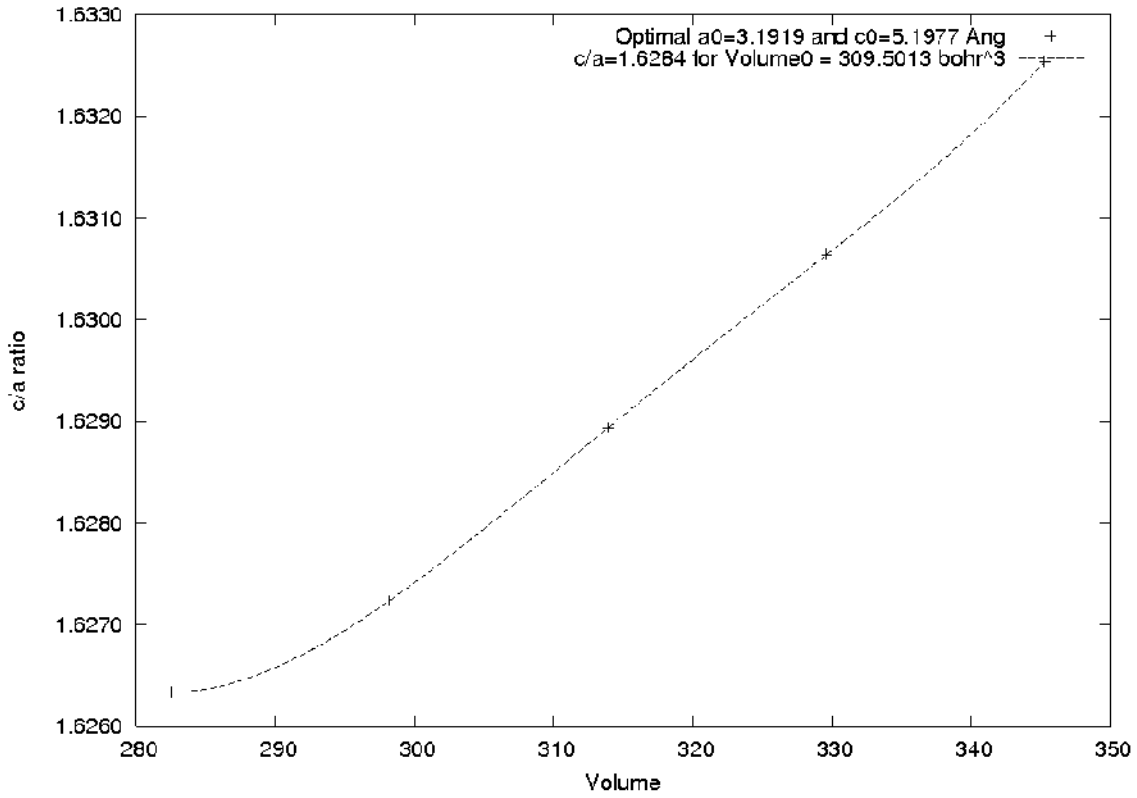
In the **Mg.outputeos** :

```
Equation of state: EOS2 (PRB52,8064)        info           2
 a,b,c,d      -801.689568        30.281633      -361.535061
1168.498137
 V0,B(GPa),BP,E0       309.5013        36.1561         4.1024

 Equation of state: Murnaghan                info           2
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0      309.4896     36.0106     4.1429   -801.338924
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
     282.5344     -801.335555     0.000000     0.000000          3.987
     298.2308     -801.338388    -0.000001    -0.000002          1.442
     313.9272     -801.338852     0.000002     0.000003         -0.498
     329.6235     -801.337480    -0.000001    -0.000003         -1.998
     345.3198     -801.334700     0.000000     0.000001         -3.171
                 Sigma:          0.000001     0.000002

 Equation of state: Birch-Murnaghan                info           2
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       309.5001     36.1388    4.1068   -801.338926
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
     282.5344     -801.335555     0.000000               3.974
     298.2308     -801.338388    -0.000001               1.447
     313.9272     -801.338852     0.000002              -0.499
     329.6235     -801.337480    -0.000001              -2.001
     345.3198     -801.334700     0.000000              -3.162
                 Sigma:          0.000001
```

In Terminal :

```
#####################################
Vol-opt= 309.5013 ,  coa-opt= 1.6284
a0= 6.03193 , c0= 9.82239 bohr
a0= 3.1919 , c0= 5.1977 Ang
#####################################
```


Mg
Murnaghan: V0,B(GPa),BP,E0
309.4896 36.0106 4.1429 -801.338924
-801.3330
-801.3340
-801.3350
-801.3360
-801.3370
-801.3380
-801.3390
270
280
290
300
310
320
330
340
350
360


Optimal a0=3.1919 and c0=5.1977 Ang
c/a=1.6284 for Volume0 = 309.5013 bohr^3
c/a ratio
1.6330
1.6320
1.6310
1.6300
1.6290
1.6280
1.6270
1.6260
280
290
300
310
320
330
340
350
Volume

	Our calculations	Exp[1]
a (Ang)	3.20	3.21
c (Ang)	5.20	5.21
B (GPa)	36.0	35.4

1) E Wachowicz and A Kiejna, J. Phys.: Condens. Matter 13 (2001) 10767–10776

Calculation 2-Dimensional of Equation Of State for hexagonal Be

```
Be
H   LATTICE,NONEQUIV.ATOMS:  1 194 P63/mmc
MODE OF CALC=RELA unit=bohr
  4.327475  4.327475  6.781153 90.000000 90.000000120.000000
ATOM  -1: X=0.33333334 Y=0.66666666 Z=0.75000000
          MULT= 2          ISPLIT= 4
      -1: X=0.66666666 Y=0.33333334 Z=0.25000000
Be1        NPT=  781  R0=0.00010000 RMT=   1.99      Z:  4.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
```

Select R_Kmax = 8 , L_max = 9 , XC = pbe, and nkpoint = 3000
Select order of fit 5 and default parameters for volume and c/a changes.
Since **Be** is not spin-polarized system, it is not necessary to modify **2Doptimize.job** file and you can run it.
After running **2Doptimize.job** file and **ana2D_lapw**, you will find the below values in Terminal and Be.outputeos file.

In the **Be.outputeos :**

```
Equation of state: EOS2 (PRB52,8064)        info           7
 a,b,c,d       -56.429582       -18.694574        -1.584227
145.328416
 V0,B(GPa),BP,E0       106.8496       122.6264         3.3392

 Equation of state: Murnaghan                info           7
 E=E0+[B*V/BP*(1/(BP-1)*(V0/V)**BP +1)-B*V0/(BP-1)]/14703.6
 Pressure=B/BP*((V0/V)**BP -1)
 V0,B(GPa),BP,E0       106.8434   122.4197     3.4062   -59.079470
         vol       energy         de(EOS2)      de(Murnaghan)
Pressure(GPa)
      98.9796      -59.076771     0.000000     0.000000         10.691
     104.4785      -59.079243     0.000000    -0.000001          2.847
     109.9774      -59.079104     0.000000     0.000001         -3.370
     115.4762      -59.076875     0.000000    -0.000001         -8.357
     120.9751      -59.072969     0.000000     0.000000        -12.399
                  Sigma:         0.000000     0.000001

 Equation of state: Birch-Murnaghan               info           2
```

```
 E = E0 + 9/16*(B/14703.6)*V0*[(eta**2-1)**3*BP + (eta**2-1)**2*(6-
4*eta**2)]
        --> eta = (V0/V)**(1/3)
 Pressure = 3/2*B*(eta**7 - eta**5)*(1 + 3/4*(BP-4)*[eta**2 - 1])
 V0,B(GPa),BP,E0       106.8517    122.7028    3.3159     -59.079470
         vol       energy         de(Birch-Murnaghan)  Pressure(GPa)
      98.9796      -59.076771     0.000000               10.651
     104.4785      -59.079243     0.000000                2.860
     109.9774      -59.079104     0.000000               -3.372
     115.4762      -59.076875     0.000000               -8.367
     120.9751      -59.072969     0.000000              -12.371
                  Sigma:          0.000000
```

In Terminal :

```
#####################################
Vol-opt= 106.8496 ,  coa-opt= 1.5709
a0= 4.28250 , c0= 6.72737 bohr
a0= 2.2662 , c0= 3.5599 Ang
#####################################
```

	Our calculations	**Exp**[1]
a (Ang)	2.27	2.29
c (Ang)	3.56	3.59
B (GPa)	107	110

1) E Wachowicz and A Kiejna, J. Phys.: Condens. Matter 13 (2001) 10767–10776

With best wishes,

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