



IR ELAST

+

WIEN2k

**A Package for calculating elastic tensors of orthorhombic
Phases *by using second-order derivative* and with Wien2k
Package**

User's guide, Elastic Orthorhombic_12.1(Release 21.02.2012)

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Installation guide

1_ Copy “**ortho-elastic.tar.gz**” file in your computer in each Directory that you would like.

```
tar -zxvf ortho-elastic.tar.gz
cd ortho-elastic
```

2_ Run **buildOIRElast_lapw**

This program helps you provide "Makefile" and then compile ortho-elastic and after that define Environment Variable ELASTO_PATH and add it at the end of **.bashrc** file.

Call Package

1_ Make struct file and then we recommend to run "sgroupcheck_lapw".

2_ Do initialization (run "instgen_lapw" and "init_lapw" in Terminal).

It is not necessary to do step 2. This program can do that.

3_ If you want to do Spin-Orbit calculations run "command_initso_lapw" in Terminal.

4_ If you want to do LDA+U calculations run "command_initu_lapw" and then "auto_initu_lapw" in Terminal.

NOTE ABOUT STEPS 3 AND 4

After using distortion for calculation C44, C55, and C66 the symmetry of orthorhombic compounds changes and maybe Number of atoms change. So when you run "command_initso_lapw" or "command_initu_lapw" ,in section name of atom, type "all name of atom" (e.g. all Mn). With this command, you use SO or LDA+U calculations for example for all Mn atoms.

5_ Run "O_set_elast_lapw" in Terminal.

6_ Now you must modify job files according to your needs.

You can run "O_modifyjob_lapw" in Terminal .

7_ Now you must run job files.

You can run "O_calljob_lapw" in Terminal . It will take time.

Note 1: When you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials) call “**command_init_lapw**” and after that choose "answscf=no" in “**ORTHO.job**” files and a new "savename" (eg. "_use_pbe_rk8").

8_ Run "O_ana_elast_lapw" in Terminal.

Optionally you can specify more cases by rerunning "**O_setupcXX**" (**XX=11, 12,22,.. see Suppose section**). Specify also your "**old**" cases. The old results will then be taken automatically into account without recalculation (unless you modify **job** files i.e: [set ansWSCF=no](#)).

NOTE ABOUT PROGRAMS

O_set_elast_lapw : makes elast-constant directory in present work directory (PWD) and c11, c12, c13, c22, c23, c33, c44, c55, and c66 directories in elast-constant directory. Moreover O_set_elast_lapw program copies information of "PWD" in c11, c12, c13, c22, c23, c33, c44, c55, and c66 directories and calls "command_init_lapw", O_setupc11, O_setupc12, O_setupc13, O_setupc22, O_setupc23, O_setupc33, O_setupc44, O_setupc55, and O_setupc66 programs.

O_modifyjob_lapw : Edits job files for modifying them according to your needs.

O_calljob_lapw : calls job files for running.

O_ana_elast_lapw : calls O_ana_elast_lapw for calculation elastic constants **and makes an output file in elast-constant directory with name case.output_elastic.**

O_ana_elastorder_lapw : **THIS PROGRAM CHECK THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT** (This program saves these data in the **output-order** file in the elast-constant directory.). **You can run it in the elats-constant directory. Moreover O_ana_elast_lapw calls O_ana_elastorder_lapw at the end of calculations.**

TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

Moreover this program predicts **Bulk modulus** of your compound by using elastic constant values.

command_init_lapw : gets informations for making "auto_init_lapw".

sgroupcheck_lapw : finds best value of tol in sgroup program and copies case.struct_sgroup as case.struct.

Suppose

Suppose we only want to calculate c33.

We do these stages as following:

- 1) Make a directory for example c33.
- 2) Make "case" directory in c33 directory.
- 3) Make "case.struct" file in "case" directory and copy it as "init.struct".
Moreover make "pwdname" file and write in it "**case.**" and save it.
- 4) Run command_init_lapw
- 5) For SO calculations, run command_initso_lapw.
- 6) For LDA+U calculations, run command_initu_lapw and auto_initu_lapw.
- 7) Run O_setupc33 program.
- 8) chmod +x ORTHO.job file.
- 9) Modify ORTHO.job file.
- 10) Call ORTHO.job
- 11) Call O_ana_elastic_lapw

Suppose we want to rerun c33 with more data points.

We do these stages as following:

- 1) cd "elast-constant" directory.
- 2) cd "c33" directory.
- 3) cd "case" directory.
- 4) Run O_setupc33 program.
- 5) If you want to rerun **job** files with modifications in (RKmax, k-mesh, XC-potentials)
call "command_init_lapw" and after that choose "answscf=no" in "**ORTHO.job**" files
and a new "savename" (eg. "_use_pbe_rk8").
- 6) Modify ORTHO.job file.
- 7) Call ORTHO.job
- 8) Call O_ana_elastic_lapw

IMPORTANT NOTE

For calculation best values of elastic constants, please find EOS and then copy case.outputeos in "case" directory within c11, c12, c13, c22, c23, c33, c44, c55, and c66 directories. **Otherwise this program set an arbitrary number for optimized volume (Vopt=999).**

Converged check

Since this package computes elastic constants by using second-order derivative ($E''(\epsilon)$) of Polynomial fit ($E=E(\epsilon)$) of Energy vs. Strains (ϵ) at zero strain ($\epsilon=0$). So, you must use values of strain around zero and **from the viewpoint of fit convergence**, we usually expect to see a minimum when we plot Energy vs. strain (this Package plots it). Moreover I recommend to check the sensitivity of the results to the order of fit. This program shows them. You can see in the example.

We recommend to use more data-points, more k-points and larger RKmax for all calculations to reduce numerical noise.

TO AVOID THE SENSITIVITY OF YOUR RESULT TO THE ORDER OF FIT, WE HIGHLY RECOMMEND TO USE VERY SMALL STRAINS.

EXAMPLE

Calculation elastic-constants for TiSi2

```
TiSi2
F LATTICE,NONEQUIV.ATOMS: 270_Fddd
MODE OF CALC=RELA unit=bohr
 15.628041  9.070689 16.157165 90.000000 90.000000 90.000000
ATOM -1: X=0.12500000 Y=0.12500000 Z=0.12500000
      MULT= 2          ISPLIT= 8
ATOM -1:X= 0.87500000 Y=0.87500000 Z=0.87500000
Ti1      NPT= 781  R0=0.00005000 RMT= 2.3850  Z: 22.0
LOCAL ROT MATRIX:  1.0000000  0.0000000  0.0000000
                   0.0000000  1.0000000  0.0000000
                   0.0000000  0.0000000  1.0000000
ATOM -2: X=0.46150000 Y=0.12500000 Z=0.12500000
      MULT= 4          ISPLIT= 8
ATOM -2:X= 0.53850000 Y=0.87500000 Z=0.87500000
ATOM -2:X= 0.71150000 Y=0.37500000 Z=0.87500000
ATOM -2:X= 0.78850000 Y=0.12500000 Z=0.12500000
Si1      NPT= 781  R0=0.00010000 RMT= 2.3500  Z: 14.0
LOCAL ROT MATRIX:  0.0000000  1.0000000  0.0000000
                   0.0000000  0.0000000  1.0000000
                   1.0000000  0.0000000  0.0000000
0          NUMBER OF SYMMETRY OPERATIONS
```

Select Xc = PBE-GGA, R_Kmax = 7, L_max = 8, and nkpoint = 5000

```
#####
# O_ana_elast_lapw analyses Elastic #
#          constant #
# C(2012) by Morteza Jamal #
#          Ali. H. Reshak #
#####
```

```

#####
# O_ana_elastc_lapw analyses Elastic      #
#           constant                      #
#           C(2012) by Morteza Jamal      #
#           Ali. H. Reshak                #
#           using case.outputeos         #
#           VstVene                       #
#           which have been created by    #
#           ORTHO.job                     #
#####
-0.020000    -5735.784670
-0.010000    -5735.786608
 0.000000    -5735.787275
 0.010000    -5735.786560
 0.020000    -5735.784891
=====
Order of fit:  2 C11 is:    315.5225 GPa, RMS: 0.532182E-04
Order of fit:  3 C11 is:    315.5225 GPa, RMS: 0.288776E-04
Order of fit:  4 C11 is:    366.7443 GPa, RMS: 0.704492E-12
*****
Polynomial fit for C11 done
A RMS of 0.532182E-04 was achieved using a polynome of degree :  2

At volume=  572.5982 bohr^3
C11 is:  0.021449 a.u or    315.5225 GPa
*****

Analyze done.....
Do you want a hardcopy? (y/N)
*****
You can find data in ELC.output file.
*****

#####
# O_ana_elastc_lapw analyses Elastic      #
#           constant                      #
#           C(2012) by Morteza Jamal      #
#           Ali. H. Reshak                #
#           using case.outputeos         #
#           VstVene                       #
#           which have been created by    #
#           ORTHO.job                     #
#####
-0.015000    -5735.785050
-0.010000    -5735.786497
-0.005000    -5735.787024
 0.000000    -5735.787152
 0.005000    -5735.786687
 0.010000    -5735.785833
=====
Order of fit:  2 C11+C22-2C12 is:    567.9293 GPa, RMS: 0.736751E-04
Order of fit:  3 C11+C22-2C12 is:    508.5687 GPa, RMS: 0.377351E-04
Order of fit:  4 C11+C22-2C12 is:    437.0956 GPa, RMS: 0.288151E-04
Order of fit:  5 C11+C22-2C12 is:    644.9911 GPa, RMS: 0.643110E-12
*****
Polynomial fit for C11+C22-2C12 done

```

A RMS of 0.736751E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3
C11+C22-2C12 is: 0.038607 a.u or 567.9293 GPa

Analyze done.....
Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

```
#####  
# O_ana_elastc_lapw analyses Elastic #  
# constant #  
# C(2012) by Morteza Jamal #  
# Ali. H. Reshak #  
# using case.outputeos #  
# VstVene #  
# which have been created by #  
# ORTHO.job #  
#####  
-0.020000 -5735.783438  
-0.010000 -5735.786563  
0.000000 -5735.787275  
0.010000 -5735.785230  
0.020000 -5735.780373
```

=====
Order of fit: 2 C11+C33-2C13 is: 687.1648 GPa, RMS: 0.584743E-04
Order of fit: 3 C11+C33-2C13 is: 687.1648 GPa, RMS: 0.153579E-04
Order of fit: 4 C11+C33-2C13 is: 714.4060 GPa, RMS: 0.704492E-12

Polynomial fit for C11+C33-2C13 done
A RMS of 0.584743E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3
C11+C33-2C13 is: 0.046712 a.u or 687.1648 GPa

Analyze done.....
Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

```
#####  
# O_ana_elastc_lapw analyses Elastic #  
# constant #  
# C(2012) by Morteza Jamal #  
# Ali. H. Reshak #  
# using case.outputeos #  
# VstVene #  
# which have been created by #  
# ORTHO.job #  
#####  
-0.015000 -5735.785319  
-0.010000 -5735.786399
```

-0.005000 -5735.786869
0.000000 -5735.787276
0.005000 -5735.787202
0.010000 -5735.786952
0.015000 -5735.786261

=====
Order of fit: 2 C22 is: 328.2530 GPa, RMS: 0.513416E-04
Order of fit: 3 C22 is: 328.2530 GPa, RMS: 0.506064E-04
Order of fit: 4 C22 is: 254.7452 GPa, RMS: 0.407217E-04
Order of fit: 5 C22 is: 254.7452 GPa, RMS: 0.372513E-04
Order of fit: 6 C22 is: 592.1555 GPa, RMS: 0.972291E-12

Polynomial fit for C22 done

A RMS of 0.513416E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3

C22 is: 0.022314 a.u or 328.2530 GPa

Analyze done.....

Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

O_ana_elastc_lapw analyses Elastic #
constant #
C(2012) by Morteza Jamal #
Ali. H. Reshak #
using case.outputeos #
VstVene #
which have been created by #
ORTHO.job #
#####

-0.020000 -5735.783464
-0.010000 -5735.786414
0.000000 -5735.787152
0.010000 -5735.785702
0.020000 -5735.782025

=====
Order of fit: 2 C22+C33-2C23 is: 566.7527 GPa, RMS: 0.371659E-05
Order of fit: 3 C22+C33-2C23 is: 566.7527 GPa, RMS: 0.321622E-05
Order of fit: 4 C22+C33-2C23 is: 561.0479 GPa, RMS: 0.000000E

Polynomial fit for C22+C33-2C23 done

A RMS of 0.371659E-05 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3

C22+C33-2C23 is: 0.038527 a.u or 566.7527 GPa

Analyze done.....

Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

```
#####
# O_ana_elastc_lapw analyses Elastic #
# constant #
# C(2012) by Morteza Jamal #
# Ali. H. Reshak #
# using case.outputeos #
# VstVene #
# which have been created by #
# ORTHO.job #
#####
```

```
-0.015000 -5735.784258
-0.010000 -5735.785627
-0.005000 -5735.786710
 0.000000 -5735.787152
 0.005000 -5735.787263
 0.010000 -5735.787098
 0.015000 -5735.786485
```

```
=====  
Order of fit: 2 C33 is: 411.4737 GPa, RMS: 0.499417E-04  
Order of fit: 3 C33 is: 411.4737 GPa, RMS: 0.388762E-04  
Order of fit: 4 C33 is: 414.4565 GPa, RMS: 0.388571E-04  
Order of fit: 5 C33 is: 414.4565 GPa, RMS: 0.117335E-04  
Order of fit: 6 C33 is: 308.1785 GPa, RMS: 0.595404E-12
```

```
*****  
Polynomial fit for C33 done  
A RMS of 0.499417E-04 was achieved using a polynome of degree : 2
```

```
At volume= 572.5982 bohr^3  
C33 is: 0.027971 a.u or 411.4737 GPa  
*****
```

```
Analyze done.....  
Do you want a hardcopy? (y/N)  
*****  
You can find data in ELC.output file.  
*****
```

```
#####
# O_ana_elastc_lapw analyses Elastic #
# constant #
# C(2012) by Morteza Jamal #
# Ali. H. Reshak #
# using case.outputeos #
# VstVene #
# which have been created by #
# ORTHO.job #
#####
```

```
-0.010000 -5735.786444
-0.005000 -5735.787020
 0.000000 -5735.787160
 0.005000 -5735.787020
 0.010000 -5735.786369
```

```
=====  
Order of fit: 2 C44 is: 100.4236 GPa, RMS: 0.231508E-04  
Order of fit: 3 C44 is: 100.4236 GPa, RMS: 0.205422E-04  
Order of fit: 4 C44 is: 63.9866 GPa, RMS: 0.575215E-12
```

Polynomial fit for C44 done
A RMS of 0.231508E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3
C44 is: 0.006827 a.u or 100.4236 GPa

Analyze done.....
Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

O_ana_elastc_lapw analyses Elastic #
constant #
C(2012) by Morteza Jamal #
Ali. H. Reshak #
using case.outputeos #
VstVene #
which have been created by #
ORTHO.job #
#####

-0.010000 -5735.786686
-0.005000 -5735.787092
0.000000 -5735.787160
0.005000 -5735.787092
0.010000 -5735.786686

=====
Order of fit: 2 C55 is: 64.6594 GPa, RMS: 0.212980E-04
Order of fit: 3 C55 is: 64.6594 GPa, RMS: 0.212980E-04
Order of fit: 4 C55 is: 26.8818 GPa, RMS: 0.406738E-12

Polynomial fit for C55 done
A RMS of 0.212980E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3
C55 is: 0.004395 a.u or 64.6594 GPa

Analyze done.....
Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

O_ana_elastc_lapw analyses Elastic #
constant #
C(2012) by Morteza Jamal #
Ali. H. Reshak #
using case.outputeos #
VstVene #
which have been created by #
ORTHO.job #
#####

-0.010000 -5735.786306
-0.005000 -5735.786990
0.000000 -5735.787160
0.005000 -5735.786990
0.010000 -5735.786206

=====
Order of fit: 2 C66 is: 120.2642 GPa, RMS: 0.276446E-04
Order of fit: 3 C66 is: 120.2642 GPa, RMS: 0.238028E-04
Order of fit: 4 C66 is: 78.0438 GPa, RMS: 0.000000E

Polynomial fit for C66 done
A RMS of 0.276446E-04 was achieved using a polynome of degree : 2

At volume= 572.5982 bohr^3
C66 is: 0.008175 a.u or 120.2642 GPa

Analyze done.....
Do you want a hardcopy? (y/N)

You can find data in ELC.output file.

Printing final Elastic constant At voulme= 572.5982 bohr^3 .

=====
C11 = 315.5225 GPa C22 = 328.2530 GPa C33= 411.4737 GPa
C44 = 100.4236 GPa C55 = 64.6594 GPa C66= 120.2642 GPa
C11+C22-2C12 = 567.9293 GPa
C11+C33-2C13 = 687.1648 GPa
C33+C22-2C23 = 566.7527 GPa
=====
C11 = 315.5225 GPa C22 = 328.2530 GPa C33= 411.4737 GPa
C44 = 100.4236 GPa C55 = 64.6594 GPa C66= 120.2642 GPa
C12 = 37.9231 GPa C13 = 19.9157 GPa C23= 86.4870 GPa
=====

Press enter key to continue....

O_ana_elastorder_lapw analyses Elastic #
constant #
C(2012) by Morteza Jamal #
Ali. H. Reshak #
using ELCorder.fit files #
#####

CHECK THE SENSITIVITY
OF YOUR RESULT TO THE ORDER OF FIT

Press enter key to continue....
Order of fit for calculations were 4,5,4,6,4
6,4,4, and 4
We select minimum value for ORDER OF FIT i.e. 4

Press enter key to continue....

ORDER OF FIT IS : 2 , At volume = 572.59821 (bohr^3) #####
(c11) = 315.523 (GPa)

(c22) = 328.253 (GPa)
(c33) = 411.474 (GPa)
(c44) = 100.424 (GPa)
(c55) = 64.659 (GPa)
(c66) = 120.264 (GPa)
(c11+c22-2c12) = 567.929 (GPa)
(c11+c33-2c13) = 687.165 (GPa)
(c22+c33-2c23) = 566.753 (GPa)

c11 = 315.523 (GPa)
c22 = 328.253 (GPa)
c33 = 411.474 (GPa)
c44 = 100.424 (GPa)
c55 = 64.659 (GPa)
c66 = 120.264 (GPa)
c12 = 37.923 (GPa)
c13 = 19.916 (GPa)
c23 = 86.487 (GPa)

=====
Pridicting Bulk mudules by using elastic constant values = 149.322
(GPa)

=====
ORDER OF FIT IS : 3 , At volume = 572.59821 (bohr^3) #####
(c11) = 315.523 (GPa)
(c22) = 328.253 (GPa)
(c33) = 411.474 (GPa)
(c44) = 100.424 (GPa)
(c55) = 64.659 (GPa)
(c66) = 120.264 (GPa)
(c11+c22-2c12) = 508.569 (GPa)
(c11+c33-2c13) = 687.165 (GPa)
(c22+c33-2c23) = 566.753 (GPa)

c11 = 315.523 (GPa)
c22 = 328.253 (GPa)
c33 = 411.474 (GPa)
c44 = 100.424 (GPa)
c55 = 64.659 (GPa)
c66 = 120.264 (GPa)
c12 = 67.603 (GPa)
c13 = 19.916 (GPa)
c23 = 86.487 (GPa)

=====
Pridicting Bulk mudules by using elastic constant values = 155.918
(GPa)

=====
ORDER OF FIT IS : 4 , At volume = 572.59821 (bohr^3) #####
(c11) = 366.744 (GPa)
(c22) = 254.745 (GPa)
(c33) = 414.456 (GPa)
(c44) = 63.987 (GPa)
(c55) = 26.882 (GPa)
(c66) = 78.044 (GPa)
(c11+c22-2c12) = 437.096 (GPa)
(c11+c33-2c13) = 714.406 (GPa)
(c22+c33-2c23) = 561.048 (GPa)

c11 = 366.744 (GPa)
 c22 = 254.745 (GPa)
 c33 = 414.456 (GPa)
 c44 = 63.987 (GPa)
 c55 = 26.882 (GPa)
 c66 = 78.044 (GPa)
 c12 = 92.196 (GPa)
 c13 = 33.397 (GPa)
 c23 = 54.076 (GPa)

=====
 Pridicting Bulk mudules by using elastic constant values = 155.031
 (GPa)
 =====

You can find these data in the output-order file.

C11 = 315.5225 GPa C22 = 328.2530 GPa C33= 411.4737 GPa
C44 = 100.4236 GPa C55 = 64.6594 GPa C66= 120.2642 GPa
C11+C22-2C12 = 567.9293 GPa
C11+C33-2C13 = 687.1648 GPa
C33+C22-2C23 = 566.7527 GPa

	Our calculations(relax)	Exp¹
C11	315.5	317.5
C22	328.2	320.4
C33	411.5	413.2
C44	100.4	112.5
C55	64.7	75.8
C66	120.3	117.5
C11+C22-2C12	567.9	579.2
C11+C33-2C13	687.2	653.8
C22+C33-2C23	566.8	561.6

[1] P. Ravindran, Lars Fast, P. A. Korzhavyi, and B. Johansson, J. Appl. Phys. **84**, (1998).

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