

If you want to use Hex-elastic package Please follow the following steps.

## FOR INSTALL

Edit "Makefile" and select your Fortran compiler ( FC ) and Fortran compiler options ( FOPT ) and the path of MKL library ( LDFLAGS ) and then save it ( you can type options that used for compiling Wien2k Package). Now type in Terminal environment:

```
make Makefile
make clean
```

## FOR USING

- 1\_ Make struct file and we recommend then run "sgroupcheck\_lapw".
- 2\_ Do initialization ( run "instgen\_lapw" and "init\_lapw" in Terminal).
- 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

Since for calculation C44 and (C11-C12) we use from Strains and then run "sgroupcheck\_lapw", may be Number of atoms in new struct file 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 "set\_elast\_lapw" in Terminal.
- 6\_ Now you must modify job files according to your needs ( you can run "modifyjob\_lapw" in Terminal ).
- 7\_ Now you must run job files ( you can run "calljob\_lapw" in Terminal ). It will take time.
- 8\_ Run "ana\_elastic\_lapw" in Terminal.

### NOTE ABOUT PROGRAMS

**set\_elast\_lapw** : makes elastic-constant directory in present work directory ( PWD ) and c11+c11, c11-c12, c33, c44, and czz directories in elastic-constant directory. Moreover set\_elast\_lapw program copies information of "PWD" in c11+c12, c11-c12, c33, c44, and czz directories and calls "command\_init\_lapw", setupc1112, setupc11m12, setupc33, setupc44, and setupczz programs.

**modifyjob\_lapw** : Edits job files for modifying them according to your needs.

**calljob\_lapw** : calls job files for running.

**ana\_elastic\_lapw** : calls ana\_elastic1112\_lapw, ana\_elastic11m12, ana\_elastic33\_lapw, ana\_elastic44\_lapw, and ana\_elasticzz\_lapw programs for calculation elastic constants and makes an output file in elastic-constant directory with name case.output\_elastic.

Moreover ana\_elastic1112\_lapw, ana\_elastic11m12, ana\_elastic33\_lapw, ana\_elastic44\_lapw, and ana\_elasticzz\_lapw programs produce case.outputc1112, case.outputc11m12, case.outputc33, case.outputc44, and case.outputczz, respectively.

**sgroupcheck\_lapw** : finds best value of tol in sgroup program and copies case.struct\_sgroup as case.struct.

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 instgen\_lapw
- 5) Run init\_lapw
- 6) For SO calculations, run command\_initso\_lapw.
- 7) For LDA+U calculations, run command\_initu\_lapw and auto\_initu\_lapw.
- 8) Run setupc33 program.
- 9) chmod +x c33.job file.
- 10) Modify c33.job file.
- 11) Call c33.job
- 12) Call ana\_elastic33\_lapw

## IMPORTANT NOTE

---

For calculation best values of elastic constants, please find EOS and then copy case.outputeos in "case" directory within c11+c11, c11-c12, c33, c44, and czz directories.

## EXAMPLE

---

### *Calculation elastic-constant for Ti*

You can find ti.struct and ti.outputeos in example-elastic directory of this package.

```
Ti
H LATTICE,NONEQUIV.ATOMS: 1 194 P63/mmc
MODE OF CALC=RELA unit=bohr
5.574694 5.574694 8.843922 90.000000 90.000000120.000000
ATOM -1: X=0.33333333 Y=0.66666665 Z=0.75000000
MULT= 2 ISPLIT= 4
```

```

-1: X=0.66666667 Y=0.33333335 Z=0.25000000
Ti1      NPT= 781 R0=0.00005000 RMT= 2.4000 Z: 22.0
LOCAL ROT MATRIX:  1.0000000 0.0000000 0.0000000
                   0.0000000 1.0000000 0.0000000
                   0.0000000 0.0000000 1.0000000

```

Select R\_Kmax = 7 , L\_max = 8 and nkpoint = 3000

When you call set\_elast\_lapw, please select number of changes for c11+c11, c11-c12, c33, and czz 11 and percent of changes -5%, -4%, -3%, -2%, -1%, 0%, 1%, 2%, 3%, 4%, 5% and for c44 select default.

After running job files, you will find the below values for ELASTIC-CONSTANT of Ti ( **do not forget to copy ti.outputeos in "ti" directory within c11+c11, c11-c12, c33, c44, and czz directories** ).

	Our calculation	Other(TB) <sup>1</sup>	Exp <sup>1</sup>
<b>C11</b>	188.3	171	160
<b>C12</b>	63.6	58	90
<b>C13</b>	61.2	46	60
<b>C33</b>	194.9	203	181
<b>C44</b>	<b>8.7</b>	64	47

**1) Michael J. Mehl and Dimitrios A. Papaconstantopoulos, PRB, 54, 1996.**

### *Calculation elastic-constant for Sc*

```

Title
H LATTICE,NONEQUIV.ATOMS: 1194_P63/mmc
MODE OF CALC=RELA unit=bohr
6.254996 6.254996 9.958861 90.000000 90.000000120.000000
ATOM -1: X=0.33333333 Y=0.66666667 Z=0.75000000
      MULT= 2 ISPLIT= 4
ATOM -1:X= 0.66666667 Y=0.33333333 Z=0.25000000
Sc      NPT= 781 R0=0.00005000 RMT= 2.4000 Z: 21.0
LOCAL ROT MATRIX:  1.0000000 0.0000000 0.0000000
                   0.0000000 1.0000000 0.0000000
                   0.0000000 0.0000000 1.0000000

```

Select R\_Kmax = 7 , L\_max = 8 and nkpoint = 3500

please select number of changes for c11+c11, c11-c12, and czz 11 and percent of changes -5%, -4%, -3%, -2%, -1%, 0%, 1%, 2%, 3%, 4%, 5% and for c33 select -10%, -5%, -3%, 0%, 3%, 5%, 10%.

After running job files, you will find the below values for ELASTIC-CONSTANT of Sc ( do not forget to copy Sc.outputeos in "Sc" directory within c11+c11, c11-c12, c33, c44, and czz directories ).

	Our calculation	Other(TB) <sup>1</sup>	Exp <sup>1</sup>
<b>C11</b>	101.7	72	99
<b>C12</b>	22.3	30	40
<b>C13</b>	31.9	31	29
<b>C33</b>	101.7	78	107
<b>C44</b>		25	28

1) Michael J. Mehl and Dimitrios A. Papaconstantopoulos, PRB, 54, 1996.

**NOTE : Example show that our package is not able to calculate c44 very good.**

---

**Morteza Jamal**  
**Email: m\_jamal57@yahoo.com**

---