

A Package for calculating elastic tensors of cubic phases using Wien2k Package

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If you want to use cubic-elastic package Please follow the following steps.
You can install cubic-elastic package in each Directory that you would like.

FOR INSTALL

1_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

2_Run “addbash_lapw” program (type addbash_lapw in terminal). This program define Environment Variable ELASTC_PATH and add it at the end of **.bashrc** file. Therefore you will able to call cubic-elastic’s programs in each Directory.

FOR USING

- 1_ Make struct file and run "init_elastc_lapw" and then change to "elast" directory.
- 2_ Run "setup_elast_lapw".
- 3_ Now you must modify job files according to your needs (you can run "modifyjobc_lapw" in Terminal).
- 5_ Now you must run job files (you can run "calljobc_lapw" in Terminal). It will take time.

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

- 6_ Run "ana_elastc_lapw" in Terminal.

Optionally you can specify more cases by rerunning “**setup_elast_lapw**”. 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

init_elastic_lapw : makes "elastic" and with in "eos", "tetra", "rhomb", and "result" directories and calls "command_init_lapw" if you decide to run "init_lapw" as automatically. Moreover "init_elastic_lapw" program copies "case.struct" file as "init.struct" and "eos.templ" and produces "tetra.templ" and "rhomb.templ" by calling "genetemplc" program and then copies them in "eos", "tetra", and "rhomb" directories and then runs "auto_init_lapw" or "init_lapw" within them.

In "result" directory, you can find all struct, scf, and clm* files.

setup_elastic_lapw : Produces structs file that will be necessary for calculations by using "setupeos", "setuptetra" and "setuprhomb" programs.

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

calljobc_lapw : calls job files for running.

ana_elastic_lapw : calls ana_elasteos_lapw, ana_elasttetra_lapw, and ana_elastrhomb_lapw programs for calculations elastic constants and makes an output file in elastic directory with name "outputs".

Moreover ana_elasteos_lapw, ana_elasttetra_lapw, and ana_elastrhomb_lapw programs produce eos.outputeos, tetra.outputtetra, and rhomb.outputrhomb in "eos", "tetra", and "rhomb" directories, respectively.

command_init_lapw : gets informations for making "auto_init_lapw".

Suppose we only want to calculate $(c_{11}+2c_{12})/3$ or $(c_{11}-c_{12})$ or $(c_{11}+2c_{12})/2+2c_{44}$.

We do these stages as following:

- 1) Make a directory with name "elastic" and within "eos" or "tetra" or "rhomb" directory.
- 2) copy "case.struct" file as "init.struct" and "eos.templ" and then copy them within "eos" or "tetra" or "rhomb" directory.
- 3) Within "tetra" or "rhomb" directory run "genetemplc" program (only for $(c_{11}-c_{12})$ or $(c_{11}+2c_{12})/2+2c_{44}$ calculations).
- 4) copy "eos.templ" as "eos.struct" within "eos" directory or copy "tetra.templ" as "tetra.struct" within "tetra" directory or copy "rhomb.templ" as "rhomb.struct" within "rhomb" directory
- 4) Run instgen_lapw and init_lapw within "eos" or "tetra" or "rhomb" directory.
- 5) Run "setupeos" or "setuptetra" or setuprhomb" within "eos" or "tetra" or "rhomb" directory, respectively.
- 6) Modify "eos.job" or "tetra.job" or "rhomb.job" file according your needs within "eos" or "tetra" or "rhomb" directory.

- 7) “chmod +x eos.job” or “chmod +x tetra.job” or “chmod +x rhomb.job”
- 8) Run job file within “eos” or “tetra” or “rhomb” directory.
- 9) Within elast directory, run “ana_elasteos_lapw” or “ana_elasttetra_lapw” or ana_elastrhomb_lapw”.

Suppose we only want to add some points to EOS calculations.

In present work directory, we go to “elast” directory and then within “eos” directory. Now run “setupeos” and select more cases. After that we modify “eos.job” file according to our needs and then run “eos.job” file (do not forget to do “chmod +x eos.job” before running). Now in “elast” directory, we run “ana_elastc_lapw”.

EXAMPLE

Calculation elastic-constant for MgO

```

MgO
F LATTICE,NONEQUIV.ATOMS: 2
MODE OF CALC=RELA unit=bohr
  7.868900  7.868900  7.868900  90.000000  90.000000  90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
        MULT= 1          ISPLIT= 8
Mg      NPT=  781  R0=0.00010000 RMT=    1.7000  Z: 12.0
LOCAL ROT MATRIX:    1.0000000  0.0000000  0.0000000
                    0.0000000  1.0000000  0.0000000
                    0.0000000  0.0000000  1.0000000
ATOM   2: X=0.50000000 Y=0.00000000 Z=0.00000000
        MULT= 1          ISPLIT= 8
O       NPT=  781  R0=0.00010000 RMT=    1.7000  Z:  8.0
LOCAL ROT MATRIX:    0.0000000  0.0000000  0.0000000
                    0.0000000  0.0000000  0.0000000
                    0.0000000  0.0000000  0.0000000

```

Select Xc = LDA , R_Kmax = 8 , L_max = 10 and nkpoint = 5000

I used default parameters for making struct files.

At final , we will have :

```

At volume = 121.7040 (bohr^3)
(c11+2c12)/3 = 172.5279 (GPa)
-----
At volume = 121.7040 (bohr^3)
(c11-c12) = 228.46455464288584488060 (GPa)
-----
At volume = 121.7040 (bohr^3)
(c11+2c12)/2+2c44 = 563.02635464510707999552 (GPa)
-----
c11 = 324.83760309525722992040 (GPa)

```

c12 = 96.37304845237138503980 (GPa)

C44 = 152.11725232255353999776 (GPa)

Have a good day...
Thomas Charpin and Morteza Jamal

	Our calculations	Thomas Charpin calculations
C11 (GPa)	325	329
C12 (GPa)	96	93
C44 (GPa)	152	151

Calculation elastic-constant for Pt

```
Pt
F LATTICE,NONEQUIV.ATOMS: 1
MODE OF CALC=RELA unit=bohr
 7.407729 7.407729 7.407729 90.000000 90.000000 90.000000
ATOM 1: X=0.00000000 Y=0.00000000 Z=0.00000000
      MULT= 1          ISPLIT= 2
Pt1      NPT= 781 R0=0.00000500 RMT= 2.5000 Z: 78.0
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000
                  0.0000000 1.0000000 0.0000000
                  0.0000000 0.0000000 1.0000000
 48      NUMBER OF SYMMETRY OPERATIONS
```

Select Xc = PBE-GGA , R_Kmax = 8 , L_max = 10 and nkpoint = 5000

I used default parameters for making struct files.

At final , we will have :

```
At volume = 105.9922 (bohr^3)
(c11+2c12)/3 = 261.1294 (GPa)
-----
At volume = 105.9922 (bohr^3)
(c11-c12) = 78.52977449540448229176 (GPa)
-----
At volume = 105.9922 (bohr^3)
(c11+2c12)/2+2c44 = 626.26100114806094925656 (GPa)
-----
c11 = 313.48258299693632152784 (GPa)
c12 = 234.95280850153183923608 (GPa)
C44 = 117.28345057403047462828 (GPa)
-----
```

Have a good day...
Thomas Charpin and Morteza Jamal

	Our calculations	Exp¹
C11 (GPa)	313	347
C12 (GPa)	234	251
C44 (GPa)	117	76

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

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