IRelast2D Package

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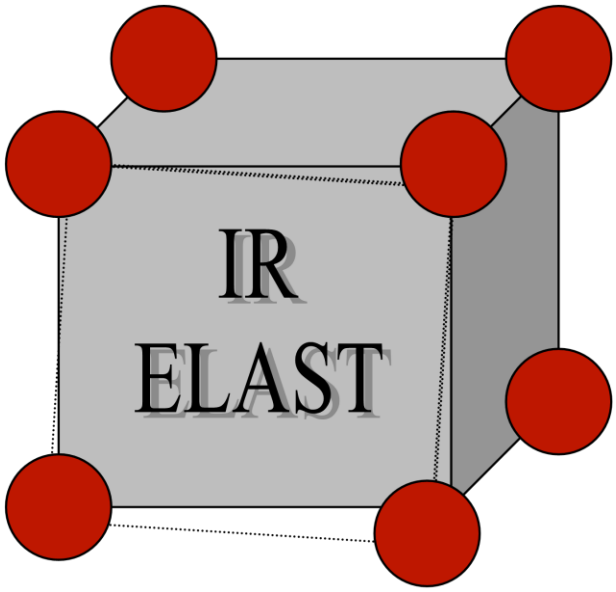
IRelast2D is a package for finding elastic constants of Oblique, Rectangular, Square and Hexagonal, crystals of 2D materials with WIEN2k package.

[03/10/2021]



IRelast2D

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WIEN2k

A Package for calculating elastic tensors of 2D materials by using second-order derivative **with WIEN2k Package**

User's guide, IRelast2D_21.1 (Release 03.10.2021)

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MANDATORY CONDITIONS:

In any publication in the scientific literature please reference the program as follows:

M. Jamal, IRelast2D, http://www.wien2k.at/ (2021).
J. Mater. Chem. C, 2019, 7, 13559--13572.

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This package calculates elastic constants for Oblique, Rectangular, Square and Hexagonal, crystals of 2D materials by using second-order derivative of polynomial fit of Energy vs. strains at zero strain. **We suppose vacume is along Z-Direction**

The package is driven by the following scripts:

- **set_elast2D_lapw**

It prepares the whole calculation and should be run in a directory with a valid **case.struct** file. It finds crystal systems (S= O(Oblique), R(Rectangular), S(Square) and H(Hexagonal)) of the case.struct file and creates the necessary subdirectories **elast-constant**, **elast-constant/c11**, **elast-constant/c22**, **elast-constant/c66**, **.....** It also copies information of present work directory into the c11, c22, c66, and .... subdirectories and calls **command_init_lapw** to get information for producing **auto_init_lapw** script for automatic initialization. Then it gets the options for running the scf-cycle in the job file by calling **command_run2D_lapw.** At the end, it generates the distorted struct-files and **SURF.job** using S2D_setupc11, S2D_setupc22, and .... programs (S= O(Oblique), R(Rectangular), S(Square) and H(Hexagonal)).

- **modifyjob2D_lapw**

It makes you possible to edit job file and modify the previously created **SURF.job** file according to your needs (spin-polarization, convergence,...) when you call it from main directory i.e. **case** directory. You can avoid from this step when you have specified proper commandline options in the earlier step.

- **calljob2D_lapw**

It makes you possible to run job files from **elast-constant/c11/case**, **elast-constant/c22/case**, **elast-constant/c66/case** , and .... subdirectories but, I recommend to run job files by hand from **elast-constant/c11/case**, **elast-constant/c22/case**, **elast-constant/c66/case** , and .... subdirectories**.**

- **ana_elast2D_lapw**

This program calls **ana_elastc2D_lapw** script and determines elastic constants as well as the Shear, and Young modulus and the Poisson's coefficient. Using elastic constants data and the auxiliary program "**stabilityJAC2D**" it checks elastic stability conditions. The main output file which is saved in the elast-constant directory is **case.output_elastic**.

Optionally you can specify more data points, for the calculation of the elastic constants, by rerunning "**S2D_setupcX" (**S= O(Oblique), R(Rectangular), S(Square) and

H(Hexagonal)) and **X=11, 12, 66,…)**. Specify also your **''old'' data points**. The old results will then be taken automatically into account without recalculation (unless you modify the **job** files i.e: set answscf=no).

Please do the following steps for this goal for example for c66.

S= (O(Oblique), R(Rectangular), S(Square) and H(Hexagonal))

1. cd to the "elast-constant" directory.
2. cd to the "c66" directory.
3. cd the "case" directory.
   3-1) To avoid step 6, you can run "command_run2D_lapw" for setting the proper commandline options for producing the "SURF.job" .
4. Run the **S2D_setupc66** program.
5. If you want to rerun the **job** files with modifications in (RKmax, k-mesh, XC-potentials) call **"command_init_lapw"** and then choose "answscf=no" in **"SURF.job"** files and a new "savename" (eg. "_use_pbe_rk8").
6. Modify the **SURF.job** file.
7. Call **SURF.job**
8. Call **ana_elastc2D_lapw**