AFLOW V 3.1.155

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*                                                                             *
*              Aflow STEFANO CURTAROLO - Duke University 2003-2018             *
*                   High-Throughput ab-initio Materials Discovery             *
*                                                                             *
*******************************************************************************
```
Thermal properties calculated using a quasi-harmonic Debye model.
This implementation in AFLOW written by Cormac Toher and Stefano Curtarolo,
and is described in the papers Phys. Rev. B 90, 90, 174107 (2014) and
Phys. Rev. Materials 1, 015401 (2017).
Based on the GIBBS program, described in the publications
 Computer Physics Communications 158, 57-72 (2004) and
 Journal of Molecular Structure (Theochem) 368, 245-255 (1996).
Please cite the 4 papers mentioned above in addition to the standard AFLOW
papers if you use results obtained using the AFLOW AGL code.
The Hugoniot calculation described in point (18) below was implemented
by Patrick Avery at University of Buffalo (email: psavery@buffalo.edu).

The current version of AGL can calculate the thermal conductivity, Debye temperature,
Gruneisen parameter, heat capacity, vibrational free energy, and other thermal properties,
as a function of temperature and pressure. The results are written in a variety of formats
in different output files. The main output file is named aflow.agl.out, and contains the
AGL results for the thermal conductivity at 300K, the traditional and acoustic Debye
temperatures, the Gruneisen parameter, the heat capacities at constant volume (Cv) and
constant pressure (Cp) at 300K, the thermal expansion at 300K, and the static and
isothermal bulk modulus at 300K. It also contains the results for the thermal conductivity,
Debye temperature, Gruneisen parameter, heat capacity, thermal expansion and bulk modulus
as function of temperature; and the Gibbs free energy, vibrational Helmholtz free energy,
vibrational internal energy, and vibrational entropy as a function of temperature. More
information can be found in the other main ouput file AGL.out, which contains the results
for the thermal properties and bulk moduli for all temperatures and pressures. The values
for the vibrational internal energy, vibrational free energy, entropy, heat capacity,
Debye temperature and Gruneisen parameter as a function of temperature at zero pressure
are written to the file AGL_THERMO, in a similar format to that used by the THERMO file
written by AFLOW APL. For further details on the output files written, see points (16)
and (17) below. Other results can be written and plotted by setting the appropriate
values in the aflow.in file, as described in point (17) below.

AFLOW AGL expects a well relaxed structure on input. There is no additional relaxation
inside the AFLOW AGL. So, you have to prepare such a structure by a separate AFLOW run
using a relaxation mode for energy and/or forces.

When AFLOW AGL is run, it will first check for the existence of the required DFT
calculations. If these exist, then it will extract the required information and
proceed to calculate the thermal properties. If these do not exist, then it will
create the required directories and aflow.in files, and then stop. By running AFLOW
with the "--D" and "--multi" flags, AFLOW will then automatically descend into these
subdirectories and run the required electronic structure calculations, after which
it will stop. The user will then have to rename or delete the LOCK file in the main
directory, and the run AFLOW again to calculate the thermal properties. This
can all be performed within a submission script as in the following example:

```
aflow --multi -D $pathname/ >> log.$PBS_JOBID
mv $pathname/LOCK $pathname/LOCK.old
aflow --multi -D $pathname/ >> log.$PBS_JOBID
```

This procedure is similar to that required to run AFLOW APL.

1) To perform a AFLOW AGL calculation the following line has to be present in aflow.in:

    [AFLOW_AGL]CALC

    AFLOW checks for the existence of this line in aflow.in. If it does not exist,

then the job is not an AFLOW AGL calculation and no other AGL settings are read.

AGL can also be run from within other parts of AFLOW, such as from APL, in order to obtain properties such as bulk modulus and equilibrium volume as a function of temperature to be used within these other parts of AFLOW. In this case, AGL will run and the other AGL settings in the aflow.in file will be read, even if the "[AFLOW_AGL]CALC" line is not present.

2) The AFLOW AGL method requires a set of energy vs. volume data, which are obtained from DFT calculations of a set of strained structures. The user has the possibility to set the number of strained structures and the size of the strain step. These parameters can be set by including the following lines in the aflow.in file:

   [AFLOW_AGL]NSTRUCTURES=number
   [AFLOW_AGL]STRAINSTEP=number

   The default setting is 28 structures and a step size of 0.01. The strain step size corresponds to the value by which each lattice vector is shortened or lengthened for each new strained structure.

3) The AFLOW AGL method allows the user to select what type of AFLOW DFT runs are performed for each strained structure (see Calderon et al., Comp. Mat. Sci. 108A, 233-238 (2015) for a description of the parameters used for the different calculation types). The default option is to perform an AFLOW STATIC calculation for each strained structure, which can be set by including the following lines in the aflow.in file:

   [AFLOW_AGL]STATIC=ON

   The other option is to run a RELAX_STATIC=2 calculation, which can be set by including the following lines in the aflow.in file:

   [AFLOW_AGL]RELAX_STATIC=ON

4) The AFLOW AGL method allows the user to select which form of the equation of state is used to fit the (E, V) data. The options include numerical, Vinet (J. Phys. Condens. Matter 1, 1941 (1989)), Birch-Murnaghan and spinodal (Baonza, Caceres, and Nunez, Phys. Rev. B 51, 28 (1995)). These options can be selected by including the following line in the aflow.in file :

   [AFLOW_AGL]IEOS=number

   The options are as follows:
   IEOS=0: Numerical equation of state (default setting)
   IEOS=1: Vinet equation of state
   IEOS=2: Birch-Murnaghan equation of state
   IEOS=3: Vinet equation fitting, but numerical calculation to obtain thermal properties
   IEOS=4: Birch-Murnaghan equation fitting, but numerical calculation to obtain thermal properties
   IEOS=5: Spinodal (BCNT) equation of state
   IEOS=6: Spinodal (BCNT) equation fitting, but numerical calculation to obtain thermal properties
   IEOS=-1: Number equation of state with minimal output, no plots generated or files other than [system name].out are written

   For the spinodal equation of state, the user also has the option to optimize the non-linear parameter beta using the following:

   [AFLOW_AGL]IOPT_G=number

   The options are as follows:
   IOPT_G=0: Beta is fixed to 0.85
   IOPT_G=1: Beta is always optimized
   IOPT_G=2: Beta is only optimized in the static calculation, and then this value is used for the finite temperature calculations

5) The AFLOW AGL method allows the user to select whether or not to calculate the Debye
   temperature self-consistently. These options can be selected by including the following
   line in the aflow.in file:

   [AFLOW_AGL]IDEBYE=number

   The options are as follows:
   IDEBYE=0: No self-consistent calculation of Debye temperature, Debye temperature calculated
         from static bulk moduli (default)
   IDEBYE=1: User contributed Debye temperatures
   IDEBYE=2: Self-consistent calculation of Debye temperatures from adiabatic bulk moduli
   IDEBYE=3: Debye temperature calculated from static bulk modulus at static equilibrium volume
   IDEBYE=-1: Static calculation only, no finite temperature properties calculated

   User contributed Debye temperatures should be given in the following format:

   [AFLOW_AGL]DEBYE_TEMP_number=number

   The first number is an integer corresponding to the number of the structure, while the second
   number is the user's value of the Debye temperature for this structure.

6) The AFLOW AGL method allows the user to choose the details of how the (E, V) curve is fitted by
   a polynomial, and in particularly how convex points in the (E, V) data are accounted for. This
   allows the user to relax the concavity restrictions on the (E, V) data being used. These options
   can be selected by including the following line in the aflow.in file:

   [AFLOW_AGL]FITTYPE=number

   The options are as follows:

   FITTYPE=0: Fits only the first concave section of the (E, V) data. If this does not include the
         minimum, it also includes a second concave section starting from the minimum, if such
      a section exists. This is the default setting.
   FITTYPE=1: Fits only (E, V) data points where the energy is monotonically decreasing until the
         minimum energy is reached, and points where the energy is monotonically increasing
      after the minimum energy is reached.
   FITTYPE=2: Fits all (E, V) data points.
   FITTYPE=3: Selects points using same method as for FITTYPE=1, but then fits these points by a
         polynomial which is used to generate a new set smoothly concave (E, V) data points.
   FITTYPE=4: Fits all points by a polynomial which is used to generate a new set of smoothly
         concave (E, V) data points.
   FITTYPE=5: The (E, V) data is read in from user-created file instead of being directly extracted
         from the results of the electronic structure calculations.

   Note that these fitting options should be used carefully, as they could give misleading results.
   They are mainly useful for testing and debugging, and for in depth exploration of certain properties
   of specific systems. For high-throughput data generation, use only the default option of FITTYPE=0,
   as this is the safest. Also, be sure to check for warnings about data points being excluded from the
   calculation. If a lot of points are excluded, you may want to recheck the (E, V) from the original
   electronic structure calculations, and if it is very noisy it would be advisable to rerun these
   calculations with a denser k-point mesh.

7) The AFLOW AGL method allows the user to set the value of the Poisson ratio to be used by including
   the following line in the aflow.in file:

   [AFLOW_AGL]POISSON=number

   The default value is 0.25.

   The AFLOW AGL method can also call the AFLOW AEL method to calculate the Poisson ratio from the
   elastic constants by including the following line in the aflow.in file:

   [AFLOW_AGL]AELPOISSONRATIO=ON

   This option will run the AEL method in full, calculating the Poisson ratio, bulk and shear moduli,

3

and other elastic properties. Note that running this method in conjunction with AGL will require
an additional aflow run followed by moving the LOCK file to a different location. See the README
file for AEL for more details on this method.

8) The AFLOW AGL method allows the user to set the number of temperature and pressure points to be used
in the calculation, as well as the size of the increments between each temperature or pressure point.
These values can be set by including the following lines in the aflow.in file:

    [AFLOW_AGL]NPRESSURE=number
    [AFLOW_AGL]SPRESSURE=number
    [AFLOW_AGL]NTEMP=number
    [AFLOW_AGL]STEMP=number

NPRESSURE is the number of pressure points and SPRESSURE is the increment between pressure points.
NTEMP is the number of temperature points and STEMP is the increment between temperature points.

The default values are as follows:

    NPRESSURE=11
    SPRESSURE=2.0
    NTEMP=201
    STEMP=10.0

9) The AFLOW AGL method allows the user to provide specific pressure values to be used in the
calculations. This option can be selected by including the following line in the aflow.in file:

    [AFLOW_AGL]SETPRESSUREVALUE=ON

Setting this option results in the specific pressure values being read in from the aflow.in file.
The default value is SETPRESSUREVALUE=OFF so that no specific values are read in. User specified
pressure values should be provided using the following format:

    [AFLOW_AGL]PRESSURE_number=number

Note that the first pressure value should always be equal to 0.0. If this is not the case,
AFLOW AGL will give a warning and insert a value of 0.0 as the first pressure value. Also,
negative pressure values will result in AFLOW AGL exiting with an error.

10) The AFLOW AGL method allows the user to set the maximum number of convergence iterations
for the Gauss-Legendre and self-consistent Debye functions. This limit prevents these
functions from getting stuck in an infinite loop. This value can be set by including the
following line in the aflow.in file:

    [AFLOW_AGL]MAXLOOPS=number

The default value is 250.

11) The AFLOW AGL method allows the user to set the value of the energy for an infinite volume.
The purpose of this is to set the zero of the energy scale.
This value can be set by including the following line in the aflow.in file:

    [AFLOW_AGL]EINF=number

The default value is 0.0.

12) The AFLOW AGL method allows the user to choose whether or not to write out the input file for
the original, non-AFLOW version of GIBBS. This can be useful for debugging and testing.
This option can be selected by including the following line in the aflow.in file:

    [AFLOW_AGL]WRITEGIBBSINPUT=option

The AGL input will be written for WRITEGIBBSINPUT=ON. The default value is WRITEGIBBSINPUT=OFF,
which does not write out the file.

13) The AFLOW AGL method allows the user to choose whether or not to check the concavity and

location of the energy minimum of the (E, V) data calculated with VASP before starting the GIBBS method. In order to fit the (E, V) data by a polynomial, the data points should be concave and include a minimum. This option can be selected by including the following line in the aflow.in file:

[AFLOWGIBBS]CHECKEVCONCAVITY=option

A value of CHECKEVCONCAVITY=ON causes the concavity check to be performed. The default value is CHECKEVCONCAVITY=OFF so no concavity check is performed prior to the GIBBS method. The GIBBS method will perform another concavity check after the (E, V) data has been passed to it, and will return an error if the data is not concave.

Problems with the (E, V) data are usually the result of incompleteness of the electronic structure calculation basis set or k-point grid. If CHECKEVCONCAVITY=ON and if the (E, V) data is not concave, then AFLOW AGL doubles value of KPPRA to increase the number of k-points, and creates a new set of directories containing aflow.in files with this new value of KPPRA. The electronuc structure calculations are rerun with the increased number of k-points, and the new set of (E, V) data is once again checked for concavity. This process is repeated until a concave data set is obtained or the maximum number of concavity check iterations is reached. The number of concavity check iterations can be set by including the following line in the aflow.in file:

[AFLOW_AGL]MAXCCITER=number

The default value for the maximum number of concavity check iterations is 1.

The AFLOW AGL method allows the user to choose whether or not to check that the (E, V) data set includes the energy minimum. In order to get a good fit, the (E, V) data should contain the minimum. This check can be initiated by including the following line in the aflow.in file:

[AFLOW_AGL]CHECKMIN=option

A value of CHECKMIN=ON causes the check of the location of the energy minimum to be performed. The default value is CHECKMIN=OFF so no check is performed.

If CHECKMIN=ON, the (E, V) data is sorted in order of increasing volume. If the lowest energy in the data set corresponds to the smallest or largest volume, then the (E, V) data set does not include the minimum. Additional strained structures are then created until the (E, V) data includes a minimum or the maximum number of minimum check iterations is reached. The number of minimum check iterations can be set by including the following line in the aflow.in file:

[AFLOW_AGL]MAXCMITER=number

The default value for the maximum number of minimum position check iterations is 5.

14) Since multiple different volume calculations are performed for a given system, there is a certain amount of redundancy towards the failure of some of these calculations, and therefore options have been implemented within AGL to allow for the skipping of one or more failed run. Failed runs can be detected automatically (by the absence of the appropriate LOCK or OUTCAR file in the directory), and the option of whether or not to skip these runs can be set by including the following line in the aflow.in file:

[AFLOW_AGL]AUTOSKIPFAILEDARUNS=option

The default is "OFF" so that no runs are skipped automatically; instead detection of a failed run will cause AGL to exit with an error unless this particular run was explicitly listed to be skipped.

Specific runs can be listed for skipping by including the following line in the aflow.in file:

[AFLOW_AGL]SKIPFAILEDARUNS=directory_name_list

where "directory_name_list" is a string with the list of directory names containing the failed runs to be skipped by the AGL fitting algorithm. If there is more than one failed run, the individual directory names should be listed on the same line, separated by commas.

AGL only permits a certain number of runs to be skipped. The maximum number of runs permitted to be skipped can be set by including the following line in the aflow.in file:

```
[AFLOW_AGL]SKIPARUNSMAX=number
```

The default value is 7, so that up to seven runs can be skipped.

15) The AFLOW AGL method will automatically calculate the thermal conductivity at the acoustic Debye temperature and as a function of temperature using the equation originally derived by Slack (see Glen A. Slack, Solid State Physics 34, 1-75 (1979) for original method and C. Toher et al., Phys. Rev. B 90, 174107 (2014) and Phys. Rev. Materials 1, 015401 (2017) for more details; these references also describe the acoustic Debye temperature). This calculation is always switched on.

The thermal conductivity can also be calculated with this equation as a function of temperature using the equilibrium volume as a function of temperature by including the following line in the aflow.in file:

```
[AFLOW_AGL]KAPPAVOLUME=option
```

The thermal conductivity will be calculated using the equilibrium volume as a function of temperature for KAPPAVOLUME=ON, and the results are written to the file "AGL_thermal_properties_temperature_vol.dat". The default value is KAPPAVOLUME=OFF, which only calculates the thermal conductivity using the equilibrium volume at the acoustic Debye temperature.

The user can also provide values to AGL for the acoustic Debye temperature and the Gruneisen parameter to be used in calculating the thermal conductivity by including the lines:

```
[AFLOW_AGL]THETA_COND=number
[AFLOW_AGL]GRUNEISEN=number
```

If both of these lines are present, the thermal conductivity is calculated with the Slack equation using the values provided by the user, and the results are written in the "AGL_thermal_conductivity_user_lib.dat". This can be useful for comparing AGL results to values in the literature for the purpose of debugging and testing the AGL code.

16) The main output file for AFLOW AGL is aflow.agl.out. It contains the AGL results for the thermal conductivity at 300K, the traditional and acoustic Debye temperatures, the Gruneisen parameter, the heat capacities at constant volume (Cv) and constant pressure (Cp) at 300K, the thermal expansion at 300K, and the static and isothermal bulk modulus at 300K, as well as recording the source and value of the Poisson ratio used to calculate the Debye temperature. It also contains the results for the thermal conductivity, Debye temperature, Gruneisen parameter, heat capacity, thermal expansion and bulk modulus as function of temperature; and the Gibbs free energy, vibrational Helmholtz free energy, vibrational internal energy, and vibrational entropy as a function of temperature.

17) The AFLOW AGL method allows the user to choose whether or not to automatically create plots of the results for the Debye temperature, heat capacity, Gruneisen parameter, and vibrational free energy as a function of temperature; as well as the energies obtained from the DFT calculations as a function of volume per atom and volume per cell. These plots are in saved as different formats depending on the input given by the user. The plots are stored in the files <sysname>_debye_temperature.*, <sysname>_heat_capacity.*, <sysname>_gruneisen_parameter.*, <sysname>_vibrational_free_energy.*, <sysname>__energy_volume_atom.* and <sysname>__energy_volume_cell.*; where "*" is dependent on the format in which the files are saved and <sysname> is the name given to the material system being calculated. These results can be plotted by including the following line in the aflow.in file:

```
[AFLOW_AGL]PLOTRESULTS=option
```

If PLOTRESULTS=ON, then the plots are generated with gnuplot. The default option is
PLOTRESULTS=OFF so that no plots are generated. Which files are kept and which formats
are used to save the plots depends on the options used to run AFLOW. In particular,
the "--keep" option controls whether or not the gnuplot script ("--keep=gnuplot")
and the eps file ("--keep=eps") are saved instead of deleted. The plots can be saved
in other file formats including png, pdf, jpeg and gif using the options "--keep=png",
"--keep=pdf", "--keep=jpg" and "--keep=gif", respectively.

If [AFLOW_AGL]IEOS=-1 or [AFLOW_AGL]IDEBYE=-1, then the plotting of these properties
is skipped.

The AFLOW AGL method also allows the user to choose whether to write additional output
files. These additional output files include the file Debye_temperature.dat, which
writes the Debye temperature, heat capacity, vibrational free energy and Gruneisen
parameter as a function of temperature in a format which is easy to plot using commonly
available graphing software such as xmgrace. This file can be written by including the
following entry in the aflow.in file:

[AFLOW_AGL]WRITEFULLRESULTS=option

The additional output files are written if WRITEFULLRESULTS=ON. The default value is
WRITEFULLRESULTS=OFF, i.e. the additional output files are not written. When this option
is active, the values of the Debye temperature, heat capacity, vibrational free energy
and Gruneisen parameter at certain temperatures are written in the file Debye_summary.dat.
These temperature values correspond to methods most often used in the literature to
determine which temperature value is used for the Debye temperature or heat capacity being
reported. If [AFLOW_AGL]IEOS=-1 or [AFLOW_AGL]IDEBYE=-1, then the writing of these files
is skipped. The specific temperature values are determined as follows:

- Best fit of Debye temperature to heat capacity:
The first temperature value is determined from the value of the Debye temperature which
produces the best fit to the heat capacity curve calculated using AGL. The heat capacity
curve is fitted using the following equation:

$$c_V = 9 n k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D / T} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

Here, c_V is the heat capacity at constant volume, n is the number of atoms in the unit
cell, k_B is Boltzmann's constant, T is the temperature, and Θ_D is the Debye temperature.
This equation is the same as that given in equation 23.26 in Solid State Physics, Ashcroft and
Mermin (1976). The temperature value at which this value of the Debye temperature is produced
by AGL is also written, along with the heat capacity, vibrational free energy, and
Gruneisen parameter at this temperature.

- Temperature where heat capacity is half Dulong-Petit value
At high temperatures, the heat capacity tends to a limit given by $3 n k_B$, where n is the
number of atoms per unit cell and k_B is the Debye temperature. This is known as the
Dulong-Petit value. The second temperature value is determined from the point at which the
heat capacity is equal to half of this value, i.e. $1.5 n k_B$. This method was used to determine
the Debye temperatures listed in table 23.3 in Solid State Physics, Ashcroft and Mermin (1976).

- Minimum value of Debye temperature
The third temperature value used it that at which the Debye temperature calculated
using the AGL method is a minimum.

- Maximum value of Debye temperature
The fourth temperature value used it that at which the Debye temperature calculated
using the AGL method is a maximum.

- 300K (~room temperature)
The final temperature used is 300K, which corresponds approximately to room temperature.

Finally, the values of the Debye temperature, Gruneisen parameter and vibrational free
energy for the temperatures corresponding to the best fit to the heat capacity, the half
Dulong-Petit value of the heat capacity, and 300K (~room temperature), respectively, are
written in a script-parsable format in the file agllib.dat. The format used is

```
        the same as that used for the file aflowlib_entry.out.

18) The energy and mass density data as a function of temperature and pressure generated
    by AGL can be used calculate the Hugoniot relation for the material. It finds the energy (E)
    and mass density (rho) at each pressure (P) and temperature so that the following Hugoniot
    expression is true:

    E - E0 = 0.5 * (P + P0)*(1.0/rho0 - 1.0/rho)

    where E0, P0 and rho0 are the reference energy, pressure and mass density for the material
    (typically the values at room temperature and pressure). The Hugoniot relation can be
    calculated using AGL by including the following line in the aflow.in file:

    [AFLOW_AGL]HUGONIOTCALC=option

    If HUGONIOTCALC=ON, then the Hugoniot calculation is performed and the results are written
    to the file AGL_Hugoniot.out. The default option is HUGONIOTCALC=OFF so that no Hugoniot
    calculation is performed.

19) EXAMPLE:  CaO FCC with default AGL settings (note that this will give the same results if
    all of the "[AFLOW_AGL]" lines except "[AFLOW_AGL]CALC" are removed or commented out):

[AFLOW] ********************************************************************************************
[AFLOW] Test file for AGL calculation of CaO (fcc)
[AFLOW] ********************************************************************************************
[AFLOW] ********************************************************************************************
[AFLOW]SYSTEM=Ca1O1_ICSD_26959
[AFLOW] ********************************************************************************************
[AFLOW] input file for aflow
[AFLOW_MODE=VASP]
[AFLOW] ********************************************************************************************
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp46s]
[AFLOW] ********************************************************************************************
[AFLOW] ********************************************************************************************
[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE]NCPUS=MAX
[AFLOW_MODE_MPI_MODE]COMMAND ="mpirun -np"
[AFLOW_MODE_MPI_MODE]AUTOTUNE
[AFLOW_MODE_MPI_MODE]BINARY="mpivasp46s"
[AFLOW] ********************************************************************************************
[AFLOW_SYMMETRY]CALC
#[AFLOW_SYMMETRY]SGROUP_WRITE
#[AFLOW_SYMMETRY]SGROUP_RADIUS=7.77
[AFLOW] ********************************************************************************************
#[AFLOW_NEIGHBOURS]CALC
[AFLOW_NEIGHBOURS]RADIUS=7.7
[AFLOW_NEIGHBOURS]DRADIUS=0.1
[AFLOW] ********************************************************************************************
#[AFLOW_APL]CALC                                       // README_AFLOW_APL.TXT
[AFLOW_APL]ENGINE=DM                                   // README_AFLOW_APL.TXT
[AFLOW_APL]DISMAG=0.015                                // README_AFLOW_APL.TXT
[AFLOW_APL]MINATOMS=100                                // README_AFLOW_APL.TXT
#[AFLOW_APL]SUPERCELL=3x3x3                            // README_AFLOW_APL.TXT
[AFLOW_APL]DC=y                                        // README_AFLOW_APL.TXT
[AFLOW_APL]DPM=y                                       // README_AFLOW_APL.TXT
[AFLOW_APL]ZEROSTATE=y                                 // README_AFLOW_APL.TXT
[AFLOW_APL]DOS=y                                       // README_AFLOW_APL.TXT
[AFLOW_APL]TP=y                                        // README_AFLOW_APL.TXT
[AFLOW_APL]TPT=0:2000:10                               // README_AFLOW_APL.TXT
[AFLOW] ********************************************************************************************
#[AFLOW_QHA]CALC                                       // README_AFLOW_APL.TXT
[AFLOW_QHA]GP_VOL_DISTORTION_PERCENTAGE=0.03           // README_AFLOW_APL.TXT
[AFLOW_QHA]DISPLACEMENTS=y                             // README_AFLOW_APL.TXT
[AFLOW_QHA]PROJECTION_DIR=1:1:1                        // README_AFLOW_APL.TXT
```

```
[AFLOW_QHA]EOS=n                                          // README_AFLOW_APL.TXT
[AFLOW_QHA]EOS_VOLRANGE_DIST=-2:4:0.5                      // README_AFLOW_APL.TXT
[AFLOW_QHA]EOS_KPOINTS_MODE=32768:10000:20:100000          // README_AFLOW_APL.TXT
[AFLOW] ************************************************************************************
#[AFLOW_AAPL]CALC                                          // README_AFLOW_APL.TXT
[AFLOW_AAPL]TDMAG=0.015                                    // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUT_SHELL=4                                    // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUT_RAD=4.5                                    // README_AFLOW_APL.TXT
[AFLOW_AAPL]SUMRULE=1E-5                                   // README_AFLOW_APL.TXT
[AFLOW_AAPL]BTE=FULL                                       // README_AFLOW_APL.TXT
[AFLOW_AAPL]THERMALGRID=21x21x21                           // README_AFLOW_APL.TXT
[AFLOW_AAPL]ISOTOPE=y                                      // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUMULATIVEK=y                                  // README_AFLOW_APL.TXT
[AFLOW_AAPL]BOUNDARY=n                                     // README_AFLOW_APL.TXT
[AFLOW_AAPL]NANO_SIZE=100                                  // README_AFLOW_APL.TXT
[AFLOW_AAPL]TCT=200:700:20                                 // README_AFLOW_APL.TXT
[AFLOW] ************************************************************************************
#[VASP_RUN]RELAX_STATIC_BANDS=2                            // GENERATE | STATIC | RELAX=N | RELAX_STATIC=N | STATIC
#[VASP_FORCE_OPTION]NEGLECT_NOMIX
[VASP_FORCE_OPTION]CHGCAR=OFF                              // ON | OFF (default ON)
#[VASP_FORCE_OPTION]KPOINTS=keyword[,keyword]             // EVEN | ODD | KSHIFT_GAMMA_EVEN | KSHIFT_GAMMA_ODD | KS
[VASP_FORCE_OPTION]SYM=ON                                 // ON | OFF  (default ON)
[VASP_FORCE_OPTION]AUTO_PSEUDOPOTENTIALS=potpaw_PBE       // pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_P
[VASP_FORCE_OPTION]NBANDS                                 // Estimate Bands (better than VASP)
#[VASP_FORCE_OPTION]SPIN=ON,REMOVE_RELAX_1                 // (ON | OFF  (default ON)), REMOVE_RELAX_1 | _2
#[VASP_FORCE_OPTION]AUTO_MAGMOM=ON                         // ON | OFF (default OFF)
[VASP_FORCE_OPTION]RELAX_MODE=ENERGY                      // ENERGY | FORCES | ENERGY_FORCES | FORCES_ENERGY (defau
[VASP_FORCE_OPTION]PREC=HIGH                              // (LOW | MEDIUM | NORMAL | HIGH | ACCURATE), PRESERVED (
[VASP_FORCE_OPTION]ALGO=FAST                              // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (
#[VASP_FORCE_OPTION]NOTUNE
[VASP_FORCE_OPTION]TYPE=DEFAULT                           // METAL | INSULATOR | SEMICONDUCTOR | DEFAULT (default D
[VASP_FORCE_OPTION]CONVERT_UNIT_CELL=SPRIM                // SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART,
#[VASP_FORCE_OPTION]VOLUME+=10.0
#[VASP_FORCE_OPTION]VOLUME*=1.05
[AFLOW] ************************************************************************************
[AFLOW] ************************************************************************************
[VASP_INCAR_MODE_EXPLICIT]START
SYSTEM=Ca1O1_ICSD_26959
NELM = 120
NELMIN=2
LPLANE=.TRUE.
LREAL=.FALSE.
LSCALU=.FALSE.
#NBANDS=XX                                                # for hand modification
#IALGO=48                                                 # for hand modification
[VASP_INCAR_MODE_EXPLICIT]STOP
[AFLOW] ************************************************************************************
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE]KSCHEME=M
[VASP_KPOINTS_FILE]KPPRA=8000
[VASP_KPOINTS_FILE]STATIC_KSCHEME=M
[VASP_KPOINTS_FILE]STATIC_KPPRA=10000
[VASP_KPOINTS_FILE]BANDS_LATTICE=FCC
[VASP_KPOINTS_FILE]BANDS_GRID=20
[AFLOW] ************************************************************************************
[AFLOW_AGL]CALC
[AFLOW_AGL]AELPOISSONRATIO=OFF
[AFLOW_AGL]POISSON=0.25
[AFLOW_AGL]NTEMP=201
[AFLOW_AGL]NPRESSURE=11
[AFLOW_AGL]NSTRUCTURES=28
[AFLOW_AGL]STRAINSTEP=0.01
[AFLOW_AGL]WRITEGIBBSINPUT=OFF
[AFLOW_AGL]WRITEFULLRESULTS=OFF
[AFLOW_AGL]PLOTRESULTS=OFF
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[AFLOW_AGL]IEOS=0
[AFLOW_AGL]IDEBYE=0
[AFLOW_AGL]CHECKEVCONCAVITY=OFF
[AFLOW_AGL]CHECKMIN=OFF
[AFLOW_AGL]FITTYPE=0
[AFLOW] *******************************************************************************************
[VASP_POSCAR_MODE_EXPLICIT]START
Ca1O1 #225 - (Ca1O1_ICSD_26959) - Ca1O1 [Ca1O1] cF8 Fm-3m CaO 225 Ca1O1_ICSD_26959 ICSD_26959  (icsd library) (V
1.224745
    0.00000000000000    1.95061033183634    1.95061033183634
    1.95061033183634    0.00000000000000    1.95061033183634
    1.95061033183634    1.95061033183634    0.00000000000000
1 1
Direct(2) [A1B1]
    0.00000000000000    0.00000000000000    0.00000000000000  Ca
    0.50000000000000    0.50000000000000    0.50000000000000  O
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *******************************************************************************************
[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE]Ca
[VASP_POTCAR_FILE]O
[AFLOW] potpaw_PBE: Ca_sv O
[AFLOW] COMPOSITION_PP=|Ca_sv1|O1|
[AFLOW] COMPOSITION=|Ca1|O1|
[AFLOW] VOLUME(A^3)=|0|0|
[AFLOW] MASS(amu)=|40.08|15.9994|
[AFLOW] *******************************************************************************************
[AFLOW] Aflow automatically generated (aflow_avasp.cpp)
[AFLOW] *******************************************************************************************
[AFLOW] aflow/aconvasp/aqe/apennsy v(30793) in ICSD/FCC/Ca1O1_ICSD_26959
[AFLOW] *******************************************************************************************
[AFLOW] SELF-MODIFICATION
[AFLOW] Recycling CONTCAR of relax1
[AFLOW] *******************************************************************************************
[VASP_POSCAR_MODE_EXPLICIT]START
Ca1O1 #225 - (Ca1O1_ICSD_26959) - Ca1O1
1.224745
    0.00000000000000    1.97560216103176    1.97560216103176
    1.97560216103176    0.00000000000000    1.97560216103176
    1.97560216103176    1.97560216103176   -0.00000000000000
1 1
Direct(2) [A1B1]
    0.00000000000000   -0.00000000000000   -0.00000000000000
    0.50000000000000    0.50000000000000    0.50000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *******************************************************************************************
[VASP_FORCE_OPTION]SPIN=OFF      // Self Correction
[AFLOW] SELF-MODIFICATION
[AFLOW] Recycling CONTCAR of relax2
[AFLOW] *******************************************************************************************
[VASP_POSCAR_MODE_EXPLICIT]START
Ca1O1 #225 - (Ca1O1_ICSD_26959) - Ca1O1
1.224745
    0.00000000000000    1.97560216103176    1.97560216103176
    1.97560216103176    0.00000000000000    1.97560216103176
    1.97560216103176    1.97560216103176    0.00000000000000
1 1
Direct(2) [A1B1]
    0.00000000000000    0.00000000000000    0.00000000000000
    0.50000000000000    0.50000000000000    0.50000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *******************************************************************************************
```