

AFLOW V 3.1.111

```
*****
*
*          aflow - STEFANO CURTAROLO Duke University 2003-2017          *
*          High-Throughput ab-initio Computing Project                  *
*
*****
LATEST VERSION OF THE FILE:          materials.duke.edu/AFLOW/aflow_aconvasp.pdf
*****
```

AFLOW POSTPROCESSING MODE (formerly called aconvasp/aqe)

aflow --help [-h]

Gives Help information.

aflow --version | -v

Gives Version Information.

aflow --machine

Gives Machine Information.

aflow --check_integrity | --checki

Check the integrity of xlib functions

aflow --abccar < POSCAR | WYCCAR

Converts the POSCAR or WYCCAR in format.

POSCAR is the usual VASP file

WYCCAR is described as

TITLE

SCALE (positive (rescaling) negative (volume))

A B C ALPHA BETA GAMMA SG# [OPTION#]

#specie0 #specie1

DIRECT (or CARTESIAN)

.. specie0

.. specie0

..

.. specie1

.. specie1

and so on. (Stefano Feb 2009)

The positions of the species will be used with the list of

symmetry operations (aflow_wyckoff.cpp) to generate all the atoms.

aflow --abinit

Transforms the POSCAR (or whichever is the input file format) to a
ABINIT GEOM format.

The geometrical file follows the ABINIT convention.

aflow --aims

Transforms the POSCAR (or whichever is the input file format) to a
AIMS GEOM format.

The geometrical file follows the AIMS convention.

aflow --ace < POSCAR

Outputs to standard out a cell standard ASCII (ace) file

based on the POSCAR input file. This can be used as input

for CarIne.

aflow --use_aflow.in=XXX

Uses XXX instead of "aflow.in" in searching/running/operating directories.

The option is very useful for compounded calculations.

aflow --aflowin < POSCAR

Output the structure inside the strings:

[VASP_POSCAR_MODE_EXPLICIT]START

structure...

[VASP_POSCAR_MODE_EXPLICIT]STOP

which is useful if you want to recycle partially ran aflow.in !

```

aflow [options] --aflow_proto=label*:speciesA*[:speciesB*][:volumeA*[:volumeB*]|:volume] [--params=.... [--h
Creates automatic aflow.in.
OPTIONS are:
--usage
--potential=pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_PBE
--potential_complete
--missing
--noautopp
--kppra=NNNN (default DEFAULT_KPPRA) --kppra_static=NNNN (default DEFAULT_KPPRA_STATIC) --bands_grid=N
--enmax_multiply=NNNN (default: VASP_PREC_ENMAX_HIGH, VASP_PREC_ENMAX_ACCURATE)
--pressure=0,1,2 (string of kB pressures separated by commas)
--potim=XXX (default 0.05) (VASP)
--relax_mode=[ENERGY | FORCES | ENERGY_FORCES | FORCES_ENERGY] (default VASP_FORCE_OPTION_RELAX_MODE_S
--precision=[LOW | MEDIUM | NORMAL | HIGH | ACCURATE], PRESERVED] (default=VASP_FORCE_OPTION_PREC_SCH
--metagga=[TPSS | RTPSS | M06L | MBJL | SCAN | MS0 | MS1 | MS2 | NONE] (default=VASP_FORCE_OPTION_META
--ivdw=[number_for_VASP_see_manual_for_IVDW | 0] (default=VASP_FORCE_OPTION_IVDW_SCHEME_DEFAULT) (VASP)
--algorithm=[(NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED] (default=VASP_FORCE_OPTION_ALGO_SCHEME_DEFA
--type=[METAL | INSULATOR | SEMICONDUCTOR | DEFAULT] (default=VASP_FORCE_OPTION_TYPE_SCHEME_DEFAULT) (
--convert_unit_cell= (SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART, FRAC, PRES)
--volume_plus_equal=XXX
--volume_multiply_equal=XXX
--ldau2
--noldau2
--bands
--neglect_nomix
--stdout
--qe
--abinit
--aims
--list
--params=.... { check aflow --readme=anrl }
--hex          { check aflow --readme=anrl }

```

This command generates the directory: `./AFLOWDATA/speciesAspeciesB/label/` and create an `aflow.in` inside with the "label" structure from HTQC library project, with `speciesAs`, `speciesBs`, .. and the volumes per atoms, `volumeAs`, `volumeBs`, .. (real in \AA^3). Aflow generates a huge number, `#speciesAs*#speciesBs...#label[*#pressures]`, of directories containing all the combinations of `./AFLOWDATA/speciesAspeciesB../label:pressure` and so on. This is helpful for generating huge databases.

Be careful to include the various "`_pv`," "`_sv`," etc" in the species so that the POTCAR makes sense.

HIGH-THROUGHPUT NOTE: `label`, `speciesA`, `speciesB`, `volumeA`, `volumeB` can be multiple strings separated by commas without spaces in between such as

Note that that `--aflow_proto label A B ...` is not supported anymore and you now need to use `--aflow_proto=label:A:B... et cetera`.

LABEL

`label*` = string of `label1`, `label2`, `label3`, ... separated by commas ", "
specify which labels/prototypes to generate

SPECIES

`speciesA*` = string of `speciesA1`, `speciesA2`, `speciesA3`, ... separated by commas ", "
specify which species in position A to consider.

`speciesB*` = string of `speciesB1`, `speciesB2`, `speciesB3`, ... separated by commas ", "
specify which species in position B to consider.

similarly you can have `speciesC*`, `speciesD*`, and so on.

VOLUMES

`volumeA*` = string of `volumeA1`, `volumeA2`, `volumeA3`, ... separated by commas ", "
specify the volumes of `speciesAs`, the number must be identical to the number of `speciesAs` otherwise you get an error.

`volumeB*` = string of `volumeB1`, `volumeB2`, `volumeB3`, ... separated by commas ", "

specify the volumes of speciesBs, the number must be identical to the number of speciesBs otherwise you get an error. similarly you can have volumeC*,volumeD*, and so on. If you want to set one volume per atom, identical to all the species, then specify only one number as species...:volume .

USAGE

With --usage a brief syntax help comes out.

POTENTIALS

The user can specify the potential type.
--potential=pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_PBE
If not specified it takes potpaw_PBE and the standard default for the species.
With --potential_complete it creates the subdirectory containing the type and date of the potentials: i.e. Ti_sv => Ti_sv:PAW_GGA:07Sep2000
With the option --noautopp, then you have to be careful to include the various "_pv,_sv, etc" in the species so that the POTCAR makes sense.

MISSING

With the option --missing it creates automatic aflow.in only for the missing . structures of the database. It checks on:

\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB1))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB2))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB3))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB4))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB5))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB6))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICDS))/LIB/	of AFLOW_MATERIALS_SERVER
\$(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_AURO))/LIB/	of AFLOW_MATERIALS_SERVER

KPOINTS SPECIFICATION

With --kppra=NNN the user can specify a NNN number of kpoints per reciprocal atom.

PRESSURE CALCULATIONS

The user can run calculations under pressure by adding --pressure (kB).

--pressure=p0[,p1][,p1]...

Example

--pressure=10,20,30

Then the data will be generated as directories containing all the combinations of

./AFLOWDATA/specieAspecieB/label:P=p0/

./AFLOWDATA/specieAspecieB/label:P=p1/

The input file aflow.in will contain the correct PSTRESS=** entry

BANDS CALCULATIONS

The user can run bands by adding --bands

POTIM PARAMETER

For some systems VASP requires POTIM smaller than the default

0.5. See the VASP Manual.

RELAX_MODE

One of the RELAX_MODEs specified in the AFLOW manual (VASP only).

[ENERGY | FORCES | ENERGY_FORCES | FORCES_ENERGY] (default VASP_FORCE_OPTION_RELAX_MODE_SCHEME_DEFAULT)

PRECISION

One of the PRECISIONs specified in the AFLOW manual (VASP only).

[(LOW | MEDIUM | NORMAL | HIGH | ACCURATE), PRESERVED] (default=VASP_FORCE_OPTION_PREC_SCHEME_DEFAULT)

ALGORITHM

One of the ALGORITHMs specified in the AFLOW manual (VASP only).

[(NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED] (default=VASP_FORCE_OPTION_ALGO_SCHEME_DEFAULT)

TYPE

One of the TYPEs specified in the AFLOW manual (VASP only).

[METAL | INSULATOR | SEMICONDUCTOR | DEFAULT] (default=VASP_FORCE_OPTION_TYPE_SCHEME_DEFAULT)

CONVERT_UNIT_CELL

One of the CONVERSIONs specified in the AFLOW manual (VASP only).
[SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART, FRAC, PRES]

VOLUME CHANGES

Volume plus equal adds XXX to the current volume.
Volume multiply equal multiplies XXX to the current volume.

LDAU CALCULATIONS (FORCING IT ON AND OFF)

The user can run bands by adding --ldau2 and the code will take the default ldaul parameters that are specified inside aflow_avasp.cpp.
If you do not like them, you can modify the cpp code OR change the lines inside aflow.in
[VASP_FORCE_OPTION]LDAU2=ON
[VASP_FORCE_OPTION]LDAU_PARAMETERS=Bi,Li,Zn;1,-1,2;0,0,7.5;0,0,0 // species;Ls;Us;Js
For some reference systems, LDAU is taken by default. Then the user can remove it with --noldau.

MIXING (TO MIX OR NOT TO MIX)

Some systems is known to be no-mix, and they will be skipped from the calculations.
To override this automatism, specify --neglect_nomix .

STDOUT output

If you specify --stdout, aflow will not write the file but print on the screen.

QUANTUM ESPRESSO output

If you specify --qe, aflow will add QUANTUM ESPRESSO code to aflow.in (experimental).

ABINIT output

If you specify --abinit, aflow will add ABINIT code to aflow.in (experimental).

AIMS output

If you specify --aims, aflow will add AIMS code to aflow.in (experimental).

LIST output

If you specify --list, aflow will not generate the aflow.ins but only report the ones to be created (useful for scripting).

ANRL: AFLOW NAVAL RESEARCH LAB PROTOTYPE LIBRARY

With respect to the article:

Mehl et al., "The AFLOW Library of Crystallographic Prototype", <https://arxiv.org/abs/1607.02532>
the code gives the possibility to define the parameters of the cell --params=...
Some rhombohedral cells can be generated in hexagonal configurations (see the article).
The choice is performed with the flag --hex.
Check aflow --readme=anrl

aflow --aflow_proto=label[:]specieA[:]specieB[:]volume

Same as above but the volume per atoms are extracted from the most dense paw_pbe values (usually the ground state) and with the Vegard's law (Vegard's law is an approximate empirical rule which holds that a linear relation exists, at constant temperature, between the crystal lattice constant of an alloy and the concentrations of the constituent elements).

HIGH-THROUGHPUT NOTE: label, specieA, specieB can be multiple strings separated by commas without spaces in between such as label1,label2,label3 generate all the labels
specieA1,specieA2,specieA3 goes through all specieAs times all Bs
specieB1,specieB2 goes through all specieBs times all As
In this case aflow generates a huge number, #labels*#specieAs*#specieB of directories containing all the combinations of
./AFLOWDATA/specieA?specieB?/label?

and so on. This is helpful for generating huge databases.

PRESSURE, POTENTIALS, BANDS calculations are allowed, see above.
STDOUT option available.

```

//DX - START
aflow --aflowSG[_label,_number][=tolerance | =tight | =loose] < POSCAR
Calculates the space group of the crystal in the ITC convention.
No assumptions are made on the input POSCAR-- may be supercell, primitive, etc.
Gives the Bravais lattice, crystal system, point group, space group number and wyckoff set.
The origin choice is always the first choice in ITC 5th edition. This is the highest symmetry
choice. (However, for Monoclinic systems, different unique axes and cell choices are examined to
ensure a spacegroup is identified.) This routine consists of an adaptive tolerance; if any symmetry
rules are broken, the tolerance is changed and everything is recalculated.
Tolerance:
  The tolerance is given in Angstroms. There are two preset tolerances:
    tight: minimum_interatomic_distance/100.0
    loose: minimum_interatomic_distance/10.0
  The default tolerance is the "tight" tolerance value.
  A value can also be specified. (Note, it must be below the minimum
interatomic distance, otherwise an error will be thrown.)
Can be called inside aflow via:
  xstructure.SpaceGroup_ITC()          (default tolerance)
  xstructure.SpaceGroup_ITC(tol)      (user defined tolerance)
AFLOW counterpart to platonSG and findsymSG.
//DX - END

aflow --alphabetic < POSCAR
Makes the structure in alphabetic order (if possible).

aflow --alpha_compound=string1,string2,...
Makes the alphabetic "compound" from the name of string. For instance
aflow --alpha_compound=Zr15.6Ag2Mg14
returns Ag2Mg14Zr15.6
aflow --alpha_species=string1,string2,...
Makes the alphabetic "species" from the name of string. For instance
aflow --alpha_species=Zr15.6Ag2Mg14
returns AgMgZr

aflow --angle=cutoff < POSCAR
Outputs to standard out the angles for each atom triplet
made up of neighbors within a distance cutoff of each other.
Actually, since this can be huge, only the first MAX_NUM_ANGLE-1
neighbours within d are used. MAX_NUM_ANGLE=21 at present and
can be set in aflow_pflow_print.cpp

//CO - START
aflow --bader -D DIRECTORY
options:
  [ --usage ]
  [ --critical_points|--cp ]
  [ --calculate|--calc=bader|voronoi ]
  [ --nocalculate|--nocalc=bader|voronoi ]
  [ --partition|--part=neargrid|ongrid ]
  [ --refine_edge_method|--rem=-1|-2|-3 ]
  [ --reference|--ref=REF_FILE ]
  [ --vacuum|--vac=off|auto|DENSITY_THRESHOLD ]
  [ --terminate|--term=known|max ]
  [ --print_all=atom|bader|both ]
  [ --print_index|--print_idx=atom|bader|both ]
  [ --print_select_atom|--print_sel_atom=[LIST OR RANGE] ]
  [ --print_select_bader|--print_sel_bader=[LIST OR RANGE] ]
  [ --print_sum_atom=[LIST OR RANGE] ]
  [ --print_sum_bader=[LIST OR RANGE] ]
  [ --quiet|--q ]
  [ --consolidate_atoms2species|--a2s ]
  [ --remove_bader_atoms|--rba ]
  [ --jvxl_all_species|--jvxl=CUTOFF1,CUTOFF2...[:DOWNSAMPLE1,DOWNSAMPLE2,..]
|CUTOFF1[,DOWNSAMPLE1:CUTOFF2,DOWNSAMPLE2:...]]

```

```
                                [CUTOFF[,DOWNSAMPLE] ]
[ --keep=jvxl_only|--jvxl_only ]
  [ -D DIRECTORY ]
```

Perform Bader charge analysis by means of FORTRAN code from the Henkelman Group at UT, Austin. <http://theory.cm.utexas.edu/bader/>

DIRECTORY is the path to the data from VASP.

If this is omitted, it will assume the desired path is the one from which the command is called.

The following files are required to be present in DIRECTORY:

CHGCAR.static|CHGCAR

OUTCAR.static|OUTCAR

POSCAR.static|POSCAR

[AECCAR0.static|AECCAR0] } OR A CORRESPONDING REFERENCE CHARGE DENSITY FILE

[AECCAR2.static|AECCAR2] } (explained below)

though they can be compressed as .bz2 or .gz files.

Description of flags and, if applicable, corresponding bader code command:

--calculate=|--calc=bader|voronoi

--nocalculate=|--nocalc=bader|voronoi

[corresponding bader code command: -c | -n < bader | voronoi >]

Turn on [-c] or off [-n] the following calculations

bader: Bader atoms in molecules (default)

voronoi: population analysis based on distance

WARNING: If you specify --nocalc=bader without a --calc command, the bader code is not expected to produce any files.

It is sufficient to specify --calc=voronoi without --nocalc=bader.

EXPECTED FILES: ACF.dat, AVF.dat, BCF.dat, LABEL_abader.out (net charges and atomic volumes calculated from bader code).

--partition=|--part=neargrid|ongrid

[corresponding bader code command -b < neargrid | ongrid >]

Use the default near-grid bader partitioning or the original on-grid based algorithm.

--refine_edge_method=|--rem=-1|-2|-3

[corresponding bader code command -r < refine_edge_method >]

By default (-r -1) , only the points around reassigned points are checked during refinements. The old method, which checks every edge point during each refinement, can be enabled using the -r -2 switch:

A new weight method developed by Yu and Trinkle and be enabled with the -r -3 switch.

--reference=|--ref=REF_FILE

[corresponding bader code command -ref REF_FILE]

By default, AFLOW will sum the AECCAR0 and AECCAR2 to form the aflow.CHGCAR_sum file.

However, this can be overridden by specifying a desired reference file.

EXPECTED FILES: aflow.CHGCAR_sum

--vacuum=|--vac=off|auto|DENSITY_THRESHOLD

[corresponding bader code command -vac < off | auto | vacuum_density >]

Assign low density points to vacuum.

auto: vacuum density cutoff is 1E-3 e/Ang³ (by default in AFLOW)

off: do not assign low density points to a vacuum volume

DENSITY_THRESHOLD: a float designating the maximum density assigned to a vacuum volume

--terminate=|--term=known|max

[corresponding bader code command -m < known | max >]

Determine how trajectories terminate

known: stop when a point is surrounded by known points

max: stop only when a charge density maximum is reached

```

--print_all=atom|bader|both
[ corresponding bader code command -p < all_atom | all_bader > ]
    Print calculated volumes (containing charge above threshold of 0.0001 electrons)
        atom: all atomic volumes
        bader: all Bader volumes
EXPECTED FILES: BvAtxxxx.dat/Bvolxxxx.dat

--print_index=|--print_idx=atom|bader|both
[ corresponding bader code command -p < atom_index | bader_index > ]
    Print corresponding volume index
        atom: atomic volume index
        bader: bader volume index
EXPECTED FILES: AtIndex.dat/BvIndex.dat

--print_select_atom=|--print_sel_atom=[LIST OR RANGE]
[ corresponding bader code command -p sel_atom [LIST OR RANGE] ]
    Print specified atomic volumes.
    List or range corresponds to 1,2,3 (comma-separated) or 1-3 (hyphen-separated).
EXPECTED FILES: BvAtxxxx.dat

--print_select_bader=|--print_sel_bader=[LIST OR RANGE]
[ corresponding bader code command -p sel_bader [LIST OR RANGE] ]
    Print specified bader volumes.
    List or range corresponds to 1,2,3 (comma-separated) or 1-3 (hyphen-separated).
EXPECTED FILES: B_wexxxx.dat (artifact of bader code)

--print_sum_atom=[LIST OR RANGE]
[ corresponding bader code command -p sum_atom [LIST OR RANGE] ]
    Print sum of specified atomic volumes.
    Consider using aflow --chgsum command instead.
    List or range corresponds to 1,2,3 (comma-separated) or 1-3 (hyphen-separated).
EXPECTED FILES: BvAt_summed.at

--print_sum_bader=[LIST OR RANGE]
[ corresponding bader code command -p sum_bader [LIST OR RANGE] ]
    Print sum of specified bader volumes.
    Consider using aflow --chgsum command instead.
    List or range corresponds to 1,2,3 (comma-separated) or 1-3 (hyphen-separated).
EXPECTED FILES: Bvol_summed.at

--quiet|--q
    No output printed to screen.

--consolidate_atoms2species|--a2s
    Combine all atomic volumes to form species volumes.
EXPECTED FILES: BvAt_SPECIES.dat

--remove_bader_atoms|--rba
    Remove individual atomic volumes.
    Useful if you only want to keep species volumes.
    Only read if --a2s specified.

--jvxl_all_species=|--jvxl=CUTOFF1,CUTOFF2...[:DOWNSAMPLE1,DOWNSAMPLE2,...]
    |CUTOFF1[,DOWNSAMPLE1:CUTOFF2,DOWNSAMPLE2:...]|
    |CUTOFF[,DOWNSAMPLE]
    Generate .jvxl files of all species volumes at the specified cutoffs.
    A .jvxl file is a space-efficient file format for surface charges read by Jmol.
    See http://chemapps.stolaf.edu/jmol/docs/misc/JVXL-format.pdf.
    You may also specify a downsample ratio.
    This will reduce the number of points on the surface by the specified factor.
    You may produce multiple .jvxl files in the following ways:
        CYCLIC MODE (:):
            Every combination of cutoff [and downsample_ratio] will be produced
        SETS MODE (:):
            Provide sets of cutoff [and corresponding downsample_ratio] to be produced

```

WARNING: while you may specify a cutoff of arbitrary precision, the label of the output file will only show precision to the nearest hundredth.
EXPECTED FILES: LABEL_Bader_CUTOFF_DOWNSAMPLE_RATIO_SPECIES.jvxl

--keep=jvxl_only|--jvxl_only
After producing .jvxl files, remove atomic and species volume files.
Only read if --jvxl specified.

NOTE:

Multiple print command can be issued, with the exception of:
--print_all=atom && --print_sel_atom=[LIST OR RANGE]
--print_all=bader && --print_sel_bader=[LIST OR RANGE]
By default, the program will ignore the latter command and only execute the former (--print_all).

All CHG files printed from bader code will have its header amended so that it may be read by Jmol.
See --prepare_chgcar_4_jmol command for more information.

Bader Charge code reference:

<http://theory.cm.utexas.edu/henkelman/code/bader/>

W. Tang, E. Sanville, and G. Henkelman. J. Phys.: Condens. Matter 21, 084204 (2009).

E. Sanville, S. D. Kenny, R. Smith, and G. Henkelman. J. Comp. Chem. 28, 899-908 (2007).

G. Henkelman, A. Arnaldsson, and H. Jonsson. Comput. Mater. Sci. 36, 254-360 (2006).

//CO - END

aflow --bandgap=bands_directory

Calculates the energy gap and band edges of a material by looking at the occupancies in the OUTCAR file
On output it produces the following background system information:

System : The system name, identical to the SYSTEM tag in the OUTCAR.
Spin tag : Whether it is a spin polarized / unpolarized calculation.
Fermi level : Obtained from the E-fermi tag in the OUTCAR.

The energy gap (Egap) and band edges (Valence Band Top, VBT, and Conduction Band Bottom, CBB) are then output in table format, with 5 significant figures.

Unpolarized example:

	VBT	CBB	Egap	Type
Net Result :	0.0000e+00	0.0000e+00	+0.0000e+00	insulator_direct

Polarized example:

	VBT	CBB	Egap	Type
Majority Spin :	0.0000e+00	0.0000e+00	0.0000e+00	insulator_indirect
Minority Spin :	-1.0000e+00	-1.0000e+00	-1.0000e+09	metal
Net Result :	0.0000e+00	0.0000e+00	0.0000e+00	insulator_direct

Special for metallic materials: the edges are arbitrarily set to -1 and the gap is arbitrarily set to -1.0E-09. The "Net Result" is the overall gap and edges of the system. Note that the band edges have been referenced to the Fermi energy.

Sample output for a Spin-polarized material, Te4V5_ICSD_42881:

System : Te4V5_ICSD_42881
Spin tag : 2
Fermi level : 5.3880e+00

	VBT	CBB	Egap	Type
Majority Spin :	-4.0090e-01	+3.6820e-01	+7.6910e-01	insulator_indirect
Minority Spin :	-8.6570e-01	+3.5710e-01	+1.2228e+00	insulator_direct
Net Result :	-4.0090e-01	+3.5710e-01	+7.5800e-01	insulator_indirect

aflow --bandgaps < dirlist

Similar to --bandgap, the directories of bands runs are stored in file "dirlist", one directory per line (see also --calculated=bandgaps)


```

aflow --bands=PROOUT < POSCAR
  Outputs the up and down bands to band.up.out and band.dn.out.
  Format is
  k-space path length (true, fractional), bands (up or down),
  nkpt, kx, ky, kz
  Uses data in PROOUT file. Uses POSCAR to get lattice to calculate
  true recipricol distances. Must run vasp with LORBIT=2 to get
  the PROOUT file.

aflow --bs | --band_structures
  Given a calculation with all the parts (static,bands) creates the
  subdirectory BANDS with the band structures files.

aflow --bzdirections | --bzd < POSCAR
  Calculates lattice and print a nice looking KPOINTS in VASP format.

aflow --bzdirections= | --bzd=LATTICE
  Print a nice looking KPOINTS in VASP format for one of the lattices,
  where the lattices are in their conventional-primitive form (kpoints
  are fractional of the reciprical lattice of the CONVENTIONAL primitive).
LATTICES = (the ones with "")
1. TRI order: kalpha,kbeta,kgamma > 90 (kgamma<kalpha, kgamma<kbeta)
   or kalpha,kbeta,kgamma < 90 (kgamma>kalpha, kgamma>kbeta)
   special case when kgamma=90
   "TRI1a" kalpha>90 kbeta>90 kgamma>90
   "TRI1b" kalpha<90 kbeta<90 kgamma<90
   "TRI2a" kalpha>90 kbeta>90 kgamma=90
   "TRI2b" kalpha<90 kbeta<90 kgamma=90
2. "MCL" unique (order b<=c)
3. MCLC (order alpha<90)
   "MCLC1" kgamma>90
   "MCLC2" kgamma=90
   "MCLC3" kgamma<90, b*cos(alpha)/c + (b*sin(alpha)/a)^2 < 1
   "MCLC4" kgamma<90, b*cos(alpha)/c + (b*sin(alpha)/a)^2 = 1
   "MCLC5" kgamma<90, b*cos(alpha)/c + (b*sin(alpha)/a)^2 > 1
4. "ORC" unique (order a<b<c)
5. "ORCC" unique (order a<b)
6. ORCF (order a<b<c)
   "ORCF1" "ORCF_invb2+invc2<inva2" for 1/a^2 > 1/b^2 + 1/c^2
   "ORCF2" "ORCF_inva2<invb2+invc2" for 1/a^2 < 1/b^2 + 1/c^2
   "ORCF3" for 1/a^2 = 1/b^2 + 1/c^2
7. "ORCI" unique (order a<b<c)
8. "TET" unique (order a a c)
9. BCT (order a a c)
   "BCT1" "BCT_c<a" for c<a
   "BCT2" "BCT_c>a" for c>a
10. "RHL1" alpha<90
    "RHL2" alpha>90
11. "HEX" unique (order 60 90 90)
12. "CUB" unique
13. "FCC" unique (order 60 60 60)
14. "BCC" unique

aflow --BZmax < POSCAR
  Calculates the distance between high-symmetry K points and Gamma point
  in the reciprocal space, and sorts them.

aflow --bzplot | --plotbz < POSCAR
  Reads POSCAR from stdin and makes brillouin zone image file "bzplot.eps" and "bzplot.png".
  The data for plotting is saved in bzplot.dat and the script to make the plot is saved in plotbz.sh.
  plotbz.sh can be modified by hand to make further adjustment of the figure.
aflow --bzplotdata < POSCAR > bzplot.dat
  Reads POSCAR and generates data for brillouin zone and kpath plotting.
  The data is outputted to stdout (cout).

```

```

aflow --bzplotuseKPOINTS=KPOINTS < POSCAR
aflow --bzplotdatauseKPOINTS=KPOINTS < POSCAR > bzplot.dat
    Analogous to --bzplot and --bzplotdata respectively, however the first word of the first line
    in KPOINTS file is used as the str_sp.bravais_lattice_variation_type to get the kpath (as opposed to
    doing --sp of the POSCAR).

aflow [--np=NP] --cages[=roughness] < POSCAR
    Returns the center, radius and coordination (with atoms number)
    of the cages for interstitial defects (SC Nov07).
    It prints all the cages generated by putting spheres between
    four, three and two points, stable and metastable respectively.
    After finding all the cages (REDUCIBLE) the algorithm removes the
    ones symmetrically equivalent (by using the space group calculated
    at the beginning). The cages that are worth simulating are the
    IRREDUCIBLE ones.
    Radius is the radius includeing the scale.
    P is the number of points used to find the sphere.
    C is the coordination of the sphere (the number of atoms on its
    surface, from radius to radius+roughness.
    T is the label of the irreducible cage. You can see in the last
    part of the output the lables of the reduced cages.
    NOTES: If you specify "--np=NP", a concurrent number of NP posix
    threads will be started to speed the calculation in a multicpu-
    multicore environent.

aflow --calculated=icsd --random
    Print one of the available calculated directories (usefull for webs).
aflow --calculated[=[=]all|icsd|lib1|lib2|lib3|lib4|lib5|lib6|auro]
    "all": print the total number of calculations in the databases.
    "icsd": print the list of calculated ICSD-structures.
    "lib1": print the list of calculated pure systems.
    "lib2": print the list of calculated binary systems.
    "lib3": print the list of calculated ternary systems (magnetic, Heusler projects, etc.)
    "lib4": print the list of calculated quaternary systems (very few)
    "lib5": print the list of calculated quaternary systems (very few)
    "lib6": print the list of calculated quaternary systems (very few)
    "auro": print the list of calculated auro database system.

aflow --cart [-c] < POSCAR
    Outputs to standard out a new POSCAR file with atom
    positions in cartesian coordinates.
aflow --chgcar2jvxl|--c2j=CHGCAR1[,CHGCAR2,...]::CUTOFF1,CUTOFF2...[::DOWNSAMPLE1,DOWNSAMPLE2,...]
    |CHGCAR1,CUTOFF1[,DOWNSAMPLE1:CHGCAR2,CUTOFF2[,DOWNSAMPLE2:...]]
    |CHGCAR,CUTOFF[,DOWNSAMPLE]

options:
    [ --usage ]
    [ --output=|--o= ]

Converts a surface data file (e.g. CHGCAR file) to a .jvxl file at a specified cutoff.
See http://chemapps.stolaf.edu/jmol/docs/misc/JVXL-format.pdf.
You may also specify a downsample ratio.
This will reduce the number of points on the surface by the specified factor.
You may produce multiple .jvxl files in the following ways:
    CYCLIC MODE (::)
        Every combination of cutoff [and downsample_ratio] will be produced
    SETS MODE (:)
        Provide sets of cutoff [and corresponding downsample_ratio] to be produced
    You may specify the name of the output file (ending with .jvxl) ONLY if sets are provided.
    WARNING: while you may specify a cutoff of arbitrary precision, the label of the
    output file will only show precision to the nearest hundredth.
aflow --chgdiff=CHGCAR1,CHGCAR2
options:
    [ --usage ]
    [ --output=|--o=CHGCAR_OUT ]

```

This takes the difference between two CHGCAR files, outputting CHGCAR1-CHGCAR2. The output is in the form of a vasp46s CHGCAR. The output file is aflow_CHGDIFF.out (unless otherwise specified).

```
aflow --chgsum=CHGCAR1,CHGCAR2,...
options:
  [ --usage ]
  [ --output=|--o=CHGCAR_OUT ]
```

This finds the sum between two or more CHGCAR files. The output is in the form of a vasp46s CHGCAR. The output file is aflow_CHGSUM.out (unless otherwise specified).

```
aflow --chgint CHGCAR
Outputs to standard out the integrated charge density around every atom. The total integrated density within the Voronoi volume is given for each atom. The code also calculates the integrated density in a surrounding sphere for each atom. This is output as a function of radius for radii from 0 to 3 angstrom in steps of 0.1 angstrom. The total,Up-Dn,Up,Dn charges are all integrated although for non-spin polarized calculations only the first gives new information. The code works on all the recent versions of vasp we have tried but they seem to change the CHGCAR formatting sometimes so it may crash on different versions (at least 4.4.1 and 4.4.5 (including PAW) work). For a large cell this can take a while (e.g., 80 atoms might take ~20 minutes). vasp4631 ok.
```

```
aflow --cif < POSCAR
Outputs to standard out a Crystallographic Information File (cif) format file based on the POSCAR input file. This can be used as input for Mercury, and is the preferred format in Gerd's structure collection.
```

```
aflow --clat=a,b,c,alpha,beta,gamma
Outputs to standard out the cartesian lattice vectors obtained from the input a b c alpha beta gamma.
```

```
aflow --clean --DIRECTORY=DIRECTORY
Cleans the directory, like aflow --clean --DIRECTORY=DIRECTORY
```

```
aflow --clean_all < LIST_DIRECTORIES
Cleans all the directories. Be careful !
(if the LIST_DIRECTORIES contain aflow.in and LOCK the substring gets removed to help the search).
```

```
aflow --cluster-expansion=... | --ce=structure_type,A,B,EA,EB
--ce structure_type A B formation_energy_A formation_energy_B
Cluster expansion
structure_type: fcc/bcc/hcp
A, B: element names
EA, EB: formation energy of pure element A and B
```

```
aflow --cluster=structure_type,atom_num_min,atom_num_max,neighbour_min,neighbour_max
Get clusters
atom_num_min, atom_num_max : minimum and maximum numbers of atoms in a cluster
neighbour_min, neighbour_max : minimum and maximum nearest neighbour pairs including in a cluster
```

```
aflow --cmp_str POSCAR1 POSCAR2 rcut
This compares the characteristics of two POSCAR files and is useful for determining if the files are the same. Characteristics compared include number of atoms, number of types, total volume, volume per atom, lattice parameters, number of neighbours of each pair type out to rcut, differences in bond lengths for neighbours of each pair type out to cutoff, and space groups. For rcut<0 the
```

```

    cutoff is set to 4*(Wigner-Seitz radius of each atom) (this is the
    radius such that num atom spheres occupies the whole volume).
aflow --compare=a,b,c,d,e,f,g,h,k,j,i,l
Outputs to standard output the % comparison between
a#g b#h c#k d#j e#i f#l in %
    cout << abs(a1-a7)/((a1+a7)/2.0) << ;
    cout << abs(a2-a8)/((a2+a8)/2.0) << ;
    cout << abs(a3-a9)/((a3+a9)/2.0) << ;
    cout << abs(a4-a10)/((a4+a10)/2.0) << ;
    cout << abs(a5-a11)/((a5+a11)/2.0) << ;
    cout << abs(a6-a12)/((a6+a12)/2.0) << ;
    cout << endl;
Useful with y-ndata to compare % relaxations.

    aflow --compare_material=POSCAR_1,POSCAR_2 [--np=xx] [--print]
Compares POSCAR_1 to POSCAR_2 if the ratios are commensurate
and types of atoms are the same (i.e. same material).
POSCARs must be in the same directory you are running in.
[--np=xx] : Number of processors (default 8). Algorithm is thread-friendly.
[--print] : (For two at a time only.) Prints comparison data.
    Check aflow --readme=compare

    aflow --compare_structure=POSCAR_1,POSCAR_2 [--np=xx] [--print]
Compares POSCAR_1 to POSCAR_2 (no requirement on type of atoms,
just stoichiometry ratios). POSCARs must be in the same
directory you are running in.
[--np=xx] : Number of processors (default 8). Algorithm is thread-friendly.
[--print] : (For two at a time only.) Prints comparison data.
    Check aflow --readme=compare

    aflow --compare_material_directory|--compare_material_dir [-D "PATH"] [--np=xx]
Determines the unique materials (same atomic species)
within a given directory. Returns a JSON and TXT file with the
results. Default Directory: "."
[-D "PATH"] : User can specify a specific directory to compare.
    Output will be placed there also.
[--np=xx] : Number of processors (default 8). Algorithm is thread-friendly.
    Check aflow --readme=compare

    aflow --compare_structure_directory|--compare_structure_dir [-D "PATH"] [--np=xx]
Determines the unique structure prototypes within a given directory.
Returns a JSON and TXT file with the results. Default Directory: "."
[-D "PATH"] : User can specify a specific directory to compare.
    Output will be placed there also.
[--np=xx] : Number of processors (default 8). Algorithm is thread-friendly.
    Check aflow --readme=compare

//CO - START
aflow --convex_hull|--chull --alloy=MnPdPt[,AlCuZn,...] [chull_options] [--path=[DIRECTORY]]
Queries the AFLOW API for relevant entries (see --load_library), calculates
the convex hull, and returns the information as a PDF (default, see --output).
--chull : Necessary flag for entering mode for calculating convex hull.
--alloy : Necessary argument, specifies system. This code is not dimension specific,
    i.e., you can calculate the convex hull for any n-ary system.
[--path=[DIRECTORY]] : Optional argument, specify the directory for the output.
    Default is "./".
[--usage] : Returns usage commands and options.
[--output=|--o=latex|pdf|json|text] : Select the output format. Latex/PDF are the same (.pdf).
    JSON and plain text have the following extensions: .json and .txt.
    Default is Latex/PDF.
[--image_only|--imageonly|--image] : Latex/PDF output mode only. Similar to --document_only,
    but the image dimensions are not necessarily for a standard page. Preferred option for
    importing into papers/presentations.
[--no_document|--nodocument|--no_doc|--nodoc|--full_page_image|--fullpageimage] :
    Latex/PDF output mode only. Exclude the report from the output. Differs from image only

```

in that the convex hull illustration will be formatted for a standard page (8.5x11in). This is good when generating lots of images that need to be the same size.

[--document_only|--documentonly|--doc_only|--doonly|--doc] : Latex/PDF output mode only.

Exclude convex hull illustration. This is the default for quaternary systems and above.

[--stability_criterion|--stabilitycriterion|--stable_criterion|--scriterion|--sc=aflow:bb0d45ab555b] : Calculates the stability criterion of the ground state structure. Will return a warning if structure is not a ground state one. It removes the point from the hull, calculates the new hull, and calculates the distance of this point from below/above (Hf/Ts) hull.

[--equilibrium_phases|--equilibriumphases|--ep] : For each ground state structure, print the equilibrium phases that contain it. Very useful for determining which structures are in N-phase equilibrium. In essence, it is the text-version of the convex hull.

[--keep_log|--keeplog|--log] : Prints a log file of relevant output.

LOADING OPTIONS:

[--load_library|--loadlibrary|--ll=icsd|lib1|lib2|lib3] : Specify libraries from which to load. Default: icsd, lib2, and lib3.

[--neglect|--ban=aflow:bb0d45ab555bc208,aflow:fb9eaa58604ce774] : Ban specific entries from the convex hull calculation, done by AUID.

[--see_neglect|--seeneglect|--sn] : Show why entries were neglected.

[--remove_extreme_points|--removeextremepoints|--remove_extrema|--rep=-1000] : Exclude points based on Hf/Ts (floor/ceiling). Units are meV/atom / K.

[--entropic_temperature|--entropictemperature|--entropemp] : Calculate the Ts convex hull (upper-half). Default is Hf hull (lower-half).

[--ldau] : Only include points with LDAU. Hulls cannot contain mix LDAU character.

[--force_output|--forceoutput|--fo] : By default, the convex hull calculation will quit if it does not identify any ground state structures. This flag will override the program exit and still produce an output file.

[--load_entries_entry_output|--loadentriesentryoutput|--leo] : Get full output for all entries loaded from the AFLOW API.

[--load_API|--load_api|--loadapi|--lapi|--api] : Force loading entries from the API (default unless on nietzsche, aflowlib, or habana).

GENERAL PLOTTING OPTIONS:

[--keep_tex|--keeptex|--tex] : Latex/PDF output mode only. Will keep latex .tex and put it in --path=[DIRECTORY].

[--plot_offhull|--plotoffhull|--offhull=true|false] : Plot off hull compounds. Will not plot unstable explicitly asked by --unstable flag. By default, is true for 2D systems, false for 3D systems.

[--unstable] : Plot unstable points (above/below 0 Hf/Ts).

[--filter_by_z|--filterbyz|--fz=200] : Latex/PDF output mode only. Similar to --remove_extreme_points but this will only remove points from the convex hull illustration, but still include them in the plot.

[--filter_by_distance|--filterbydistance|--f_dist|--fdist|--fd=200] : Latex/PDF output mode only. Similar to --filter_by_z, but will filter based on distance from convex hull, and not Hf/Ts.

[--include_endpoints|--includeendpoints] : Latex/PDF output mode only. Include endpoints in the convex hull illustration. Default is off.

[--no_color_gradient|--nocolorgradient|--noccg] : Latex/PDF output mode only. Turns off all colors.

[--labels=both|none|off|compound|prototype] : Latex/PDF output mode only. Labels for compounds on the convex hull illustration. Default is compound. You can change to prototype, both (compound::prototype), or none/off.

[--plot_reduced_composition|--plotreducedcomposition|--plot_reducedcomposition|--rc=true|false] : Latex/PDF output mode only. Show reduced composition label. By default, this is false for 2D systems, true for 3D systems.

[--labels_off_hull|--labelsoffhull] : Latex/PDF output mode only. Similar to --labels, but for non ground state structures.

[--meta_labels|--metalabels] : Latex/PDF output mode only. Include metadata in the labels on the convex hull illustration. This includes Hf, Ts, and distance to hull.

[--no_hyperlinks|--nohyperlinks] : Latex/PDF output mode only. Turn off all hyperlinks to websites.

[--no_links|--nolinks] : Latex/PDF output mode only. Turn off all links from the convex hull illustration to the report.

[--kill_all_links|--killalllinks|--kal] : Latex/PDF output mode only. Turn off all links/hyperlinks.

[--large_font|--largefont|--large|--lf] : Latex/PDF output mode only. Prints a "larger" font size for convex hull illustration.

[--helvetica_font|--helveticafont|--helvetica] : Latex/PDF output mode only. Change font to helvetica.

`--no_bold_labels|--noboldlabels|--nobl` : Latex/PDF output mode only. Turn off any bold font.
`--no_rotate_labels|--norotatelabels|--norl` : Latex/PDF output mode only. Labels are rotated for space (default). This flag turns that option off.
`--composition_header_report|--compositionheaderreport|--composition_header|--compositionheader` : Latex/PDF output mode only. In the report, will print out stoichiometry group headers (compounds) with fractional compositions. Default is to show compositions in reduced form (reduced by greatest common multiple).
`--compounds_column_report|--compoundscolumnreport|--compounds_column|--compoundscolumn|--compound_colu`
 Latex/PDF output mode only. Include a column for the compound name. Compounds are grouped by stoic but each prototype will have a different atom count.
`--small_banner|--smallbanner|--sb` : Latex/PDF output mode only. Does not include AFLOW logo, count and date on the convex hull illustration.
`--no_banner|--nobanner|--nob` : Latex/PDF output mode only. Turns off banner information.
`--no_aflow_logo|--noaflowlogo|--noal` : Latex/PDF output mode only. Prints text logo instead of PDF va
`--latex_output|--latexoutput` : Latex/PDF output mode only. See full latex output.
 Good for troubleshooting.
`--latex_interactive|--latexinteractive` : Latex/PDF output mode only. Allows you to interact with latex as it compiles. Good for troubleshooting.

2D PLOTTING OPTIONS:

`--reverse_axis|--reverseaxis|--ra|--flip_axes|--flipaxes|--fa` : Latex/PDF 2D output only.
 Flips the top and bottom axes and reverse the order of the points.

3D PLOTTING OPTIONS:

`--no_color_bar|--nocolorbar|--nocb` : Latex/PDF output mode only. Hides color bar, but keeps colors.
`--no_heat_map|--noheatmap|--nohm` : Latex/PDF output mode only. Turns off colors from facets, but keep points colored.
`--no_color_ternaries|--nocolorternaries|--nocts` : Latex/PDF 3D output mode only. Ternary labels are black (not white).
`--color_ternaries_yellow|--colorternariesyellow|--cty` : Latex/PDF 3D output mode only. Ternary labels are white by default. This makes them yellow.
`--light_contrast|--lightcontrast|--lcl` : Latex/PDF output mode only. Modifies the convex hull illustration color scheme to be lighter.
`--hull_drop_shadow|--hulldropshadow|--hull_dropshadow|--dropshadow` : Latex/PDF 3D output mode only. Changes facet lines to be thin, white lines with thicker black background. Default is off (thick black facet lines).
`--draw_all_facet_lines|--drawallfacetlines|--daf1` : Latex/PDF 3D output mode only. Facet lines are only drawn if they have not already been drawn (overlapping lines) by default. This flag will draw all facet lines. Helpful if manipulating .tex file.

//DX - END

`aflow --corners | --corner < POSCAR`

Add to the POSCAR the corner and face atoms so it looks good when you plot the unit cell with rasmol/jmol and so on.. This option is just for visualization and should not be used to transform POSCARS to run. You will get super-imposed atoms!

`aflow --data < POSCAR`

Outputs to standard out basic data about the structure in the POSCAR input file. Output includes volume, a b c alpha beta gamma, reciprocal lattice, reciprocal lattice volume.

`aflow --data1=rcut < POSCAR`

This is basically like `cmp_str` except that it works on 1 str. Slightly different data is given: No space groups, All bond lengths.

`aflow --data2 < POSCAR`

Outputs to standard out basic data about the structure in the POSCAR input file. Similar to `--data` but with another style (SC).

`aflow --debye=THERMO`

Usage: `aflow --debye=THERMO[bz2]`

Fits Debye temperature to heat capacity data in THERMO or THERMO.bz2 file as calculated using APL. Writes results to file `debye_temperature.dat` and plots results in `debye_temperature.png`. Also calculates value for Debye temperature which best fits all heat capacity data in the range given in the THERMO file, and writes this value in the file `debye_temperature.dat`.

See Ascroft & Mermin, Solid State Physics, equation 23.26 for expression for heat capacity in terms of θ_D . The following files must reside in DIRECTORY as in the AFLOW written form or as .bz2 compressed files.

THERMO
aflow.in

The aflow.in file is used to determine the number of atoms per unit cell.
If the files are found in .bz2 form, the compressed files are preserved and temporary files are written and deleted.
The generation of the THERMO file is controlled by the command
[AFLOW_APL]TP
See README_APL, especially 3). for more details.

aflow --diff=POSCAR1,POSCAR2
Gives the difference in energy of the two structures within the PARTIAL OCCUPATION force field.

aflow --disp=cutoff < POSCAR
Outputs to standard out the displacement from each atom to all neighbors within a distance cutoff. Also gives which unit cell the neighbour is in.

aflow --dist=cutoff < POSCAR
Outputs to standard out the distances for each atom to all neighbors within a distance cutoff. Also gives which unit cell the neighbour is in.

aflow --delta_kpoints=number < POSCAR [or --dkpoints=number | -dkpoints=number | -dk=number]
Gives the k1,k2,k3 so that the delta_kappa is less-equal than "number"
See also --kpoints.

aflow --edata < POSCAR
Outputs to standard the information given by --data in addition to lattice-, superlattice- and reciprocal-lattice types.

aflow --edos ispin
ispin(1=nonspin,2=spin), Outputs to standard out the DOS, format:
Energy DOSup DOSdown
The integrated DOS is not outputted since it can be calculated from the energy bins and DOS. Needs DOSCAR and POSCAR files. DOS for spin down is given in (negative) sign.
See also --kband

aflow --edos ispin s d
aflow --edos ispin d s
See --edos. Outputs total DOS and DOS of orbital s and d. The sDOS or dDOS is per species as given in POSCAR. Output format:
Energy DOSup DOSdown s_up_spec1 s_down_spec1...s_up_specN s_down_specN d_up_spec1 d_down_spec1...d_up_specN

aflow --equivalent | --equiv | --iatoms < POSCAR
Calculate point/factor/space group and use them to label equivalent and inequivalent atoms. On the output, each structure atom has number_label_of_atom[equivalent_to_label]* (* if inequivalent).
(SC1107).

aflow --eigcurv=bands_directory
Perform a graph decomposition of the BZ paths found in a BANDS calculation into component vertices and edges. These are then organized into a data structure that contains information on the branching associated with each edge in the graph. Once this is in place, short walks are performed along these edges and their branches for the purpose of detecting maxima and minima in the band structure, as well as their corresponding curvatures. The curvatures are currently calculated using the 5 point central difference approximation,
 $f''(f) = (-f_1+16f_2-30f_3+16f_4-f_5)/(12h^2)$
which has an O(4) error. Note that the curvatures are not reliable, given that angular information is lost in the vicinity of the vertices.

aflow --effective-mass | --em directory_name
Calculate the carrier effective masses.
If the data is generated by aflow, DOSCAR.static, POSCAR.static, and EIGENVAL.static are used. Otherwise, DOSCAR, POSCAR, and EIGENVAL are used.
Output format:
compound_name
1. Band index:
Carrier type:
Carrier Spin:
Effective masses along principle axes (m0):

```

    Number of equivalent valleys:
    DOS effective mass (m0):
    DOS electron effective mass (m0): {me_spin_up, me_spin_down}
    DOS hole effective mass (m0): {mh_spin_up, mh_spin_down}

aflow --enum | --multienum < POSCAR
    Call MULTIENUM and convert a POSCAR with partial occupation into regular POSCARs.

aflow --enumsort | --multienumsort < POSCAR
    Call MULTIENUM and convert a POSCAR with partial occupation into regular POSCARs, and sort POSCARs using

aflow --ewald[=eta] < POSCAR
    Finds the electrostatic energy of the POSCAR file using the
    Ewald sum. Charges must be entered after each atom position.
    E.g., Co 0.00 0.00 0.00 +2. This is easy to do using the --names
    option. Eta is a real space screening parameter. Setting
    eta<=0 or leaving it out will cause aflow to choose it
    automatically (and hopefully optimally). Eta->0 is no
    screening and the Ewald reciprocal term will be zero. Eta->inf
    is total screening and the Ewald real term will be zero. The
    Ewald sum itself should always be the same and eta will only
    affect the efficiency of the calculation.

aflow --extract_kpoints | --xkpoints aflow.in
    Extract to stdout the kpoints embedded in the aflow.in file.
    Useful for scripting (SC0209).
aflow --extract_incar | --xincar aflow.in
    Extract to stdout the incar embedded in the aflow.in file.
    Useful for scripting (SC0209).
aflow --extract_poscar | --xposcar aflow.in
    Extract to stdout the poscar embedded in the aflow.in file.
    Useful for scripting (SC0209).
aflow --extract_potcar | --xpotcar aflow.in
    Extract to stdout the potcar embedded in the aflow.in file.
    Useful for scripting (SC0209).
aflow --extract_symmetry | --xsymmetry aflow.in
    Extract the symmetry (pgroup,fgroup,iatoms) from the poscar
    embedded in the aflow.in file. Must use this for aflow<2947
    to fix the fgroup bug.
    Useful for scripting (SC0209).

aflow --factorgroup < POSCAR
    Calculates factor group symmetry of the cell {R|t} and writes
    in the aflow.fgroup.out file. See documentation of aflow.
    The point group is required for the factor group, therefore
    the aflow.pgroup.out file will be generated as well.

aflow --findsym[=tolerance_relative: default 1.0e-3] < POSCAR
    Runs and prints out the output of the program findsym
aflow --findsym_print[=tolerance_relative: default 1.0e-3] < POSCAR
    This prints out the input file structure for findsym.
aflow --findsymSG[=tolerance_relative: default 1.0e-3] < POSCAR
    This prints out the space group without bothering with wrap ups.
    findsym must be accessible on the path !
aflow --findsymSG_label[=tolerance_relative: default 1.0e-3] < POSCAR
    Same as above but prints ONLY the space group name.
aflow --findsymSG_number[=tolerance_relative: default 1.0e-3] < POSCAR
    Same as above but prints ONLY the space group number.

aflow --fix_bands POSCAR KPOINTS.bands.old EIGENVAL.bands.old KPOINTS.bands.new EIGENVAL.bands.new
    Resample the PATH following the standard definition of the POSCAR and the standard path.
    If there are not nearby points, it will ask to redo the nbands step.

//DX - START
aflow --aflowSYM|--aflowsym|--full_symmetry|--full_sym|--fullsym[=tolerance | =tight | =loose] [--no_scan] < POSCAR

```


Calculates the full symmetry of a crystal: point group lattice, point group crystal, factor group, space group, site point group, inequivalent/equivalent atoms, and the point group of the k lattice. This routine calculates the full symmetry suite at a certain tolerance. If symmetry rules are broken, the code automatically changes tolerance and recalculates.

Tolerance:

- The tolerance is given in Angstroms. There are two preset tolerances:
 - tight: minimum_interatomic_distance/100.0
 - loose: minimum_interatomic_distance/10.0
- The default tolerance is the "tight" tolerance values.
- A value can also be specified. (Note, it must be below the minimum interatomic distance, otherwise an error will be thrown.)

Options:

- [--no_scan] : Will not perform tolerance scan.

//DX - END

aflow --frac [-f,-d,--fract,--fractional,--direct] < POSCAR
 Outputs to standard out a new POSCAR file with atom positions in direct (fractional) coordinates.

aflow --getTEMP[s] [--runstat | --runbar | --refresh=X | --warning_beep=T | --warning_halt=T]
 If available, the command outputs the hostname and temperatures of the machine. Useful to find hardware with --runstat the command continuously prints the temperature, refreshing every XX refresh seconds; with --runbar the command prints a bar with the temperature, refreshing every XX refresh seconds; with --refresh=X you can specify the refresh time (DEFAULT below) with --warning_beep=T, if the max temp goes beyond T(C, DEFAULT below), the command beeps the computer with --warning_halt=T, if the max temp goes beyond T(C, DEFAULT below), the command halts the computer (aflow DEFAULT VALUES in aflow.h

```
#define AFLOW_CORE_TEMPERATURE_BEEP_      56.0 // Celsius
#define AFLOW_CORE_TEMPERATURE_HALT_     65.0 // Celsius, you need to run aflow as root to halt
#define AFLOW_CORE_TEMPERATURE_REFRESH_  5.0  // seconds
```

aflow --gulp < POSCAR
 Outputs to standard out a gulp formatted input file based on the POSCAR input file. The formatting is for a distance calculation in gulp. If you want atom names you must put them after each atom position in the POSCAR file (see --names). If any names are missing they are defaulted to H.

aflow --hkl=h,k,l[,bond] < POSCAR
 Returns the planar density and number of broken bonds per unit area along the Miller plane (h k l). The calculations returns also the bonds broken for each type and all types.
 Note: the indices are with respect to the unit cell, not the conventional cell, and the result is in #atoms/A² (scale included).
 BOND: (default BOND_DEF):
 If you specify a "bond", all the bonds shorter than bond*nearest_neighbour_bond (between all types or combination of them) that are cut by the plane will contribute to the broken bond density Nb(#/AA).
 NOTE2: the 1st atom is taken to be the origin (all the other atoms are shifted).

aflow --hkl_search=[khlmx[,bond[,step]]] < POSCAR
 Returns the planar density and number of broken bonds per unit area along the Miller plane (h k l). The calculations returns also the bonds broken for each type and all types.
 Note: the indices are with respect to the unit cell, not the conventional cell, and the result is in #atoms/A² (scale included).
 Search from -hmax<=h<=hmax, -kmax<=k<=kmax, -lmax<=l<=lmax, where the boundaries are (-4,-4,-4) to (4,4,4) unless the HKLMAX is specified.
 HKLMAX:
 If you specify a hklmax, then the search is -hklmax<=h<=hklmax, -hklmax<=k<=hklmax, -hklmax<=l<=hklmax

BOND: (default 1.3):
 If you specify a "bond", all the bonds shorter than bond*nearest_neighbour_bond (between all types or combination

of them) that are cut by the plane will contribute to the broken bond density Nb(#/AA).

STEP: (default 1):
 If you specify STEP then the update of h,k,l, is done in steps of step.

aflow --hkl_search_simple[=cutoff[,bond[,khlmax[,step]]]] < POSCAR
 aflow --hkl_search_complete[=cutoff[,bond[,khlmax[,step]]]] < POSCAR
 Returns the planar density and number of broken bonds per unit are along the Miller plane (h k l). The calculations returns also the bonds broken for each type and all types.
 Note: the indices are with respect to the unit cell, not the conventional cell, and the result is in #atoms/A² (scale included).
 The simple search is fast but it might miss some planes!
 The complete search should not miss planes but can be very slow!

CUTOFF (default 1.3):
 If you specify a cutoff, the command will look for all the planes generated with triplets of atoms in a radius cutoff*|a1+a2+a3|. The algorithm to find the density of atoms is quite complex, and it relies on a sum of four triangles (one triangle v1,v2,v3 generated by hkl) plus three triangles generated by adding the v's and subtracting one. This guarantees that we span 2 unit cells "rhombi" in independent directions. The algorithm also plots the number of atoms in the radius, so you can choose a decent cutoff'. For bcc/fcc cutoff=1.5 usually good. If you do not specify the cutoff, a value of 1.3 is take by default. Be careful with the cutoff ! The complexity grows as cutoff³ !

BOND: (default 1.3):
 If you specify a "bond", all the bonds shorter than bond*nearest_neighbour_bond (between all types or combination of them) that are cut by the plane will contribute to the broken bond density Nb(#/AA).
 HKLMAX (default "dims" given by cutoff)
 If you specify a hklmax, then the search is
 -hklmax<=h<=hklmax, -hklmax<=k<=hklmax, -hklmax<=l<=hklmax

STEP (default simple: 1 complete 1/12)
 If you specify STEP then the update of h,k,l, is done in steps of step.

NOTE1: The algorithm will be implemented in aflow as automatic surfaces generation.
 NOTE2: the 1st atom is taken to be the origin (all the other atoms are shifted).

aflow --hnf n < POSCAR
 Given a POSCAR and a volume 'n' (determinant of the Hermite normal form), it generates the set of supercells of POSCAR having volume n and being unique. In more details: it calculates the HNF matrices, the point group of the POSCAR lattice, then reduces the supercells by symmetry and print the unique POSCARs in aflow.in START/STOP format, ready for high-throughput calculation.
 If the volume is chosen negative, then all the supercells with HNF from 2 to -n will be generated with the same algorithm.

aflow --hnftol [eps] < PARTCAR
 Given a PARTCAR, it calculates the HNF size to get the right concentration spread of partial occupation within the tolerance. If eps is zero, negative or it is not given, aflow takes the tolerance from the PARTCAR, and if this is not available, it takes the default value. PARTCAR

```

PARTCAR of Ag8.8Cd4Zr3.2      // EXAMPLE
-191.600 0.02                // POSCAR scale and tolerance if>0)
5.76 5.76 5.76 90 90        // usual a1,a2,a2 or ABCCAR or WYCKCAR definitions)
8*1+1*0.7333 4*1 1*0.266+3*1 // needs keywords * and + to determine the species and the occupations)
Direct Partial              // you need to specify Partial, the "P" is mandatory)
0.25 0.25 0.25 Ag
0.75 0.75 0.25 Ag
0.75 0.25 0.75 Ag
0.25 0.75 0.75 Ag
0.25 0.25 0.75 Ag
0.75 0.75 0.75 Ag
0.25 0.75 0.25 Ag
0.75 0.25 0.25 Ag

```

```

0.50 0.50 0.50 Ag
0.00 0.00 0.00 Cd
0.00 0.50 0.50 Cd
0.50 0.00 0.50 Cd
0.50 0.50 0.00 Cd
0.50 0.50 0.50 Zr
0.50 0.00 0.00 Zr
0.00 0.50 0.00 Zr
0.00 0.00 0.50 Zr
aflow --hnfcell < POSCAR
Convert a POSCAR with partial occupation into regular POSCARs, and generate a LOG.POCC file in working
Given a PARTCAR, it calculates the HNF size and generate supercells.
PARTCAR Example:
PARTCAR of Se0.75Sn1Te0.25 [Sn1Se0.75Te0.25]
1.0 -4 (0.001) //POSCAR scale and [HNF size if <0 (useful when you kn
0.0000000000000000 3.0268425330530309 3.0268425330530309
-3.0268425330530309 3.0268425330530309 0.0000000000000000
-3.0268425330530309 0.0000000000000000 3.0268425330530309
1*0.75 1*0.25 1 //different species mut be separated by blank space
Direct Partial
0.5000000000000000 0.5000000000000000 0.5000000000000000 Se
0.5000000000000000 0.5000000000000000 0.5000000000000000 Te
0.0000000000000000 0.0000000000000000 0.0000000000000000 Sn
Another PARTCAR Example:
Se1.75Sn2
1.0 -4
2.1393597183461157 -5.9785152916018083 0.0000000000000000
2.1393597183461157 5.9785152916018083 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.2994759406996081
1*0.75+1 2
Direct P
0.6424479395478624 0.3575520604521376 0.7500000000000000 Se
0.3575520604521376 0.6424479395478624 0.2500000000000000 Se
0.8714903476790070 0.1285096523209930 0.7500000000000000 Sn
0.1285096523209930 0.8714903476790070 0.2500000000000000 Sn

aflow --icsd Pb Sn Se < ternary.icsd
aflow --icsd Sn 34 Pb < ternary.icsd
aflow --icsd 34 82 50 < ternary.icsd
Output to standard out in "ICSD-format" (the NIST's Inorganic
Crystal Structure Database) all Pb-Sn-Se ternary-compounds.
The arguments for --icsd can be the elements' symbol or atomic number.
The input is from stdin ICSD-format in this example is streamed in
from file "ternary.icsd".
"ICSD-format" is generated by exporting the entry (hit) in NIST's Inorganic
Crystal Structure Database in long format using "FindIt" software (the stand-alone ICSD browser).
Examples are /common/NIST/binary.icsd and /common/NIST/ternary.icsd
More information on ICSD: http://www.nist.gov/srd/nist84.htm
(2009, wahyu@alumni.duke.edu)
aflow --icsd_alllessthan Ra < input.icsd
(see --icsd). Output compounds if ALL elements in a compound have Z<Z_Ra
aflow --icsd_allmorethan Ra < input.icsd
(see --icsd_alllessthan).
aflow --icsd_basislessthan 20 < input.icsd
aflow --icsd_basismorethan 20 < input.icsd
(see --icsd). Output all compounds having number of basis atoms in the PRIMITIVE cell
lessthan or morethan the specified parameter.
aflow --icsd_chem MgB4 < input.icsd
(see icsd). Extract MgB4 compound.
aflow --icsd_cubic < ternary.icsd
aflow --icsd_triclinic < ternary.icsd
aflow --icsd_monoclinic < ternary.icsd
aflow --icsd_orthorhombic < ternary.icsd
aflow --icsd_tetragonal < ternary.icsd
aflow --icsd_rhombohedral < ternary.icsd

```

```

aflow --icsd_trigonal < ternary.icsd
aflow --icsd_hexagonal < ternary.icsd
aflow --icsd_cubic --icsd_orthorhombic < ternary.icsd
    (see --icsd). Output all compounds which belong to the specified system.
    If multiple options, the relational is "OR".
aflow --icsd_tri < input.icsd
aflow --icsd_mcl < input.icsd
aflow --icsd_mclc < input.icsd
aflow --icsd_orc < input.icsd
aflow --icsd_orcc < input.icsd
aflow --icsd_orcf < input.icsd
aflow --icsd_orci < input.icsd
aflow --icsd_tet < input.icsd
aflow --icsd_bct < input.icsd
aflow --icsd_rhl < input.icsd
aflow --icsd_hex < input.icsd
aflow --icsd_cub < input.icsd
aflow --icsd_fcc < input.icsd
aflow --icsd_bcc < input.icsd
    (see --icsd). Output compounds which belong to the specified lattice type:
    tri (trigonal)
mcl (monoclinic)
mclc (c-centered monoclinic)
orc (orthorhombic)
orcc (c-centered orthorhombic)
orcf (face-centered orthorhombic)
orci (body-centered orthorhombic)
tet (tetragonal)
bct (body-centered tetragonal)
rhl (rhombohedral/trigonal)
hex (hexagonal)
cub (simple cubic)
fcc (face-centered cubic)
bcc (body-centered cubic)
aflow --icsd_denslessthan 4.5 < ternary.icsd
aflow --icsd_densmorethan 5.5 < ternary.icsd
aflow --icsd_densmorethan 4.5 --icsd_denslessthan 8.3 < ternary.icsd
    (see --icsd). Output all compounds with density (in g/cm3) lessthan and/or morethan
    the specified argument.
aflow --icsd_id 11120 < input.icsd
    (see --icsd). Extract compound with entry ID number 11120 of the original ICSD database.
aflow --icsd_lessthan Pb < binary.icsd
aflow --icsd_lessthan 82 < binary.icsd
    (see --icsd). Output all compounds in binary.icsd that contains AT LEAST
    ONE element with atomic number Z<Z_Pb (Z<82).
aflow --icsd_listmetals
    Output to stdout a list of metallic elements used in the --icsd_removemetals option.
aflow --icsd_makelabel < input.icsd
    Output to stdout a list of labels compatible to generate aflow.in from icsd database.
    The label uses the following format: chemicalformula_ICSD_entrynumber
    The chemicalformula is ascendingly sorted based on the element symbol and the
    concentration must be explicitly included eventhough it is 1.
    The entrynumber is the entry number of the compound in the ICSD database.
    e.g. Zn1Zr1_ICSD_106235
aflow --icsd_morethan Pb < binary.icsd
aflow --icsd_morethan 82 < binary.icsd
aflow --icsd_morethan Pt --icsd_lessthan Hg < binary.icsd
aflow --icsd_morethan 78 --icsd_lessthan 80 < binary.icsd
    (see --icsd_lessthan and --icsd).
aflow --icsd_n_ary 2 < input.icsd
    (see --icsd). Output all binary compounds
aflow --icsd_n_ary 3 < input.icsd
    (see --icsd). Output all ternary compounds. and so on
aflow --icsd_nobrokenbasis < input.icsd
    (see --icsd). Some compounds reported in the ICSD database have missing wyckoff position

```

of some of the constituents. This option extracts only the ones with complete wyckoff pos.

```

aflow --icsd_nopartialocc < input.icsd
  (see --icsd). Output only compounds with full occupancies
aflow --icsd_proto #Nspecies1 #Nspecies2 #Nspecies3 ... < input.icsd
aflow --icsd_proto 2 1 7 < input.icsd
  (see icsd). Output all ternary compounds with general chemical formula A2BC7, AB2C7, A7B2C, and all
  other possible cyclic permutations.
aflow --icsd_remove Pu < input.icsd
  (see --icsd). Remove compounds which contain Pu.
aflow --icsd_removemetals < input.icsd
  (see --icsd). Remove compounds that are composed ENTIRELY by metallic elements.
  Metallic elements:
  Alkali metals, Alkaline earth metals, Transition metals,
  Lanthanoids, Actinoids, Other metals (Al, Ga, In, Sn, Tl, Pb, Bi).
  To list all metallic elements used in this option, use --icsd_listmetals
aflow --icsd_sg 62 < binary.icsd
aflow --icsd_sglessthan 62 < binary.icsd
aflow --icsd_sgmorethan 45 < binary.icsd
aflow --icsd_sgmorethan 194 --icsd_sglessthan 231 < binary.icsd
  (see --icsd). Output all compounds where the space group number satisfies the
  specified arguments.
aflow --icsd_unique < input.icsd
  (see --icsd). Discard redundant compounds based on SG# AND ChemicalFormula

aflow --icsd_check_raw > output.dat
Checks the validity of the current vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/ dirs and files
(POSCAR KPOINTS DOSCAR and EIGENVAL)
with respect to vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/LIB/
output.dat will contain:
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/./././ OK
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/./././ OK
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/./././ ERROR file1 file2 ...
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/./././ NotInLIB
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/RAW/./././ NotInLIB
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/LIB/./././ NotInRAW
vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD)/LIB/./././ NotInRAW
and so on.
aflow --icsd_check_raw 0 > output.dat
same as the default --icsd_check_raw
aflow --icsd_check_raw 1 > output.dat
use the list of RAW and LIB dirs that have been compiled in aflow
i.e. XHOST.vGlobal.at(X) (ICSD_LIB); // aflow_data_calculated.cpp
    XHOST.vGlobal.at(X) (ICSD_RAW); // aflow_data_calculated.cpp

aflow --icsd2aflowin < input.icsd
  Convert input.icsd (ICSD-format) to aflow.in
aflow --icsd2poscar < input.icsd
  Write output to stdout POSCAR from stdin ICSD-format
aflow --icsd2proto < input.icsd
  Write output to stdout in ICSD_PROTO-format from stdin ICSD-format
aflow --icsd2wyck < ternary.icsd
  Write output to file WYCKCAR (WYCKCAR-format) from stdin ICSD-format
  in this example is streamed in from file "ternary.icsd".
  If the input contains multiple compounds, a subfolder will
  be created for each compound using the following folder name template:
    CompoundFormula_ICSD_ICSDid/
  The ICSDid is the compound id in the original ICSD database.
  ONLY compounds with elements having full occupation (sof=1) will be processed.
aflow --icsd2wyck --sof < ternary.icsd
  (see --icsd2wyck). In this case, all compounds will be processed.
  If partial occupation is detected, the sof will be written as part of
  the label of the element and WARNING will be written in the title and cerr.
aflow --icsdproto2aflowin < input.proto
  Convert ICSD-PROTOTYPE-format to aflow.in
  (2007-2011, wahyu@alumni.duke.edu)

```

aflow --identical < POSCAR
 Makes all the atoms identical. Useful to find the properties of the superlattice.

aflow --incell < POSCAR
 Outputs to standard out a POSCAR file with all atoms mapped to their images within the unit cell.

aflow --incompact < POSCAR
 Similar to --incell
 Outputs to standard out a POSCAR file where all the atoms are mapped through the unit and neighbours cells to minimize the shortest possible bond with an adjacent atom
 This option is very useful if you run big and complicate molecules where atoms exit of the unit cell and you have problems understanding where they are because visualization packages do not show bonds anymore ...
 Anyway, it is easier to test than to describe. (SC 6 Aug 04)

aflow --insphere radius < POSCAR
 Similar to --incell and --incompact
 Outputs in XYZ format (rasmol standard), the positions of all the atoms inside a sphere of radius "radius" centered in the origin.
 If you want another origin, you must shift the atoms first.
 The radius is in cartesian format. (SC 6 Aug 04)

aflow --intpol=file1,file2,nimages,nearest_image_flag
 Creates nimages image POSCAR files by interpolating linearly between structures in file1 and file2. File1 and file2 should both be POSCAR like files with corresponding atoms. The nearest_image_flag is set to 'e' for exact interpolation and 'n' or 'N' for nearest-image interpolation. Exact interpolation means that all the positions are taken exactly as they are input. Nearest-image interpolation means that the interpolation between two corresponding atoms in file1 and file2 is actually done between the atom in file1 and the nearest image of the corresponding atom in file2. This is useful, e.g., if the positions (in direct coordinates) are 0.01 (file1) and 0.99 (file2). These are far apart in exact interpolation but very close in nearest-image interpolation. The POSCAR output files are numbered and output to the present directory. The code also creates numbered subdirectories and copies the appropriate POSCAR files into those. This option makes it easy to set up a rubber band calculation in vasp.

aflow --inwignerseitz [--inws] < POSCAR
 Outputs to standard out a POSCAR file where all the atoms are mapped to their images in the Wigner-Seitz cell. (SC 10Jan04)

aflow --inflate_lattice=coefficient | --ilattice coefficient=coefficient < POSCAR
 Inflate/deflate POSCAR lattice of coefficient.

aflow --inflate_volume=coefficient | --ivolume coefficient=coefficient < POSCAR
 Inflate/deflate POSCAR lattice of coefficient.

aflow --kpath [--grid=XX] < POSCAR
 Outputs to stdout a KPOINTS in line mode useful for bandstructure calculations. The k-points path is chosen to cover all possible pair combinations of special k-points in the irreducible BZ (IRBZ). a special k-point is either:

- (1) a center of a face in IRBZ, or
- (2) a corner of IRBZ, or
- (3) a midpoint (say M) of a line-edge (say AB) IF the Gamma-M-A makes a 90 degrees angle.

 The coordinates are given in fractionals of the k-vectors, in which derived from the "standard" lattice used in AFLOW.
 To find out the standard lattice of the POSCAR, use --sp option.
 Optional: --grid=XX specifies the density of the grid, if not specified it takes --grid=16.
 NOTE: If grid is negative real number, e.g. --grid=-0.01, then its value is taken as the deltaK during the path which is constructed as uniformly as possible in the k-space.
 The option works both for VASP, QE style mode inputs (ABINIT and AIMS in the future).

Example: `aflow --proto=3:Ag:Zr [--qe | --abinit | --aims] | aflow --kpath=-0.01`

`aflow --kpoints=KDENS [or --kppra=KDENS,-k=KDENS] < POSCAR`
This function prints a set of Monkhorst-Pack kpoint mesh values (divisions along each reciprocal lattice parameter) based on the desired KDENS density and the lattice parameters. The values assure the most even distribution of KDENS along the lattice params consistent with the kpt density. See `--delta_kpoints`

`aflow --jmol[=n1[,n2[,n3[,color[,true/false]]]] < POSCAR`
Similar to `--xyz`. Starts jmol (must be available) with a file based on the POSCAR input file. If you want to use atom names you must put them after each atom position in the POSCAR file (see `--names`). If any names are missing they are defaulted to H. If no numbers are specified, aflow takes "1,1,1". (SC/Dec09)
Background color may be chosen (e.g., white, brown, beige, etc...). Default background color is white. The flag "true" specifies that the cif file is to be saved. Default is "false." (RHT/Mar11)

`aflow --jmolanimation | --animation | --print=gif [gif_file] < POSCAR`
Generate animated gif file of rotated structure from POSCAR by using jmol and ImageMagick. If no output gif file name is given, the default name "animantion_" + process id + ".gif" will be used. The setting parameters of jmol cannot be changed by users currently. User must have valid DISPLAY for jmol to open its window and "Convert" command is used to generate multi-gif by combining gif files generated by jmol.

`aflow --join_strlist strlist1 strlist2`
Outputs to standard out a sequence of structures in POSCAR format. The structures consist of those in strlist1 with the atoms from strlist2 added in. The positions are taken from strlist2, transformed into Cartesian coordinates, and then inserted into strlist1. All inserted atoms are added as new types. If one file has more structures than the other then the shorter file is padded with copies of the last structure. For more information on a strlist see `--make_strlist`.

`aflow --kband ispin`
ispin(1=nospin,2=spin). Outputs to standard out Eband vs K for band structure plot. Needs EIGENVAL and KPOINTS files. Format:
Kpoint upEband1 upEband2...upEbandN downEband1 downEband2...downEbandN
The Kpoint column is constructed by cascading each KPOINT-segment specified in KPOINT file.

`aflow --latticereduction | -latreduction POSCAR`
Lattice Reduction to Max Orthogonality (Minkowski) and then to Niggly Form. This procedure has been shown to give the best unit cell for the lattice in terms of Minkowski optimization and most symmetric representation. For the bcc and fcc it gives the standard, most symmetric, unit vectors.
It also helps in the primitive cell search, as it has been included by default inside. (SC0902).

`aflow --lattice_type | --lattice | --lattice_crystal < POSCAR`
Returns the lattice type and the conventional lattice type of the CRYSTAL following the tables of Setyawayn-Curtarolo [<http://dx.doi.org/10.1016/j.commatsci.2010.05.010>].

`aflow --lattice_lattice_type | --lattice_lattice < POSCAR`
Returns the lattice type and the conventional lattice type of the LATTICE following the tables of Setyawayn-Curtarolo [<http://dx.doi.org/10.1016/j.commatsci.2010.05.010>].

`aflow --latticehistogram < POSCAR`
Outputs the lattice calculated respect to tolerance of histogram of symmetry.

`aflow --use_LOCK=XXX`
Uses XXX instead of "LOCK" in freezing/searching/operating directories.

The option is very useful for compounded calculations.

```
aflow --ltcell=a11,a12,a13,a21,a22,a23,a31,a32,a33 < POSCAR
```

```
aflow --ltcell=a11,a22,a33 < POSCAR
```

```
aflow --ltcell=file < POSCAR
```

Outputs to standard out the linear transform of the input POSCAR file. This simply multiplies cell parameters and atom positions by the 3x3 matrix values. This can be used to rotate the cell, swap x and y coordinates, etc. This cannot create a supercell (see --supercell for that). The nine numbers must be separated spaces, and they form the nine elements a11,a12,a13,a21,a22,a23,a31,a32,a33 of the 3x3 supercell matrix, respectively. If you specify only 3 numbers, the other six are taken zero. If you use the "file" syntax, nine numbers are read from file. They can be on one or multiple lines. New algorithm by SC (aug07).

The new lattice is (by column) (a1 a2 a3)*=LT*(a1 a2 a3).

```
aflow --ltcellfv=v1,v2,v3,phi < POSCAR
```

Rotates the lattice vectors and atoms by angle phi (in degrees) around vector (v1,v2,v3). Outputs to standard out the new POSCAR. This can be used to rotate the cell, swap x and y coordinates, etc.

```
aflow --magpara=directory | --magpara (./)
```

Output shows the magnetic momentum, cell of volume and spin polarization around Fermi level. If a directory is not specified, it loads "./"

EXAMPLE: aflow --magpara

```
MAGNETIC MOMENTUM CELL : 2.74234
MAGNETIC MOMENTUM ATOM : 0.685586
VOLUME CELL           : 53.43
VOLUME ATOM           : 13.3575
SPIN DECOMPOSITION    : 0.032,1.447,1.447,-0.062
POLARIZATION FERMI    : 0.755068
```

```
aflow --slab=h,k,l[#filled_layers[#vacuum layers]] < POSCAR
```

Produces a slab unit cell in POSCAR format. The normal of the slab is specified by the Miller indices of the orthogonal plane. Thus, make sure you know how the original POSCAR is specified. For example, (100) is not what you think for fcc primitive. Each point (hkl) in the reciprocal lattice corresponds to a set of lattice planes (hkl) in the real space lattice. The reciprocal lattice vector points in a direction normal to the real space planes.

```
aflow --make_strlist OUTCAR XDATCAR
```

Outputs to standard out a sequence of structures in POSCAR format. The strlist file created contains a list of structures, each formatted exactly like a POSCAR file, with an empty line after all but the last one. The file must have no extra lines at the end or all routines that read it will crash. The lattice parameters are pulled out from the OUTCAR and the positions from XDATCAR. If OUTCAR has too few lattice parameters then copies of the last set are used for the remaining XDATCAR.

```
aflow --maxatoms=N | --max_atoms=N | --atoms_max=N | --atomsmax=N < POSCAR
```

Limits the input POSCAR to N atoms (it writes an error if atoms>N).

This is a useful option for online wrappers.

```
aflow --minkowski_basis_reduction | --minkowski | --mink < POSCAR
```

Converts the unit cell with the Minkowski reduction. This routine takes a set of basis vectors (that form a lattice) and reduces them so that they form the shortest possible basis. The reduction is performed so that each vector "a_i" is as close as possible to the origin while remaining in the affine plane which is defined by "a_j", "a_k" but shifted by "a_i", for any choice of even permutations of i,j,k in 1,2,3.

See Lecture notes in computer science, ISSN 0302-974, ANTS - VI : algorithmic number theory, 2004, vol. 3076, pp. 338-357
ISBN 3-540-22156-5

Written by Gus Hart in F90, recoded by SC in C++ (Sep/08).
<http://www.farcaster.com/papers/sm-thesis/node6.html>

aflow --miscibility | --mix strings ..
Tells if in the library the system (on of the strings) was found to be miscible, immiscible or unknown.

aflow --mix AgMg
returns AgMg MISCIBILITY_SYSTEM_MISCIBLE

aflow --mom < POSCAR
Gets the mass moments of the POSCAR file. Gets only the first (center of mass) at this point. The scale is used in the calculation.

aflow --msi < POSCAR
Outputs to standard out a msi file based on the POSCAR input file. This can be used as input for cerius.
In the functions that output the msi format I do something to put the lattice vectors in a form that cerius2 can read happily. It involves making the third lattice vector parallel to Z, the second once in the YZ plane, and the letting the first lattice vector have all 3 components. It is confusing and probably done in a silly manner, but it seems to work.
If you want atom names you must put them after each atom position in the POSCAR file (see -names). If any names are missing they are defaulted to H. For an msi file one needs the atomic numbers. These are coded into the program for most atoms. If you use atoms with atomic numbers over 86 or f-electron atoms (Lanthanides and Actinides) then you will have to increase the database. For the list of all coded atomic numbers see the constructor for the structure class in structure.cc.

aflow --names A1 A2 ... < POSCAR
Outputs to standard out a POSCAR file with names A1,A2, ... after the atom positions. Each name Ai is assigned to all atoms of type i.

aflow --natoms | --numatoms < POSCAR
Outputs to standard out the number of atoms in the POSCAR. Useful for scripting. (SC0902).

aflow --nanoparticle radius distance < POSCAR
Starting from the input poscar, aflow prints a nanoparticle POSCAR with the radius and appropriate lattice making the particles as far as "at least distance". The origin of the particle is taken to be point 0,0,0 in the unit cell.
You can translate the origin before with the command --setorigin (see below) to an atom, a point in cartesian or fractional coordinates.
The radius and distance are in Angstroms and not scale normalized (all scales are set to 1.0).
If not specified the parameters are taken to be 10A. (SC Apr/08)

aflow --ndata < POSCAR
Outputs to standard output the following normalized data:
a1 a2 a3 phi(a2,a3) phi(a3,a1) phi(a1,a2)
a1,a2,a3 are NORMALIZED over $V^{1/3}$ and phi are in degrees.

aflow --niggli POSCAR
Converts the unit cell to the standardized Niggli form. The form is unique (up to some signs, I think). The transformation makes use of only the lattice vectors and does not depend on the basis atoms. This will work on any cell, but it treats the given cell as primitive, and it will not reduce the cell to primitive if it is not primitive already. At present the algorithm seems to hang if I force more than about 6 digits of accuracy so be aware that small errors might be introduced (these can break symmetry!).

aflow --nn < POSCAR
Outputs to standard out the nearest neighbour distance.

aflow --noorderparameter < POSCAR
Outputs to standard out a POSCAR without all the order parameter

```

stuff in it. (SC0903).
aflow --nosd < POSCAR
Outputs to standard out a POSCAR without selective dynamics
formatting. Combined with the above --sd option this allows
easy movement between POSCAR files with and without selective
dynamics formatting.
aflow --numnames A1 A2 ... < POSCAR
Same as names except appends an increasing integer to
each different atom type. Starts counting at 1 again
for each new atom type.
aflow --nspecies | --numspecies < POSCAR
Outputs to standard out the number of species in the POSCAR.
Useful for scripting. (SC0902).

aflow --OrthoDefect < POSCAR
Computes the orthogonality defect of the lattice of POSCAR.
The orthogonality defect is defined as the ratio of the product of
lattice vector magnitudes to the volume of the parallelepiped defined
by the lattice vectors. So, for three orthogonal vectors, this ratio
would be unity. (R. Taylor).

aflow --pdb < POSCAR
Outputs to standard out a protein database (PDB) format file
based on the POSCAR input file. This can be used as input
for many viewing programs. Note that I don't really know
anything about PDB but it seems to be an annoyingly column
formatted. Therefore, all the widths I use must tbe kept as is.
This means that if we have width W for variable X, and prec P,
then X takes up P+1 for for the decimal part and decimal point,
and we have only R=W-(P+1)-1=W-P-2 remaining digits (the -1 is
because if X takes up all of W then you run into the previous
field). So we have the constraints
Cell vectors: W=9,P=3,R=4 => <=10^5
Cell angles: W=7,P=2,R=3 => <=10^3 (which always works since
angles are given as >=0 and <=360)
Cartesian positions: W=12,8,P=3,R=7,3 => <=10^8,10^4 (>0)
and <=10^7,10^3 (<0 since you need a space for the -- sign)
This is all probably fine unless an atom makes it to more
negative than -999.999.
aflow --pdos pdos.in PROOUT
Writes the projected DOS for any desired combination of atoms,
kpoints, bands, and lm values. The output consists of 6
columns, spin up, down, up-down, and the cumulative DOS for
each of those. Only up spin data is given for non
spin-polarized calculations. The PDOS should look like
an equivalent vasp output but will not be identical since
vasp uses a different smearing method to get the PDOS.
However, I think these PDOS are basically correct, at least
qualitatively. To make this work you must
-- Use slightly altered version of vasp
-- set LORBIT=2 in INCAR
-- Set ISYM=0 in INCAR
-- Set RWIGS in INCAR (see below)
The details explaining all this are given above in the --pocc
section. The input file has the following format

# Input for aflow --pdos.

# These values you supply once.
EMIN = --20.01477264 # default: 0.5eV below lowest energy.
EMAX = 6.90250559 # default: 0.5ev above highest energy.
NBINS = 300 # default: 300
SMOOTH_SIGMA = 0.1 # Gaussian smoothing of the DOS.
# default: 1 bin width.
PRINT_PARAMS = 1 # 0=prints only data (easy to plot).

```

```

# 1=prints all the input parameters.
# default: 0

# You can have as many cases as you want.
# They are all added together.

# case 1
ATOMS = 1 # default: all atoms.
KPOINTS = # default: all kpoints.
BANDS = # default: all bands.
LMVALUES = # default: all s,p,d,f.

# case 1
ATOMS = 2 # default: all atoms.
KPOINTS = 1 2 3 # default: all kpoints.
BANDS = 1 # default: all bands.
LMVALUES = 3 # default: all s,p,d,f.

All # denote comment lines. Each case is started when the token
ATOMS is used. Following an ATOMS token, all KPOINTS, BANDS,
LMVALUES tokens will apply to the atoms denoted in the preceding
ATOMS token until the next ATOM token. The KPOINTS, BANDS,
LMVALUES tokens can be left out in which case their default values
will be used. You can have any number of cases. The above
example will calculate a PDOS with projections onto atom 1
for all kpoints, bands, and s,p,d, and f (case 1) added to the
projection onto atom 2 for kpoints 1-3, band 1, and the Pz orbital.
I believe you can create any desired projections with this input
file. The LMVALUES use the following correspondence between
numerical input and orbitals projected.

Input number: 1 2 3 4 5 6 7 8 9 10 11
Orbitals: S Py Pz Px Ptot Dxy Dyz Dz2 Dxz Dx2-y2 Dtot
Input number: 12 13 14 15 16 17 18 19 20
Orbitals: F1 F2 F3 F4 F5 F6 F7 Ftot Tot

I have not done the work to figure out which of the standard
f-orbital functions correspond to F1-F7.

This is only tested for version 4.4.5.

aflow --pearson_symbol | --pearson < POSCAR
Returns the Pearson symbol of the structure.

aflow --planedens dens2d.in CHGCAR
This finds the charge density in a plane. The input file dens2d.in
has the form
D # Coordinates for following points (Direct/Cartesian)
scale # Scale factor - edges of plane get mult. by this (but not origin).
x y z # origin point
x y z # X axis
x y z # Y axis
Nx Ny # Number of X and Y grid points
Middle # Location for origin (Middle/Corner).
Ortho # Whether to use Y orthogonal to X (Ortho/Strict).
The output consists of 4 files, dens.[tot/diff/up/dn].out. Each
has the same format, consisting of rows of density values, each
row corresponding to a value along the X axis and each column
to a value along the Y axis. The format can be read directly
into Excel and easily into MatLab. This routine uses the same
routine as --chgint to read in the CHGCAR and should work
for the same versions of vasp (see --chgint for more information).
aflow --platon[=EQUAL | EXACT][,ang,d1,d2,d3] < POSCAR
This finds the space group. aflow is creating an output
file, which is piped into a script platonSG, which uses the

```

```

program platon.
Wraps input file for Platon ADDSYM package:
CALC ADDSYM (EQUAL) (EXACT) (ang d1 d2 d3)
where:
EQUAL - Search with all atom type treated as equivalent.
EXACT - All atoms should fit for given criteria.
ang - Angle criterium in search for metrical symmetry of the
      lattice (default 1.0 degree).
d1 - Distance criterium for coinciding atoms for non-inversion
     (pseudo)symmetry elements (default 0.25 Angstrom).
d2 - Distance criterium for coinciding atoms for (pseudo)
     inversion symmetry (default 0.25 Angstrom).
d3 - Distance criterium for coinciding atoms for (pseudo)
     translation symmetry (default 0.25 Angstrom).
The defaults are specified in aflow_xatom.cpp as
#define PLATON_TOLERANCE_ANGLE 1.0
#define PLATON_TOLERANCE_D1 0.25
#define PLATON_TOLERANCE_D2 0.25
#define PLATON_TOLERANCE_D3 0.25
To get the space group, type
  aflow -platon < POSCAR | platonSG
To just get see the output file from aflow, type
  aflow -platon < POSCAR
To check for errors and see output from platon, type
  aflow -platon < POSCAR | platon -o
Note that the added flags above do not seem to work. To change tolerance
create output file from aflow, and then add the four tolerances
after CALC ADDSYM (on the same line). Then pipe this file to platonSG.
Aflow will use your atom labels if they are there. If you
give no atom labels it will use defaults for each atom type,
(these are He,Li,Be,B,C, and then W for all remaining atom types).
WARNING: If you have more than 6 atom types the W default
will give the wrong space group. The equal flag may not work.
Atoms labeled with H do not get read by default in platon.
Do not use H labels.
SEE: http://www.cryst.chem.uu.nl/platon/pl000401.html
Note: it works with platon.f and xdrv.c > 51108
platon must be accessible on the path !
aflow --platonSG[=EQUAL | EXACT][,ang,d1,d2,d3] < POSCAR
This prints out the space group without bothering with the wrap ups.
Note: it works with platon.f and xdrv.c > 51108
platon must be accessible on the path !
aflow --platonSG_label[=EQUAL | EXACT][,ang,d1,d2,d3] < POSCAR
Same as above but prints ONLY the space group name.
aflow --platonSG_number[=EQUAL | EXACT][,ang,d1,d2,d3] < POSCAR
Same as above but prints ONLY the space group number.

aflow --plotband[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Generate bandstructure plot using GNUPLOT
In this function, the spin-polarized DOS plot can be generated!
The following files must reside in the directory:
  DOSCAR.static
  EIGENVAL.bands
  KPOINTS.bands
  OUTCAR.static
Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2
Example:
  aflow --plotband=/common/DATA/ZnO,-8,6 or
  aflow --plotband=/common/DATA/ZnO,-8,6,1.2
aflow --plotband2[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
In this function, the DOS is the sum of spin-up and spin-down!

```

The following files must reside in the directory

DOSCAR.static
EIGENVAL.bands
KPOINTS.bands
OUTCAR.static

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

aflow --plotband_spinsplit[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
This function generates spin-up and spin-down electronic band structure plots, respectively.
The following files must reside in the directory:
EIGENVAL.bands
KPOINTS.bands
OUTCAR.bands

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

aflow --plotbanddos[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Generate bandstructure plot and DOS plot using GNUPLOT
This function equals to "aflow --plotband" & ""aflow --plotdos"
The following files must reside in the directory

DOSCAR.static
EIGENVAL.bands
KPOINTS.bands
OUTCAR.static

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

aflow --plotdos[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Generate DOS plot using GNUPLOT
The following files must reside in the directory:
DOSCAR.static
OUTCAR.static

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

Examples:
aflow --plotdos=/common/DATA/ZnO,-8,6
aflow --plotdos=/common/DATA/ZnO,-8,6,1.2

aflow --plotdosweb[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Generate DOS plot using GNUPLOT
The following files must reside in the directory
DOSCAR.static

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

aflow --plotpedos[=directory[,number_atom[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]]
Generate PDOS plot using GNUPLOT
The following files must reside in the directory
DOSCAR.static
OUTCAR.static

Defaults.
Directory: default = ./
Number atom: default = 1

Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2

Example:
aflow --plotpedos=/common/DATA/ZnO,1
aflow --plotpedos=/common/DATA/ZnO,1,-8,6
aflow --plotpedos=/common/DATA/ZnO,1,-8,6,1.2

aflow --plotpedosall_nonquivalent[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Usage: aflow --plotpedosall_nonquivalent[=directory[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]
Generate PDOS plots of all the inequivalent atoms using GNUPLOT.
The following files must reside in the directory

DOSCAR.static
OUTCAR.static
POSCAR.relax1

Defaults.
Directory: default = ./
Emin: The minimum value of the DOS plot. Default value -10
Emax: The maximum value of the DOS plot. Default value 10
DOSSCALE: The scale value of the DOS plot. Default value 1.2
Use --keep=gnuplot (--keep=GPL) to keep the GNU plot code.

aflow --plotphonondispersion | --pphdis (--rcm | --meV | --THz | --hz) [--print=eps | --print=pdf | --print=png | --print=jpg | --print=gif]
Usage: aflow --pphdis --rcm /common/DATA/ZnO
Generate Phonon dispersion, phonon DoS, F_vib, S_vib, and C_v plots in .eps form using GNUPLOT. The flags [--rcm | --meV | --THz | --hz] specifies the units used in the graphs; --rcm is default
--rcm reciprocal centimeters
--meV mili-electron Volts
--THz teraHertz
--hz Hertz

The optional flags [--print=pdf | --print=png | --print=jpg | --print=gif] will trigger the conversion from
The following files must reside in DIRECTORY as in the AFLOW written form or as .bz2 compressed files
PDIS

PDOS
THERMO

If the files are found in .bz2 form, the compressed files are preserved and temporary files are written and deleted.
The generation of these files is controlled by the commands
[AFLOW_APL]DC
[AFLOW_APL]DOS
[AFLOW_APL]TP
See README_APL, especially 3). for more details.

aflow --pocc_dos[=directory[,T[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]]
Generate density of states (DOS) plot at different temperature for a partial occupation structure.
If not specified, default directory is ./, temperature is 300K, DOS_Emin=-5 eV, DOS_Emax=5 eV, and DOSSCALE=1
Example: aflow --pocc_dos=./,300
More details about how to do this can be found in "README_AFLOW_POCC.TXT".

aflow --pocc_mag[=directory[,T[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]]
Calculate magnetic moment at different temperature for a partial occupation structure.
If not specified, default directory is ./, temperature is 300K, DOS_Emin=-5 eV, DOS_Emax=5 eV, and DOSSCALE=1
Example: aflow --pocc_mag=./,300
More details about how to do this can be found in "README_AFLOW_POCC.TXT".

aflow --pocc_bandgap[=directory[,T[,DOS_Emin[,DOS_Emax[,DOSSCALE]]]]]
Calculate band gap at different temperature for a partial occupation structure.
If not specified, default directory is ./, temperature is 300K, DOS_Emin=-5 eV, DOS_Emax=5 eV, and DOSSCALE=1
Example: aflow --pocc_bandgap=./,300
More details about how to do this can be found in "README_AFLOW_POCC.TXT".

aflow --pocc PROOUT
aflow --pocc PROOUT

Outputs occupations calculated from projections onto spherical harmonics for each ion for many combinations of L, M, bands, and kpoints. This works with version 445 and has not been tested on any other version (and probably won't work). To make this work you need to do the following
-- Use slightly altered version of vasp (see below)

```
-- set LORBIT=2 in INCAR (see below)
-- Set ISYM=0 in INCAR (see below)
-- Set RWIGS in INCAR (see below)
```

Here is why you need to do these things (feel free to skip this). The --pocc option reads the PROOUT file, which is produced by running vasp with LORBIT=2 in the INCAR file. There is an annoying subtle point here. I am not sure I totally get this but here is my best understanding. The projection onto the spherical harmonics actually uses some atomic like radial functions (bessel functions). This means that for each spherical harmonic there are multiple states, corresponding to different atomic energy levels and radial functions. Write the projection of band n, at kpt k, onto spherical harmonic with angular quantum numbers l,m and energy level e as Pnklme. As compiled, the vasp code outputs projections Pnklm, summing over the e parameter. This makes each projection a sum of complex numbers, allowing some cancellations. However, for occupations, like those output in PROCAR (LORBIT=1) and OUTCAR, the summations over e are done with the squares of the Pnklme. This makes sense, since you want to add up probabilities, not amplitudes, to get an occupation. Unfortunately, from the output Pnklm one cannot reconstruct the Pnklme, so the output in PROOUT is not enough to reproduce the occupations. Therefore, I suggest the following. Recompile vasp with following modifications to sphpro.F

change line 252

```
WRITE(IUP,'(9F12.6)') CSUM_PHASE
```

to

```
write(IUP,'(9F12.6)') CSUM_ABS
```

CSUM_ABS is a complex variable but the imaginary part is zero. It is the squared amplitude for each projection. Note that this is a probability. You use it directly (do not square it) to get occupations. Note that the augmentations are added to this real number, and are therefore probabilities, not amplitudes. This makes sense when you look at the code in sphpro.F that calculates the augmentation portion. The augmentations can be <0, which I assume corresponds to reducing the probability of finding electrons. This makes me a little uncomfortable but I guess it is OK. At this point the aflow code assumes the above modification and uses the magnitude of the projections to calculate all occupations (not the magnitude squared).

Also, there is another subtle point with the kpoints. If you use symmetry certain sets of symmetry equivalent kpoints (a star) are represented by a single irreducible kpoint. We are used to ignoring this and simply weighting things associated with the irreducible kpoint appropriately to account for the whole star. However, the projections onto different orbitals are not the same for all the points in a star. For example, the kpoints (0.1,0,0),(0,0.1,0),(0,0,0.1) may all be in the same star in fcc, but states associated with them will project differently onto Px orbitals. Therefore, if you use irreducible kpoints you will get the wrong projections (it seems like you do get the right totals for S,P, and D, but I am not sure that is always the case). To be safe, don't use any symmetry -- i.e., set ISYM=0 in the INCAR file.

You must set RWIGS so that the code knows the radius of the spheres onto which it projects.

To make sure all is in order you can look at the total occupations for each ion in OUTCAR. These should match the Occupations vs. ION:LM values in the output of aflow (the last lines in the output). A more detailed check is to run vasp with LORBIT=1 and compare the PROCAR file with the output of aflow. I am not sure that this will all work the same way with PAW potentials.

```

aflow --pointgroup | --pgroup < POSCAR
    Calculates the point group symmetry of the lattice {R} and writes
    it in the aflow.pgroup.out file. See documentation of aflow.
aflow --pointgroupklattice | --pgroupk < POSCAR
    Calculates the point group symmetry of the klattice {K} and writes
    it in the aflow.pgroupk.out file. See documentation of aflow.
aflow --pointgroup_crystal | --pgroup_crystal | --pgroup_xtal < POSCAR
    Calculate the point group symmetry of the crystal {R+atoms} and
    writes it the aflow.pgroup_xtal.file.
aflow --pgl < POSCAR
    Calculate the point group symmetry of the lattice {R} and
    prints it to stdout.
aflow --pgx < POSCAR
    Calculate the point group symmetry of the crystal {R+atoms} and
    prints it to stdout.

aflow --pomass[=directory]
    Outputs from the available POTCAR/OUTCAR the sum of POMASS.
aflow --pomass_atom[=directory]
    Outputs from the available POTCAR/OUTCAR and POSCAR/CONTCAR the POMASS of the cell per atom.
aflow --pomass_cell[=directory]
    Outputs from the available POTCAR/OUTCAR and POSCAR/CONTCAR the POMASS of the whole cell.

aflow --poscar < ABCCAR | WYCCAR
    Converts the ABCCAR in POSCAR format.
    ABCCAR is described as:
        TITLE
        SCALE (positive (rescaling) negative (volume))
        A B C ALPHA BETA GAMMA
        #specie0 #specie1 ....
        DIRECT (or CARTESIAN)
        .. .. . specie0
        .. .. . specie0
        . . .
        .. .. . specie1
        .. .. . specie1
        and so on. (Stefano Feb 2009)
    Converts the WYCCAR IN POSCAR format.
    WYCCAR is described as
        TITLE
        SCALE (positive (rescaling) negative (volume))
        A B C ALPHA BETA GAMMA SG# [OPTION#]
        #specie0 #specie1 ....
        DIRECT (or CARTESIAN)
        .. .. . specie0
        .. .. . specie0
        . . .
        .. .. . specie1
        .. .. . specie1
        and so on. (Stefano Feb 2009)
    The positions of the species will be used with the list of
    symmetry operations (aflow_wyckoff.cpp) to generate all the atoms.

aflow --poscar2aflowin < POSCAR
    Makes an "almost standard" aflow.in starting from the poscar.
    Useful for scripting (SC100630).

aflow --poscar2enum < POSCAR
    Convert a POSCAR into an input format for MULTIENUM (partial occupation).
    This is useful for debugging MULTIENUM.

aflow --poscar2gulp < POSCAR
    Convert a POSCAR into an input format for gulp program.

aflow --poscar2wyckoff < POSCAR

```


Outputs to Wyckoff positions using findsym.

Note that you may find more detailed information just using `aflow --findsym < POSCAR` if you can not und

```
aflow --prepare_chgcar_4_jmol|--prep4jmol=CHGCAR1[,CHGCAR2,...]
```

options:

```
[ --usage ]  
[ --outcar=OUTCAR ]  
[ --zip ]
```

Modify the header of a CHGCAR file so it can be read by Jmol.

Jmol requires species to be specified in the comment line of the CHGCAR file (first line).

This code requires an OUTCAR to read in the species.

Unless specified, it will first look for OUTCAR file in the directory of the CHGCAR, then it will look in the directory from which the command is called.

The CHGCAR and OUTCAR files may be compressed, and the edited CHGCAR file can be recompressed (if it was previously) by specifying the `--zip` command.

```
aflow --prim < POSCAR
```

Outputs to standard out a POSCAR file with a primitive unit cell. In the primitive cell finding function I look for a primitive cell by considering as candidate cell vectors every possible triad of 3 vectors that can be made from the original cell vectors or the basis vectors which translate the lattice onto itself. I then take the triad with the smallest volume to be the primitive cell. If there are multiple candidates I take the ones with the largest projections onto the original lattice vectors. See the routine GetPrim.cc for more information. NOTE: the algorithm is by SC different from the old DM aflow approach).

```
aflow --primr | --fastprimitivecell | --fprim < POSCAR
```

Returns the primitive, Minkowski reduced cell, using a fast(er) routine. (R. Taylor).

```
aflow [options] --proto=label*[:specieA*[:specieB*]..[:volumeA*[:volumeB*].. | :volume]] [ --params=..... [--]
This command prints out a prototype of label="label" with speciesA,speciesB,... (non mandatory)
of volumes per atom "volumeA, volumeB..." (not mandatory) or with standard volume per atom = "volume".
Note that that --proto label A B ... is not supported anymore and you now need to use
--proto=label:A:B... et cetera.
```

QUANTUM ESPRESSO output

If you specify `--qe`, aflow will add QUANTUM ESPRESSO code to `aflow.in` (experimental).

ABINIT output

If you specify `--abinit`, aflow will add ABINIT code to `aflow.in` (experimental).

AIMS output

If you specify `--aims`, aflow will add AIMS code to `aflow.in` (experimental).

ANRL: AFLOW NAVAL RESEARCH LAB PROTOTYPE LIBRARY

With respect to the article:

Mehl et al., "The AFLOW Library of Crystallographic Prototype", <https://arxiv.org/abs/1607.02532>

the code gives the possibility to define the parameters of the cell `--params=...`

Some rhombohedral cells can be generated in hexagonal configurations (see the article).

The choice is performed with the flag `--hex`.

Check `aflow --readme=anrl`

```
aflow --prototypermult | --PROTOTYPERMULT <POSCAR
```

Inputs 3 to 10 ary POSCARS, outputs the first alloy of prototype group, which is categorized by `--protoclassify`, from ICSD database.

```
aflow --prototypes | --protos
```

Give the list of prototypes (file LIST.txt) from the DMQC-HTQC project (SC oct 08)

```

aflow [--server=XXXXXXXX] --prototypes_icsd[=N] | --protos_icsd[=N]
Give the list of prototypes from the ICSD database included in the code.
If N is passed, then it returns ONLY the N-ary compounds.
If the ICSD_AFLOW_LIBRARY is not available, the code switches to downloading
information from the server=aflowlib.duke.edu database.
You can force downloading from different servers:
--server=aflowlib.duke.edu
--server=materials.duke.edu
--server=default (switches to aflowlib.duke.edu)

aflow [--server=XXXXXXXX] [--vasp|--qe|--abinit|--aims] --proto_icsd=label
Returns the prototype labeled with the string label, from the
ICSD database.
Example: aflow --proto_icsd=Ba1Ga4_ICSD_659522
Example: aflow --aflowlib.duke.edu --proto_icsd=Ba1Ga4_ICSD_659522
If the ICSD_AFLOW_LIBRARY is not available, the code switches to downloading
information from the server=aflowlib.duke.edu database.
You can force downloading from different servers:
--server=aflowlib.duke.edu
--server=materials.duke.edu
--server=default (switches to aflowlib.duke.edu)
The label can be of this type:
--proto_icsd=ICSD_number.{ABC}[:speciesA*[:speciesB*]..[:volumeA*[:volumeB*].. | :volume]]"
--proto_icsd=label_ICSD_number"

aflow --qe
Transforms the POSCAR (or whichever is the input file format) to a
QUANTUM ESPRESSO GEOM format.
The geometrical file follows the QE convention (see ibrav in QE manual).

aflow --qmvasp [--static] [-D directory]
Given the current directory (or the one specified by -D), aflow
produces the file aflow.qmvasp.out containing thermodynamic information
from relax2 CONTCAR/OSZICAR/OUTCAR (or .static if --static is specified).

aflow --rasmol[=n1[,n2[,n3]]] < POSCAR
Similar to --xyz. Starts rasmol (must be available) with a file
based on the POSCAR input file. If you want to use atom names
you must put them after each atom position in the POSCAR
file (see -names). If any names are missing they are defaulted to H.
If no numbers are specified, aflow takes "1 1 1". (SC/OCT07,OCT14)

aflow --raytrace rtfiler
Outputs jpeg or mpeg pictures created by ray tracing. This
is a rather elaborate routine. The basic idea is that it
takes as input a list of structures (in POSCAR like format)
and converts them into a dat file, inputs that into the ray
tracing program tachyon, then takes the tga file output by
tachyon and uses convert to make it a jpeg, then if needed
takes all the jpegs and puts them together into and mpg using
mpeg_encoder. Therefore the following programs must be
installed and in your path: tachyon, convert, mpeg_encoder
(only if making a movie). There is an input file rtfiler
which contains tokens setting characteristics of the calculation
and the ray traced picture. This input file looks like the
following:

# These set the input for the ray tracing program tachyon
CALCTYPE = 0 #0=strlist
INFILE = strlist # For CALCTYPE=0
OUTFILE = XXX # All output will have this prefix.
RESX = 600 # X pixels in images.
RESY = 500 # Y pixels in images.
ZOOM = 1.5 # Like a zoom lens.
ASPECTRATIO = 1 # Y height / X height.

```

```

ANTIALIASING = 0 # Something to do with extra accuracy.
RAYDEPTH = 12 # Number of reflections to keep in ray trace.
# x,y,z of camera location. Changes incrementally each frame
# from initial to final value. format is ciX cfX ciY cfY ciZ cfZ,
# where i,f denote initial and final, respectively.
# Default is displaced along -Y from structure center.
#CENTER = 1 1 -2 -2 2 4
#VIEWDIR = 1 0 0 # Direction of camera viewing.
#UPDIR = 0 0 1 # Up direction for picture.
BACKGROUND = 0.3 0.1 0.1 # Background lighting (all lights are R G B).
LIGHT = -20 -20 -20 0.01 1.0 1.0 1.0 # Spherical light source: center(3) radius(1) color(3)
LIGHT = 20 20 20 0.01 1.0 1.0 1.0 # Spherical light source: center(3) radius(1) color(3)
ATOMTEXTURE = 1 0.1 0.9 0.0 1.0 # atomtype ambient diffuse specular opacity
ATOMTEXTURE = 2 0.1 0.9 0.0 1.0 # atomtype ambient diffuse specular opacity
ATOMTEXTURE = 3 0.1 0.9 0.0 1.0 # atomtype ambient diffuse specular opacity
ATOMTEXTURE = 4 0.2 0.9 0.3 1.0 # atomtype ambient diffuse specular opacity
ATOMCOLOR = 1 1.0 0.75 0.3 # atomtype(1) color(3)
ATOMCOLOR = 2 0.2 0.4 1.0 # atomtype(1) color(3)
ATOMCOLOR = 3 1.0 1.0 1.0 # atomtype(1) color(3)
ATOMCOLOR = 4 1.0 0.0 0.0 # atomtype(1) color(3)
ATOMRAD = 1 0.6 # atomtype rad
ATOMRAD = 2 0.3 # atomtype rad
ATOMRAD = 3 1.0 # atomtype rad
ATOMRAD = 4 0.8 # atomtype rad
SHADING = mediumshade # fullshade,mediumshade,lowshade,lowestshade
# A supercell matrix given as 9 reals: a11 a12 a13 a21 a22 a23
# a31 a32 a33. Note that using this moves all atoms into images
# the unit cell.
# Default = 1 0 0 0 1 0 0 0 1
SUPERCELL = 1 0 0 0 1 0 0 0 1
# Rotation around x,y,z axis through structure_origin
# (counterclockwise). Rotation take place incrementally each
# frame. Rotation goes from initial to final value.
# format is riX ifX riY rfY riZ rfZ, where i,f denote initial
# and final, respectively.
# Default = 0 0 0 0 0 0
ROTATION = 0 0 0 0 -180 180
# The zero for the structure coordinates and lattice parameters.
# Rotations occur around this point.
# Default = First moment of atom positions.
STRUCTURE_ORIGIN = 0 0 0
PLANE = 1 # 0 for no plane, 1 for plane.
PLANECENTER = 0 0 -9.21016 # X Y Z for center of plane.
PLANENORMAL = 0 0 1 # Direction of plane normal.
PLANECOLOR = 1 1 1 # R G B for plane color.
PLANETEXTURE = 0.3 0.6 0.8 1.0 # ambient diffuse specular opacity for plane.

```

Tokens can be in any order, whitespace is ignored, and anything following a # on a line is ignored. The CENTER, VIEWDIR, and UPDIR depend on the structure and can be a pain to set by hand so they have fairly elaborate defaults that seem to usually work fine. The other values are not bad places to start. For more info about these check out the tachyon documentation.

For a single structure the output consists of XXX.dat, XXX.tga, XXX.jpg, XXX.enc, XXX.mpg. Having all these files is useful if some part of the program did not execute properly and you need to do steps by hand (tachyon XXX.dat produces XXX.tga, convert XXX.tga XXX.jpg produces XXX.jpg, and mpeg_encode XXX.enc produces XXX.mpg). For more than one structure the XXX.dat and XXX.tga files are erased to avoid clutter. The XXX.enc file is used for the mpeg_encode programs and is totally set in aflow and the user has not control over it from the rfile. If you want to alter it after it is output go ahead but I know almost nothing about how it works. To make your own mpg from

the jpg type: mpeg_encode XXX.enc
The tga, jpg files can be viewed with xv and the mpg with mpeg_play.XXX
Note: this routine was written by Dane and readapted by Stefano.
It might not work but require slightly modifications in the C++ source.

TACHYON WEB: <http://jedi.ks.uiuc.edu/~johns/raytracer/>
MPEG_ENCODER: http://bmrc.berkeley.edu/frame/research/mpeg/mpeg_encode.html
CONVERT: <http://www.imagemagick.org/script/index.php>

LINUX: Debian 4.0r1 contains convert ("imagemagick") and
the mpeg_encoder ("ucbmpeg").

aflow --rbanal nim nearest_image_flag
This is meant to allow you to analyse a rubber band calculation
to get energy vs. distance along activation path. The distance
is given a cumulative from the 00 to END images (a line integral),
and also as the total distance from 00 and END for each image.
The first is the activation path, the others are for double checking.
The rubber band run must have had nim images. The distance
between two images is defined to be the square root of the
sum of all the squared distances between all the atoms in the
two images. The distances depend on the
setting of nearest_image_flag (see --intpol). The code works
in two steps. First it gets energies and distances from the
OSZICAR and POSCAR/CONTCAR files, respectively. This
requires that it be run in the directory above all the image
directories. The distances are obtained from POSCAR files
for the first and last images, which are not actually calculated
so now CONTCAR files exists. For intermediate images the
POSCAR files are used. The energies are pulled from the
OSZICAR files. First, these do not exist in the first and
last image directories, so you must put them their yourself
based on other runs (if you leave them out then no energies
will be obtained but you can add the energies later, as described
below). Second, the output format for OSZICAR in a parallel
vasp rubber band run is all messed up. Therefore, the energies
are not E0 values (which are not the energy values of the
images) but the free energy from the line just before the
last E0. This numbers differ somewhat from E0 values. This
whole output formatting problem changes with version of vasp --
I set it up for version 4.4.1 beta. It should also work with
v 454. We should change it to use E0 as soon as possible.
Once the distances and energies have been obtained then they
are interpolated with a cubic spline curve. The spline
interpolation assumes that the derivatives at the end points
are 0. The E.vs.dist data and the spline interpolation are
both output to standard out. If there is any problem with
the energy data (e.g., you need to add end members) then
you can fix it and run the spline interpolation again
independently (see --spline). The spline interpolation is
done on 50 points by default. This can be
changed by setting DEFAULT_NPT_FOR_SPLINE in aflow_pflow_funcs.cpp.

aflow --rbdist POSCAR1 POSCAR2 n|N|e|E
Gets the distance between two POSCAR files. Uses lattice params
of POSCAR1. For use of n|N|e|E see --intpol.

aflow --rdf[=rmax[,nbins[,sigma]]] < POSCAR
Get the radial distribution function (rdf) for a POSCAR file
rmax: The radius out to which the rdf is calculated.
nbins: The number of bins for the rdf.
sigma: The sigma of the gaussian used to smear the rdf.
This also finds the nearest-neighbor shells by looking at
where the rdf has minima. The output gives the rdf and nn shells
for each atom and for each type of neighbour, including a sum
of all neighbour types. If you want to treat all atoms as the
same (e.g., to look at the parent lattice) just set one
type in the POSCAR file. You may need to play with sigma
and the nbins to get atoms grouped together that you want in
one shell but not to group atoms you want in different shells.

One approach is to choose enough bins to make sure to distinguish every shell of interest and then increase sigma until you group desired atoms together.

rmax default = 5
nbins default = 25
sigma default = 0 (zero does no smearing).

aflow --rdfcmp=rmax,nbins,sigma,nshmax,POSCAR1,POSCAR2
Uses the radial distribution functions (rdf) for POSCAR 1 and 2 to assess how close the structures are. For each atom the rdf and radial shell function (rsf - this gives the coordination numbers for each shell) are found for each type. The shells are found by looking at the derivatives of the rdf. Then the atoms of the same types are compared and the rms errors in the rsf for POSCAR1 and POSCAR2 are computed. Then we step through the atoms of POSCAR1, matching them up with the atoms of POSCAR2, based on the minimum rms. When a POSCAR2 atom is matched it is not considered for later matches. The total rms based on these best matches is found by averaging all the individual atom RMS's. The total RMS and the rsf for the best matched atoms are output.

rmax: The radius out to which the rdf is calculated.
nbins: The number of bins for the rdf.
sigma: The sigma of the gaussian used to smear the density.
nshmax: The farthest possible shell used for computing RMS with the rsf (if <nshmax shells are found then fewer will be used).

I think this works but large changes in shape give rsf that are too different to compare exactly and the RMS!=0. However, looking at the output can make it clear how the shells are related. At this point the 2 structure must have the same number of atoms of each type. If you want to compare 2 POSCARs where one is a multiple of the other in terms of atoms of each type you can create supercell (see --supercell) to make this function usable.

aflow --revsg [#] [n] [l] [m]
Constructs a POSCAR of a specified space group and with specified wyckoff positions
is the space group number
n multiplicity of wyckoff site (e.g., do position 4 g 1 twice)
l specifies multiplicity group (e.g., positions with multiplicity 2)
m position within multiplicity group (e.g., 2 would indicate the second position with multiplicity defined by l). (R. Taylor).

aflow --rm_atom iatom < POSCAR
Outputs to standard out a POSCAR where iatom has been removed.
iatom must be between 0 to N-1.

aflow --rm_copies < POSCAR
Outputs to standard out a POSCAR where only the first appearance of each cartesian position of the same type atom has been kept. Useful if you have multiple copies of atoms at the same positions for some reason. Note. This routine does not compare equivalent lattice positions so you are not sure that equivalent atoms are not in the same place.

aflow --rsm < POSCAR
Outputs to standard out a Rasmol (rsm) format file based on the POSCAR input file. This output can be saved as .rsm file and is designed to be visualized in simpler version of Rasmol which is called RasTop program. It might work in Rasmol program directly. The format includes the plotting of the unit cell wireframe and spacefill 150 for the atomic radius. (WS Sept07)

aflow --rsm --z z_type1 z_type2 ... z_typeNtypes < POSCAR
Similar to aflow -rsm, with additional option of atom labeling based on the atomic number (z) of each type. If --z option is not used, the default is --z 1 2 3 ... Ntypes. (WS Sept07)

aflow --sc | --std_conv | --standard_conventional | --sconv < POSCAR

Output POSCAR in a standard conventional lattice
 (use `--sp` | `--std_prim` | `--standard_primitive` | `--sprim`
 to output POSCAR in a standard primitive lattice) (WS & SC Nov09)
 REF: Setyawan Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010

`aflow --scale=s < POSCAR`
 Outputs POSCAR file giving same volume as input but
 with scale = s.

`aflow --sd AA1 AA2 ... < POSCAR`
 Outputs to standard out a POSCAR with selective dynamics
 formatting. AAi gives the selective dynamics setting for
 atoms of type i and has the form AAi=TTT,TTF,etc.. If there
 are fewer AAi than atom types then the remaining types are
 defaulted to TTT. A warning will be printed and the default
 value of TTT will be used if the AAi strings are shorter
 than three characters. (SC0907)

`aflow --setcm cm1 cm2 cm3 < POSCAR`
 Sets to center of mass to (cm1,cm2,cm3) by shifting all the
 atom positions. Use `--mom` to check the shift was correct.

`aflow --setorigin r1 r2 r3 | atom# < POSCAR`
 With r1 r2 r3, it sets the origin to r1,r2,r3 by shifting all the
 atom positions. Coordinates (r1,r2,r3) are considered fractional
 is the POSCAR is in fractional, and cartesian otherwise.
 With atom#, it sets the origin to the position of atom#
 (atom# goes from 0 to size-1).

`aflow --sewald eta < POSCAR`
 Finds the screened electrostatic energy of the POSCAR file using a
 real space sum. eta is now the screening length (ie, all
 coulomb interactions are multiplied by $\exp(-\eta * R)$.
 Charges must be entered after each atom position.
 E.g., Co 0 0 0 +2.

`aflow --shell=ns,r1,r2,name,dens < POSCAR`
 Based on the structure in POSCAR, this outputs to standard
 out all points with ns neighbors in a shell define by inner
 radius r1 and outer radius r2 ($r1 < r2$). The shell is
 restricted to only consider atoms of type name (name=NONE (""))
 is unrestricted). The dens is the linear density of
 candidate points. So for example, to search for all sites with
 4 oxygen around them between 1.8 and 2.2 Angstrom you could type
`aflow --shell=4,1.8,2.2,0,20`
 This would construct a 20x20x20 grid of puts in the cell and
 print out all points that met the shell criteria. The output
 gives all the points and their shells meeting the shell criteria.
 However, since many points are in the same shell it is
 convenient to find unique shell environments. Therefore, aflow
 reduces the complete list to keep only one representative point
 from each unique shell. The shells are distinguished by their
 centers of mass. The unique points and their shells are output
 as all unique points meeting the shell criteria. The
 representative point for each shell is the shell center of mass.
 This routine is great for finding open tetrahedral and octahedral
 sites where one might put an intercalant. This routine can
 take a while to run (usually a 20x20x20 mesh is enough, and might
 take a couple of minutes for a big cell - start small!).

`aflow --shift=Sx,Sy,Sz[,cCdD] < POSCAR`
 Outputs to standard out a POSCAR with all positions shifted by
 $S=(Sx,Sy,Sz)$. The shifted is added to the positions. The shift
 is assumed to be given in Cartesian coordinates unless you specify
 c or C for Cartesian or d or D for direct at the end.

`aflow --sitepointgroup | --agroup < POSCAR`
 Calculates the site point group symmetry for every atom in the
 unit cell and writes it in the aflow.agroup.out file.
 See documentation of aflow.

`aflow --spacegroup radius < POSCAR`
 Calculates space group symmetry of the cell {R|t+T} with

translations as big as |T| and writes it in the aflow.sgroup.out file. See documentation of aflow.

Be careful because the size of the space group increases as the radius³ times the size of the factor roup.

The point and factopr groups are required for the space group, therefore the aflow.pgroup.out and aflow.fgroup.out files will be generated as well.

```
aflow --sqs=structure_type,atom_num,neighbour_num,sl_num_min,sl_num_max,A,B | --special-quasirandom-structure
Generate special-quasirandom-structure (SQS)
structure: bcc/fcc/hcp
atom_num : maximum number of atoms in a cluster
neighbour_num : maximum number of nearest neighbour pairs in a cluster
sl_num_min : minimum number of the base structure in the superlattice
sl_num_max : maximum number of the base structure in the superlattice
```

To generate sqs bcc structure, one needs first to generate a 'cluster' file and a bcc superlattice file. Use the following commands to get sqs bcc from 5 to 8 atom/cell of AuCu alloy with energy calculated by using cluster expansion method with cluster containing up to 6th nearest neighbour pairs.

=====

1. Get cluster file. Number of atoms in a cluster is from 1 to 2 and distance of two atoms in a cluster is from the 1st to the 6th neighbour distance.

```
aflow --cluster=bcc,1,2,1,6
```

2. Get all supercell configuration. Here we get supercell with 8 atom. The first 5 is the smallest number of atoms in a supercell and the second one is the largest number.

```
aflow --superlattice=bcc,6,8
```

3. Get SQS. Check correlations of clusters with up to 2 atoms and 6th neighbour distance. You can give any two element names for the last two arguments.

```
aflow --sqs=bcc,2,6,5,8,Au,Cu
```

```
aflow --species < POSCAR
Outputs the species names, as taken from the 1st representative atom of each set.
```

```
aflow --spline npt < file
Outputs to standard out a cubic spline interpolation of npt evenly spaced points. The input file must be two columns giving X and Y(X). The derivatives at the endpoints are assumed to be zero. To change this, change yp1 and ypn in the SetSpline function in the aflow_pflow_funcs.cpp file.
```

```
aflow --sp | --std_prim | --standard_primitive | --sprim < POSCAR
Output POSCAR in a standard primitive lattice
(use --sc | --std_conv | --standard_conventional | --sconv
to output POSCAR in a standard conventional lattice) (WS & SC Nov09)
REF: Setyawan Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010
```

```
aflow --statdiel OUTCAR*
Extracts and diagonalizes the static dielectric constant tensor from the output of a DFPT run (see the aflow "DIELECTRIC_STATIC" tag). The input OUTCAR can be in one of two formats: plain text (regular VASP output), or compressed with the bzip2 utility (OUTCAR*.bz2). The routines attempt to symmetrize the tensor to within a tolerance (currently set to 1.0e-5) prior to diagonalization. The output is a single row containing 6 numbers. The first three are the real-valued diagonal terms of the tensor eps(xx), eps(yy), epz(zz); while the second set of three contain any imaginary eigenvalues that would result from a failure of the ad-hoc symmetrization procedure. Example corresponding to Al1As1_ICSD_67784:
input: aflow --statdiel OUTCAR.dielectric_static.bz2
output: 8.772122 8.772122 8.772122 0.000000 0.000000 0.000000
```

```

aflow --suffix=[directory,]"from2to"
Change the suffixes of VASP files. Easy conversion between AFLOW format and VASP format. (KESONG Dec. 2012)
Mnemonic: from2to with from/to =[n=none;r1=relax1;r2=relax2;r3=relax3;s=static;b=bands] or without abbreviation
Changes suffix of all VASPFILES from VASPFILE*"from" to VASPFILE*"to".
If a directory is specified (e.g. aflow --suffix=abc,n2s)
then it change abc/VASPFILE*"from" to abc/VASPFILE*"to"
Example: aflow --suffix=n2s (or --suffix=none2static)
Change VASPFILE* to VASPFILE*.static
Example: aflow --suffix=s2n (or --suffix=static2none)
Change VASPFILE*.static to VASPFILE*

```

```

aflow --sumpdos pdos.in PROOUT

```

```

Works for vasp.46x
This allows you to sum up projected DOS together for convenient
plotting. It only works when you have run with the following
INCAR file settings. LORBIT=1 or 2 and set RWIGS, or
LORBIT = 11 or 12 and no RWIGS (only works when using PAW PP).
If you are running parallel you must set NPAR=1. The
input file is similar to --pdos above but somewhat simpler
so I give a full example here.

```

```

# Input for aflow --sumpdos.

# These values you supply once.
SPIN = 1 # 1 = non-spin polarized, 2 = spin polarized
# Default 1
EFERMI = -999 # This will be subtracted from the energies.
# Set to 0 to subtract nothing, -999 to use
# the E_Fermi in the DOSCAR. Default -999.
NLM = 9 # number of orbitals, 9 (spd:1+3+5) or 16 (spdf:1+3+5+7)
# Default 9
PRINT_PARAMS = 0 # 0=prints only data (easy to plot).
# 1=prints all the input parameters.
# default: 0

# You can have as many cases as you want.
# They are all added together.

# case 1: t2g on atom 1
ATOMS = 1 # default: no atoms
LMVALUES = 5 6 8 # default: no lm
# case 2: eg on atoms 2 and 3
ATOMS = 2 3 # default: no atoms
LMVALUES = 7 9 # default: no lm

```

```

All # denote comment lines and can be put anywhere.
Each case is started when the token ATOMS is used.
Following an ATOMS token, all LMVALUES tokens
will apply to the atoms denoted in the preceding
ATOMS token until the next ATOM token. You can have any number
of cases, and the results for all cases are added together.
WARNING: make sure to use SPIN to set if it is a spin polarized
calculation, make sure to use EFERMI to your desired reference,
and make sure to set NLM to 9 (spd) or 16 (spdf).
The lm values correspond to orbitals by the following scheme.

```

```

Input number: 1 2 3 4 5 6 7 8 9
Orbitals:      S Py Pz Px Dxy Dyx Dz2 Dxz Dx2-y2
Input number: 10 11 12 13 14 15 16
Orbitals:      F1 F2 F3 F4 F5 F6 F7

```

```

aflow --supercell=a11,a12,a13,a21,a22,a23,a31,a32,a33 < POSCAR

```

```

aflow --supercell=a11,a22,a33 < POSCAR

```

```

aflow --supercell=file < POSCAR

```

```

Outputs to standard out a supercell of the input POSCAR file.
This lattice vectors of the supercell are given by multiplying

```


the original cell parameters by the 3x3 matrix a_{ij} coefficients. The supercell need not be integral combinations of the original lattice vectors, although using fraction may cause you to end up with a lattice inequivalent to your original. This can be used to build big supercells, swap lattice vectors, etc. The nine numbers must be separated spaces, and they form the nine elements $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}$ of the 3x3 supercell matrix, respectively. If you specify only 3 numbers, the other six are taken zero. If you use the "file" syntax, nine numbers are read from file. They can be on one or multiple lines. New algorithm by SC (aug07).

```

aflow --supercell_strlist=a11,a12,a13,a21,a22,a23,a31,a32,a33,strlist
aflow --supercell_strlist=a11,a22,a33,strlist
aflow --supercell_strlist=file,strlist

```

Outputs to standard out a sequence of structures in POSCAR format. The structures are supercells formed using the supercell matrix $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}$. If only 3 values are specified the other are taken to be zero. If you use the "file" syntax, nine numbers are read from file. They can be on one or multiple lines. For more information on supercells see --supercell. For more information on a strlist see --make_strlist.

```

aflow --superlattice=structure_type,n_min,n_max < POSCAR
      --superlattice=VASP,structure_type,A,B < superlattice_name
Generate a superlattice of base structure POSCAR
structure_type : fcc/bcc/hcp
n_min, n_max : minimum and maximum numbers of base structures in the superlattice

```

```

aflow --swap specie1 specie2 < POSCAR
Swap the specie number 1 with the specie number 2.
It is useful if you forgot to put the POSCAR in alphabetic mode.

```

```

aflow --terdata=Aa:Bb:Cc [--fonts=XX | --keep=eps | --print=jpg | --print=gif | --print=png]
Inputs are the elements in alphabetic order. Output is ternary convexhull named
"phasediagram_AaBbCc.num.pdf". The num is the calculated number of compounds.
EX:
aflow --terdata=Nb:Pt:Rh
No matter the order of the elements, the list is alphabetized.
Options
--fonts=XX  specity the size of gnuplot fonts, default 50
--keep=eps  avoid to delete the postscript before making the pdf
--print=jpg  adds the jpg picture
--print=gif  adds the gif picture
--print=png  adds the png picture

```

```

acovasp --terdata_exist list
The list is the one containing each element for the systems for a certain format.
Each element should be alphabetical order. Put 2 strings before each elements.
EX:
aflow --terdata_exist system

```

INPUTS EX:

```

empty empty Al Co Mn
empty empty Co Ge Mn

```

```

aflow --terdata A B C list
Inputs are the elements in alphabetic order and extra data for the list. Output is ternary convexhull named
"phasediagram_ABC.num.pdf". The num is the calculated number of compounds.
list type is:
ADDRESS1  COMPOUND_NAME1
ADDRESS2  COMPOUND_NAME2
...      ...
EX:
aflow --terdata terdata Nb Pt Rh list

```

```

aflow --uffenergy | --ue < POSCAR
    Output the energy of the structure using the simplified Universal Force Filed (UFF) method [JACS, 114,

aflow --vasp
    Transforms the GEOMETRICAL (or whichever is the input file format) to a
    VASP format.

aflow --volume v < POSCAR
    Outputs POSCAR file giving having volume equal to v.
aflow --volume*= x < POSCAR
aflow --volume+= x < POSCAR
    Outputs POSCAR with volume changes as *=, += actor (like in c,c++).

//DX - START
aflow --wyccar[=tolerance | =tight | =loose] < POSCAR
    Prints the wyccar file (the poscar file with wyckoff positions) for the input POSCAR
    The wyccar format presents the lattice in standard conventional form and the wyckoff
    positions with their associated labels and site symmetry. If variability in the
    Wyckoff positions exists, the algorithm finds the Wyckoff positions with the "smallest"
    lettering scheme ("a" being the smallest). (R. Taylor/ D. Hicks)
//DX - END

aflow --xray=lambda < POSCAR
    Outputs to standard out the powder xray scattering pattern for
    the structure specified in the POSCAR input file. The
    wavelength of the scattering radiation is taken to be 1.
    The xray calculation is almost nothing more that the structure
    factor, although it includes approximate treatments of the
    Debye-Waller terms and the Lorentz-polarization. In the xray
    calculations there are a number of terms that require a lot of
    information to really do right so I approximate them. First,
    scattering factors default to the atomic number. In some cases
    I coded more accurate values taken from tables for lambda=1.5418.
    No lambda dependence of the scattering factors is presently
    included. For the list of all coded atomic scattering factors
    see the constructor for the structure class in structure.cc.
    I include the Lorentz-polarization and an approximate
    Debye-Waller factor (DWF). The DWF is found assuming T=300,
    T_Debye=300, and within the high-temperature Debye aproximation.
    The atomic mass defaults to twice the atomic number but I
    have input a few more accurate values in the code. For the
    list of all coded atomic masses see the constructor for the
    structure class in structure.cc. This simulation should
    give very accurate peak locations and qualitative relative
    integrated intensities (peak heights). I am still not
    happy with why the peak intensities do not reproduce other
    codes better. The output contains formats with and without
    peaks at the same 2theta grouped together. It also contains
    data ready for plotting. Each type of data has a keyword on
    every line so you can grep it out easily.
aflow --xrd_dist=h,k,l < POSCAR
    Compute Miller plane distance (distance between planes of atoms). The triplet h,k,l
    defines the plane spanned by the three points a/h,b/k,c/l, where a b c
    are the CONVENTIONAL lattice vectors. You may enter h,k,l as integers
    (e.g., 1 2 3), decimal numbers (e.g., 0.56 .4 .5), or fractions (e.g., 1/2 3/4 4/5)
    or any combination of the three. The POSCAR must be in conventional form to get
    meaningful results. You may first use the aflow command "aflow --sc < POSCAR" to get
    standard conventional. For example,
    cat POSCAR | aflow --sc | aflow --xrd_dist=1,0,0
aflow --xyz[=n1[,n2[,n3]]] < POSCAR
    Outputs to standard out an xyz file based on the POSCAR input
    file. This can be used as input for rasmol, xmol, etc..
    If you want atom names you must put them after each atom
    position in the POSCAR file (see -names). If any names are
    missing they are defaulted to H.

```

```

aflow --xyzwignerseitz [--xyzws] < POSCAR
  Performs "aflow --xyz=1,1,1" but moves the images
  of the atoms in the Wigner-Seitz cell. This parameter
  is usefull to fight against VASP trend of moving atoms
  in different (but traslationally equivalent) positions
  of the unit cell. (SC 10Jan04).

aflow --zval[=directory]
  Outputs from the available POTCAR/OUTCAR the sum of ZVAL.
aflow --zval_atom[=directory]
  Outputs from the available POTCAR/OUTCAR and POSCAR/CONTCAR the ZVAL of the cell per atom.
aflow --zval_cell[=directory]
  Outputs from the available POTCAR/OUTCAR and POSCAR/CONTCAR the ZVAL of the whole cell.

```

FROZSL MODE

```

aflow --frozzsl_vaspsetup_aflow | --frozzsl_vaspsetup < FROZSL.output
  Takes the FROZSL.output (the one containing all representations
  and deformations) and makes the POSCAR part of the aflow.in.
  All the calculations are ready to be ran as they are enclosed
  in START.XXXX/STOP.XXXX frameworks and a AFLOW_POSTSCRIPT is
  generated to extract all the energies for the various directories.
  If another parameter is passed: i.e.
  aflow --frozzsl_vaspsetup_aflow --file
  then the command used to make the POSCARs is printed.
  (Mike Mehl Dec 09).

aflow --frozzsl_vaspsetup_poscar < FROZSL.output
  Takes the FROZSL.output (the one containing all representations
  and deformations) and makes all the POSCARs.
  If another parameter is passed: i.e.
  aflow --frozzsl_vaspsetup_poscar --file
  then the command used to make the POSCARs is printed.
  (Mike Mehl Dec 09).

aflow --frozzsl_analyze < aflow.frozzsl.out
aflow --frozzsl_readme | --frozzsl_help
  A short introduction to frozzsl calculations.

```

APENNSY MODE (this routines are available only in duke.edu domine)

```

aflow --xfixX system structure
  Repairs the convex-hull calculation by removing
  $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB2))/LIB/RAW/system/structure
  and copying
  $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB2))/LIB/LIB/system/structure
  into
  $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB2))/LIB/FIX/system/structure
  You have to go by hand and check the problem (rare) and
  probably clean and rerun the structure.
  The exact command is included in pflow::XFIXX which
  is inside aflow_pflow_main.cpp

```

ALL LIBRARIES MODES

```

aflow [--force] --lib2raw=all[,directory]
  Searches all the subdirectories of 'pwd'/LIB/ and updates 'pwd'/RAW/ and 'pwd'/WEB/
  entries for the missing ones. With directory specified, it searches on directory/LIB/
  It works only on AFLOW_MATERIALS_SERVER (defined in aflow.h).
  With "--force" it overwrites the old raw files if they exist.

```

LIB1/LIB2/LIB3/LIB4/LIB5/LIB6 MODE (this routines are available only in duke.edu domine)

```

  Scripts for the production/maintenance of the LIB* libraries.
  The "all" works only if 'pwd' = $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB*))

```

```

aflow [--force] --lib2raw=directory
aflow [--force] --lib2raw=Al_h/bcc
  From the $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB*))/LIB/directory_including_lattice
  calculation generates the RAW library
  $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_LIB*))/RAW/directory_including_lattice
  which includes the files necessary for the LIB* project
  analisys: aflow.in LOCK
If *static files are present, the DOS is calculated.
If *bands files are present, the electronic structure is calculaterd.
  It works only on AFLOW_MATERIALS_SERVER (defined in aflow.h),
  and it has been written for the LIB* project.
  It can be used also for LIB* directories.
  With "--force" it overwrites the old raw files if they exist.

```

ICSD LIBRARY MODE

```

  Scripts for the production/maintenance of the ICSD library.
  The "all" works only if 'pwd' = $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD))
aflow [--force] --lib2raw=directory
aflow [--force] --lib2raw=FCC/La1Se1_ICSD_27104
  From the $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD))/LIB/directory_including_lattice
  calculation generates the RAW library
  $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_ICSD))/RAW/directory_including_lattice
  which includes the files necessary for the ICSD project
  analisys: aflow.in LOCK DOSCAR.static. EIGENVAL.bands
  KPOINTS.bands POSCAR.bands.
  It works only on AFLOW_MATERIALS_SERVER (defined in aflow.h),
  and it has been written for the ICSD project.
  With "--force" it overwrites the old raw files if they exist.

```

LIB1/LIB2/LIB3/LIB4/LIB5/LIB6/AURO LIBRARY MODE

```

  Scripts for the production/maintenance of the LIB1/LIB2/LIB3/LIB4/LIB5/LIB6/AURO library.
  The "all" works only if 'pwd' = $(vAFLOW_PROJECTS_DIRS.at(LIB*)) or
  The "all" works only if 'pwd' = $(vAFLOW_PROJECTS_DIRS.at(XHOST_LIBRARY_AURO))
aflow [--force] --lib2raw=directory

```

AFLOWLIB MODE

```

aflow --aflowlib=entry
  Create the WEB/PHP page for the entry specified as auid or aurl. It works where the complete
  databases have been installed.

aflow --aflowlib_auid2aurl=auid1,auid2... | --auid2aurl=...
  Searches the available AUIDs and reports the AURLs if found.
Comp. Mat. Sci. 93, 178 (2014). [doi=10.1016/j.commatsci.2014.05.014] for more information.

aflow --aflowlib_aurl2auid=aurl1,aurl2... [ --aurl2auid=...
  Searches the available AURLs and reports the AUIDs if found.
Comp. Mat. Sci. 93, 178 (2014). [doi=10.1016/j.commatsci.2014.05.014] for more information.

aflow --aflowlib_auid2loop=auid1,auid2... | --auid2loop=...
  Searches the available AUIDs and reports the postprocessed "loop" if found.
Comp. Mat. Sci. 93, 178 (2014). [doi=10.1016/j.commatsci.2014.05.014] for more information.

aflow --aflowlib_aurl2loop=aurl1,aurl2... [ --aurl2loop=...
  Searches the available AURLs and reports the postprocessed "loop" if found.
Comp. Mat. Sci. 93, 178 (2014). [doi=10.1016/j.commatsci.2014.05.014] for more information.

```

```

*****
*
*           aflow - STEFANO CURTAROLO Duke University 2003-2017
*           High-Throughput ab-initio Computing Project
*
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