

AFLOW V 3.1.137

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*
*           aflow - STEFANO CURTAROLO Duke University 2003-2017
*           High-Throughput ab-initio Computing Project
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LATEST VERSION OF THE FILE:           materials.duke.edu/AFLOW/aflow_apennsy.pdf
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APENNSY MODE (SC 2009-2014: the pennsy project)
aflow --apennsy ... then --help OR
Load library options are:
--lib2 (loads LIB2 of binary alloys)
--alloy Element1Element1...
--list (gives a list of available alloys)
One of the two options MUST be specified to enter in apennsy mode.

MODIFIERS

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--server=aflow.org
Connects to aflow.org and download the list of servers containing
thermodynamic informations.
Uses the aflowlib REST-API to download the data (default if apennsy
does not find the LIB* directories in the server).
--neglect=1,2,3,4,5,662.AB,
Neglects structure /1/ /2/ ... /662.AB/ ... from the phase diagram
--noclean
In this case you need to specify the correct alloy with pseudopotential,
e.g. --alloy AgMo_pv, and you will receive the file with the right name.
Output options are:
--hull (prepare gnuplot/matlab code for the convex hulls)
it will run as "gnuplot code" or "matlab -nodesktop -r file ..."
--shull (prepare matlab code for the small convex hulls)
it will run as "gnuplot code" or "matlab -nodesktop -r file ..."
--matlab (use matlab to plot)
--gnuplot (use gnuplot to plot DEFAULT)
--energy (prepare the latex code for the pdf analisys)
--nolatex (remove latex stuff from output)
--print=html (makes html code when appropriate)
--print=hyperlinks (add hyperlinks to the LATEX/HTML code)
--reference (|ref) gives the reference paper for that system
--update (loads the alloy, makes the picture and makes the pdf)
--keep="fileextensions_separated_by_commas"
"tex" keeps *.tex during the process (if appropriate)
"eps" keeps *.eps during the process (if appropriate)
"dvi" keeps *.dvi during the process (if appropriate)
"toc" keeps *.toc during the process (if appropriate)
"GPL or gnuplot" keeps gnuplot code during the process (if appropriate)
"MAT or matlab" keeps matlab code during the process (if appropriate)
"jpg" keeps *.jpg during the process (if appropriate)
"png" keeps *.png during the process (if appropriate)
"gif" keeps *.gif during the process (if appropriate)

--cite add appropriate \\cite{} after the alloy title
--snapshot
wrap up containing --update, --keep=tex, --cite, --print=hyperlinks
--data (prints raw data in self-explanatory form for other codes)
--web (prints input file for the web awrapper page)
--all --fcc --bcc --hcp
--uncle (prints input file for uncle cluster expansion program)
--fcc --bcc --hcp
--Htot | --enthalpy_total
(print the total enthalpy of the unit cell)
--Hat | --enthalpy_atom
(print the enthalpy per atom in the unit cell)
(if no enthalpy mode is chosen, then Htot is the default).
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--Hfat | --enthalpy_formation_atom
    (prints the enthalpy per atom in the unit cell)
    (if no enthalpy mode is chosen, then Htot is the default).
--mix | --miscibility
    (makes the aflow_nomix.cpp file for automatic miscibility
    determination, cutoff is MISCIBILIT_SYSTEM_CUTOFF
    and it is in aflow.h)

--information
    Prints information of each calculation in seconds
    time(secs) cores(int) time*cores(secs) mem(MB)

--experiments
    Prints the prototype of the aflow_mix_experiments.cpp file
--miedema
    Prints the Miedema predictions
--humerothery
    Prints the Hume-Rothery predictions
--statistics
    Prints statistics
--order
    Order project (values in meV)
--rules
    Rules project for LIBRARYU
--protocheck
Check the relaxed POSCARs and fix name in phase diagram
--oss=cout
    Prints in "cout" mode.

Output pictures format are (through matlab code):
--print=eps (not necessary, it will always write eps pictures) // XHOST.vflag
--print=jpg (make the matlab code to create the jpg pic) // XHOST.vflag
--print=pdf (make the matlab code to create the pdf pic) // XHOST.vflag
--print=gif (make the matlab code to create the gif pic) // XHOST.vflag
--print=png (make the matlab code to create the png pic) // XHOST.vflag
--quiet (writes less on the picture, usefull for websites)

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EXAMPLE

If you have gnuplot and wget available, this command should produce a pdf:
aflow --alloy AgCd --hull --energy

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