

AFLOW V 3.1.146

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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.
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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
  (prints the total enthalpy of the unit cell)
--Hat | --enthalpy_atom
  (prints 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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