

## AFLOW V 2998.05

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*           AFlow - STEFANO CURTAROLO MIT/DUKE 2003-2009           *
*           High Throughput Ab-initio Computing Project           *
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Contributors: 2000-2009, Stefano Curtarolo (aflow aconvasp apennsy)
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LATEST VERSION OF THE FILE:      http://materials.duke.edu/auro/apennsy.pdf
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APENNSY MODE (SC 2009: the pennsy project)

aconvasp --apennsy

Switch to pennsy mode. You must have the RAW files in  
/common/GNDSTATE/LIBRARY\*/RAW

Currently installed only in nietzsche.mems.duke.edu.

Instead of "aconvasp --apennsy" you can use "apennsy".

Library options are:

--libraryG (loads LIBRARYG)

--libraryU (loads LIBRARYU)

--libraryX (loads LIBRARYX)

--alloy AA|AABB (load all alloys \*AA\* or \*AABB\*)

Output options are:

--hull (prepare matlab code for the convex hulls)

it will run as "matlab -nodesktop -r file ..."

--shull (prepare matlab code for the small convex hulls)

it will run as "matlab -nodesktop -r file ..."

--energy (prepare the latex code for the pdf analisis)

--data (prints raw data in self-explanatory form for other codes)

--uncle (prints input file for uncle cluster expansion program)

--fcc (pick the fcc structures)

--bcc (pick the bcc structures)

--hcp (pick the hcp structures)

--etot | --energy\_total

(prints the total energy of the unit cell)

--eat | --energy\_atom | --energy\_atomic

(prints the energy per atom in the unit cell)

(if no energy mode is chosen, then E\_tot 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)

--time

Prints the times of each calculation in seconds

--xaflowauto

Makes the xaflowauto for the qsub input file

--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

Output pictures format are (through matlab code):

--eps (not necessary, it will always write eps pictures)

--jpg (make the matlab code to create the jpg pic)

--gif (make the matlab code to create the gif pic)

--png (make the matlab code to create the png pic)

--htm (creates the htm loading code)

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