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_pocc.pdf
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One example of the high-throughput first-principle calculations for partial occupied
structure (mostly written by Kesong Yang).

1) Prepare your aflow.in input files:

[AFLOW] ***************************************************************************************************
[AFLOW]SYSTEM=Ga0.25In0.75P
[AFLOW] ***************************************************************************************************
[AFLOW] input file for aflow
[AFLOW_MODE=VASP]
[AFLOW] ***************************************************************************************************
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp46s]
[AFLOW] ***************************************************************************************************
[AFLOW] ***************************************************************************************************
#[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE]NCPUS=MAX
[AFLOW_MODE_MPI_MODE]COMMAND ="mpirun -np"
[AFLOW_MODE_MPI_MODE]AUTOTUNE
[AFLOW_MODE_MPI_MODE]BINARY="mpivasp46s"
[AFLOW] ***************************************************************************************************
[AFLOW_SYMMETRY]CALC
#[AFLOW_SYMMETRY]SGROUP_WRITE
#[AFLOW_SYMMETRY]SGROUP_RADIUS=7.77
[AFLOW] ***************************************************************************************************
#[AFLOW_NEIGHBOURS]CALC
[AFLOW_NEIGHBOURS]RADIUS=7.7
[AFLOW_NEIGHBOURS]DRADIUS=0.1
[AFLOW] ***************************************************************************************************
#[AFLOW_APL]CALC                                    // README_AFLOW_APL.TXT
[AFLOW_APL]ENGINE=DM                                // README_AFLOW_APL.TXT
[AFLOW_APL]DMAG=0.015                               // README_AFLOW_APL.TXT
[AFLOW_APL]MINATOMS=100                             // README_AFLOW_APL.TXT
#[AFLOW_APL]SUPERCELL=3x3x3                         // README_AFLOW_APL.TXT
[AFLOW_APL]DC=y                                     // README_AFLOW_APL.TXT
[AFLOW_APL]DPM=y                                    // README_AFLOW_APL.TXT
[AFLOW_APL]ZEROSTATE=y                              // README_AFLOW_APL.TXT
[AFLOW_APL]DOS=y                                    // README_AFLOW_APL.TXT
[AFLOW_APL]TP=y                                     // README_AFLOW_APL.TXT
[AFLOW_APL]TPT=0:2000:10                            // README_AFLOW_APL.TXT
[AFLOW] ***************************************************************************************************
#[AFLOW_QHA]CALC                                    // README_AFLOW_APL.TXT
[AFLOW_QHA]GP_VOL_DISTORTION_PERCENTAGE=0.03        // README_AFLOW_APL.TXT
[AFLOW_QHA]DISPLACEMENTS=y                          // README_AFLOW_APL.TXT
[AFLOW_QHA]PROJECTION_DIR=1:1:1                     // README_AFLOW_APL.TXT
[AFLOW_QHA]EOS=n                                    // README_AFLOW_APL.TXT
[AFLOW_QHA]EOS_VOLRANGE_DIST=-2:4:0.5               // README_AFLOW_APL.TXT
[AFLOW_QHA]EOS_KPOINTS_MODE=32768:10000:20:100000   // README_AFLOW_APL.TXT
[AFLOW] ***************************************************************************************************
#[AFLOW_AAPL]CALC                                   // README_AFLOW_APL.TXT
[AFLOW_AAPL]TDMAG=0.015                             // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUT_SHELL=4                             // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUT_RAD=4.5                             // README_AFLOW_APL.TXT
[AFLOW_AAPL]SUMRULE=1E-5                            // README_AFLOW_APL.TXT
[AFLOW_AAPL]BTE=FULL                                // README_AFLOW_APL.TXT
[AFLOW_AAPL]THERMALGRID=21x21x21                    // README_AFLOW_APL.TXT
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[AFLOW_AAPL]ISOTOPE=y                                    // README_AFLOW_APL.TXT
[AFLOW_AAPL]CUMULATIVEK=y                                // README_AFLOW_APL.TXT
[AFLOW_AAPL]BOUNDARY=n                                   // README_AFLOW_APL.TXT
[AFLOW_AAPL]NANO_SIZE=100                                // README_AFLOW_APL.TXT
[AFLOW_AAPL]TCT=200:700:20                               // README_AFLOW_APL.TXT
[AFLOW] ****************************************************************************************************
[VASP_RUN]RELAX_STATIC_BANDS=2                           // GENERATE STATIC RELAX=N RELAX_STATIC=N STATIC_BANDS RE
#[VASP_FORCE_OPTION]NEGLECT_NOMIX
[VASP_FORCE_OPTION]CHGCAR=ON                            // ON | OFF (default ON)
[VASP_FORCE_OPTION]KEEPK
#[VASP_FORCE_OPTION]KPOINTS=EVEN                         // EVEN | ODD (default none)
#[VASP_FORCE_OPTION]KPOINTS_KSHIFT_GAMMA=EVEN           // EVEN | ODD (default none)
#[VASP_FORCE_OPTION]KPOINTS_KSCHEME=MONKHORST_PACK      // MONKHORST_PACK | GAMMA (manual)
#[VASP_FORCE_OPTION]KPOINTS_GAMMA
#[VASP_FORCE_OPTION]KPOINTS_IBZKPT
[VASP_FORCE_OPTION]SYM=ON                                // ON | OFF  (default ON)
[VASP_FORCE_OPTION]AUTO_PSEUDOPOTENTIALS=potpaw_PBE     // pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_P
[VASP_FORCE_OPTION]NBANDS                                // Estimate Bands (better than VASP)
[VASP_FORCE_OPTION]SPIN=OFF   // (ON | OFF  (default ON)), REMOVE_RELAX_1 | _2
[VASP_FORCE_OPTION]AUTO_MAGMOM=ON                       // ON | OFF (default OFF)
[VASP_FORCE_OPTION]RELAX_MODE=FORCES                     // ENERGY | FORCES | ENERGY_FORCES | FORCES_ENERGY (defau
[VASP_FORCE_OPTION]PREC=HIGH                             // (LOW | MEDIUM | NORMAL | HIGH | ACCURATE), PRESERVED (
[VASP_FORCE_OPTION]ALGO=FAST                             // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (
[VASP_FORCE_OPTION]RELAX
#[VASP_FORCE_OPTION]NOTUNE
[VASP_FORCE_OPTION]TYPE=INSULATOR                        // METAL | INSULATOR | SEMICONDUCTOR | DEFAULT (default D
[VASP_FORCE_OPTION]CONVERT_UNIT_CELL=SPRIM       // SPRIM, SCONV, NIGGLI, MINK, INCELL, INCOMPACT, WS, CART, FR
#[VASP_FORCE_OPTION]VOLUME+=10.0
#[VASP_FORCE_OPTION]VOLUME*=1.05
[AFLOW] ****************************************************************************************************
[AFLOW] ****************************************************************************************************
[VASP_INCAR_MODE_EXPLICIT]START
SYSTEM=Ga0.25In0.75P
#NELM = 120
NELMIN=2
LPLANE=.TRUE.
LREAL=.FALSE.
LSCALU=.FALSE.
PSTRESS=000                                              # for hand modification
#NBANDS=XX                                               # for hand modification
#IALGO=48                                                # for hand modification
[VASP_INCAR_MODE_EXPLICIT]STOP
[AFLOW] ****************************************************************************************************
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE]KSCHEME=G
[VASP_KPOINTS_FILE]KPPRA=1000
[VASP_KPOINTS_FILE]STATIC_KSCHEME=G
[VASP_KPOINTS_FILE]STATIC_KPPRA=3000
[VASP_KPOINTS_FILE]BANDS_LATTICE=AUTO
[VASP_KPOINTS_FILE]BANDS_GRID=20
[AFLOW] ****************************************************************************************************
[AFLOW] ****************************************************************************************************
[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE]Ga
[VASP_POTCAR_FILE]In
[VASP_POTCAR_FILE]P
[AFLOW] ****************************************************************************************************
[AFLOW] ****************************************************************************************************
[POCC_MODE_EXPLICIT]START.POCC_STRUCTURE
Ga0.25In0.75P
1.224745  0.001
   0.00000000000000   2.24076438492221   2.24076438492221
   2.24076438492221   0.00000000000000   2.24076438492221
   2.24076438492221   2.24076438492221   0.00000000000000
1*0.25 1*0.75 1
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Direct(2) P
   0.00000000000000   0.00000000000000   0.00000000000000  Ga
   0.00000000000000   0.00000000000000   0.00000000000000  In
   0.75000000000000   0.75000000000000   0.75000000000000  P
[POCC_MODE_EXPLICIT]STOP.POCC_STRUCTURE
[AFLOW] ************************************************************************************************
[AFLOW_POCC]CALC



2) Once the appropriate aflow.in file is finished, you have to prepare the input with
aflow --pocc_input
This command will analyze your partially occupied structure from aflow.in file, which is between the lines:
[POCC_MODE_EXPLICIT]START.POCC_STRUCTURE
...
[POCC_MODE_EXPLICIT]STOP.POCC_STRUCTURE
In addition, the command will also generate a series of nonequivalent structures according to your partially oc
The log will be save in "LOG.POCC" file.

3) let your aflow daemon run your new aflow.in. The code will do the calculations for all the structures.
Once in a while you should check if there is an OUTCAR that has not been touched for a while. This indicates in
If the process gets stuck somewhere, delete the directory of the OUTCAR which is not been finished,
then delete the LOCK file of aflow, and restart aflow. The completed directories will not be modified.
The running step does not require an internet connection, so it is safe to run the displacements in a supercomp

A simple trick. If you want to speed up the calculation, after aflow starts and creates its LOCK, you can renam
This  will not interfere with the running process since the code keeps a pointer to the physical file.

4) when all the directories have finished, run
4.1) aflow --pocc_dos=DIRECTORY,TEMPERATURE
Firstly, this command will analyze your aflow.in, scan through all the subdirectories, warn you if there are mi
If this is a complete calculation, then this command will generate the density of states (DOS) plot for the par
a specified temperature.

4.2) aflow --pocc_bandgap=DIRECTORY,TEMPERATURE
This command will produce the band gap of the partially occupied structure at the specified temperature. The ba
density of states (DOS).

4.3) aflow --pocc_mag=DIRECTORY,TEMPERATURE
This command will produce the magnetic moment of the partially occupied structure at the specified temperature.

Good luck.
Kesong
July. 18th, 2013


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