AMP^2 Manual

0.9.0

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Contents:

CHAPTER 1

Installation and execution

1.1 Installation

1.1.1 System requirements

AMP^2 is written in Python 2.7. Currently, the package is not compatible with lower or higher version than 2.7. AMP^2 is utilizes Python modules in the following with link to each site.

- numpy [https://www.numpy.org]
- scipy [https://www.scipy.org]
- spglib [https://atztogo.github.io/spglib]

These modules should be pre-installed. In addition, AMP^2 needs gnuplot to draw various figures.

1.1.2 Installation

To use AMP^2, please download the file from https://github.com/MDIL-SNU/AMP2 under the working directory.

1.2 Basic setup

1.2.1 Setting for python

As we mentioned, AMP^2 was written in Python 2.7. Thus, to use AMP^2, you should set to execute Python 2.7 from 'python' command.

1.2.2 Setting of configuration file

AMP^2 uses YAML style configuration file. All setting parameters used in AMP^2 can be controlled in "config.yaml". Before using AMP^2, proper pathes and mpi program command should be set to be suitable for your system. Following commands are the essential directories and programs to be set.

```
Directory:
  submit:
  src:
  pot_path_gga:
  pot_path_lda:
Program:
  vasp_std:
  vasp_gam:
  vasp_ncl:
  gnuplot:
  mpi_command:
```

Details for the commands are in *Configuration*.

1.3 Execution

You can execute AMP^2 using Python command as following.

```
python [src_path]/main.py [path for configuration file] [path for nodefile] [the␣
↪number of cores]
```

- [src_path] is the path for directory of source codes for AMP^2.
- [path for configuration file] is the path for configuration file (config.yaml).
- [path for nodefile] is used to record the information of computing nodes.
- [the number of cores] is the number of cores to be used in parallel computing.

For the convenience, we provide the shell script file (run.sh) as following.

```
echo 'node information' > nodefile
NPROC=16       # The number of cores for parallel computing

### set path of config.yaml ###
conf=./config.yaml
################################

### Do not change #############
src_path=`grep 'src_path' $conf | tr -s ' ' | cut -d " " -f 3`
################################

python $src_path/main.py $conf nodefile $NPROC >& stdout.x
```

Before execution, you need to modify *'node information'*, *NPROC* and *conf*. Then, you can execute AMP^2 using shell script as following.

```
sh run.sh
```

The shell script file can be easily integrated with job scheduler program such as portable batch system (PBS).

CHAPTER 2

Overview

2.1 Preparing input files

Before running AMP[2], two input files should be prepared such as YAML style configuration file (config.yaml) and structure file. The details for input files are explained in *Input files*. The basic format of config.yaml and structure files are like below:

config.yaml:

```
directory:
  submit: ./Submit                        # the path of structure file or the␣
↪directory containg structure files
  output: ./Output                        # the path of the directory where␣
↪calculation is conducted
  done: ./Done                            # the path of the directory where␣
↪results are saved
  error: ./ERROR                          # the path of the directory where␣
↪the materials with error are saved
  src_path: ./src                         # the path of the directory of AMP2␣
↪source codes
  pot_path_gga: /data/vasp4us/pot/PBE52 # the path of directory for GGA␣
↪pseudopotential
  pot_path_lda: /data/vasp4us/pot/LDA52 # the path of directory for LDA␣
↪pseudopotential

program:
  vasp_std: /data/vasp4us/vasp_std      # the path of standard version of␣
↪VASP
  vasp_gam: /data/vasp4us/vasp_gam      # the path of gamma-only version of␣
↪VASP
  vasp_ncl: /data/vasp4us/vasp_ncl      # the path of noncollinear version␣
↪of VASP
  gnuplot: /gnuplot                       # the path of executable file for␣
↪gnuplot
```

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```
  mpi_command: mpirun                    # mpi command (ex. mpirun, mpiexec, .
↪..)

vasp_parallel:
  npar: 2                                # the number of bands that are␣
↪treated in parallel. It is same to NPAR tag in VASP.
  kpar: 2                                # the number of kpoints that are␣
↪treated in parallel. It is same to NPAR tag in VASP.
```

Structure file (VASP structure file format):

```
Primitive Cell
   1.000000000
      0.0    2.714895    2.714895
      2.714895    0.0    2.714895
      2.714895    2.714895    0.0
    Si
    2
Selective dynamics
Direct
    0.5    0.5    0.5  T  T  T ! Si1
    0.75    0.75    0.75  T  T  T ! Si1
```

2.2 Running AMP^2

You can execute AMP^2 using shell script as following.

```
sh run.sh
```

The details for shell script are mentioned in the section, "Execution AMP^2" in *Installation and execution*.

2.3 Outputs

After starting the calculation, new directory is formed in *output_path* as the name of the structure file. (*name* directory is formed from *name.cif* or *POSCAR_name*.) Then, if calculation is well finished, the directory moves to *done_path*. If not, it moves to *error_path*. The following data are the examples of calculation results for Cr_2O_3. More details for output files are written in *Output*.

POSCAR_GGA:

```
relaxed poscar
1.000000000
    2.53085784423    1.46119145764    4.60391533726
    -2.53085784423    1.46119145764    4.60391533726
    0.0    -2.9223829153    4.60391533726
    Cr    O
    4    6
Selective dynamics
Direct
    0.348055231569    0.348055231569    0.348055231569  T  T  T ! Cr1_up
    0.848055231569    0.848055231569    0.848055231569  T  T  T ! Cr1_up
    0.151944768431    0.151944768431    0.151944768431  T  T  T ! Cr1_down
```

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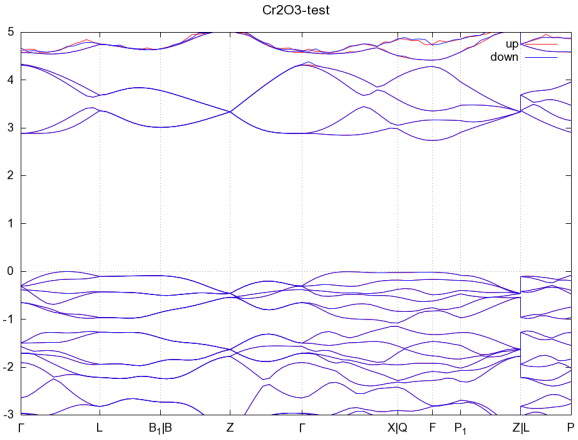
```
    0.651944768431    0.651944768431    0.651944768431  T  T  T ! Cr1_down
    0.553903778143    0.946096221857    0.25  T  T  T ! O1
    0.946096221857    0.25    0.553903778143  T  T  T ! O1
    0.25    0.553903778143    0.946096221857  T  T  T ! O1
    0.0539037781426    0.75    0.446096221857  T  T  T ! O1
    0.75    0.446096221857    0.0539037781426  T  T  T ! O1
    0.446096221857    0.0539037781426    0.75  T  T  T ! O1
```

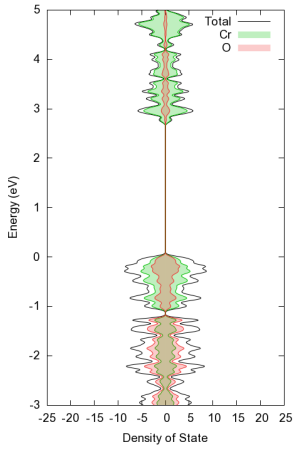
Band_gap_GGA.log:

```
Band gap:      2.734 eV (Indirect)

VBM: 0.2916667  0.0  0.0   :      3.366 eV
CBM: 0.42206  0.42206  -0.01078659   :      6.100 eV

nVBM: 30  spin: 1
nCBM: 31  spin: 1
```

band_GGA.png:



dos_GGA.png:



CHAPTER 3

Input

3.1 Input files

3.1.1 Structure file

The valid formats for structure file are that for VASP and cif format. In the cif files, symmetry operator (_space_group_symop_[] or _symmetry_equiv_[]), atomic label (_atom_site_label), occupancy (_atom_site_occupancy) and fractional positions (_atom_site_fract_[]) must be included. The name of structure files must be formatted as name.cif or POSCAR_name where tag is used for identification.

VASP structure file format:

```
Primitive Cell
   1.000000000
      0.0    2.714895    2.714895
      2.714895    0.0    2.714895
      2.714895    2.714895    0.0
    Si
    2
Selective dynamics
Direct
    0.5    0.5    0.5  T  T  T ! Si1
    0.75    0.75    0.75  T  T  T ! Si1
```

3.1.2 Configuration

All of parameters can be tuned in the configuration file as following. The detail for each parameter is explained in *Configuration*.

config.yaml:

```
directory:
  submit: ./Submit                          # the path of structure file or the␣
↪directory containg structure files
  output: ./Output                          # the path of the directory where␣
↪calculation is conducted
  done: ./Done                              # the path of the directory where␣
↪results are saved
  error: ./ERROR                            # the path of the directory where␣
↪the materials with error are saved
  src_path: ./src                           # the path of the directory of AMP2␣
↪source codes
  pot_path_gga: /data/vasp4us/pot/PBE52 # the path of directory for GGA␣
↪pseudopotential
  pot_path_lda: /data/vasp4us/pot/LDA52 # the path of directory for LDA␣
↪pseudopotential

program:
  vasp_std: /data/vasp4us/vasp_std      # the path of standard version of␣
↪VASP
  vasp_gam: /data/vasp4us/vasp_gam      # the path of gamma-only version of␣
↪VASP
  vasp_ncl: /data/vasp4us/vasp_ncl      # the path of noncollinear version␣
↪of VASP
  gnuplot: /gnuplot                         # the path of executable file for␣
↪gnuplot
  mpi_command: mpirun                       # mpi command (ex. mpirun, mpiexec, .
↪..)

calculation:
  magnetic_ordering: T                  # On/Off for the calculation to␣
↪idetify most stable magnetic spin ordering
  band: T                                   # On/Off for the calculation for␣
↪band structure and band gap
  density_of_states: T                  # On/Off for the calculation for␣
↪density of states
  hse_oneshot: T                            # On/Off for the calculation for␣
↪HSE@PBE
  dielectric: T                             # On/Off for the calculation for␣
↪dielectric constant
  effective_mass: T                         # On/Off for the calculation for␣
↪effective mass
  potential_type: GGA                       # calculation scheme (LDA or GGA)

vasp_parallel:
  npar: 2                                   # the number of bands that are␣
↪treated in parallel. It is same to NPAR tag in VASP.
  kpar: 2                                   # the number of kpoints that are␣
↪treated in parallel. It is same to NPAR tag in VASP.

cif2vasp:
  pot_name:                                 # the pseudopotential potential for␣
↪element.
    GGA:                                    # (Ex. GGA:\n    Ge:Ge_d\n    Cu:Cu_
↪pv)
    LDA:
  soc_target:                               # the elements to carry out spin-
↪orbit coupling calculation (Ex. soc_target:\n    - Bi\n    -Pb)
```

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```
  u_value:                                  # U values for PBE+U calculation (Ex.
↪ u_value:\n    La: 7.5\n    Ce: 8.5)

hybrid_oneshot:
  alpha: 0.25                               # mixing parameter for hybrid␣
↪calculation. If "Auto" is set, the mixing parameter is set to be one of␣
↪permittivity and PBE0 calualation is performed.
  cutoff_df_dvb: 0.3                        # DF/DVB used to classify␣
↪semiconductor candidates. (See paper)
  band_structure_correction: True           # On/Off for the band structure␣
↪correction

effective_mass:
  carrier_type:                             # carrier type of effective mass to␣
↪be estimated
    - hole
    - electron
```

3.2 Configuration

AMP^2 uses YAML style configuration file. All configurations for AMP^2 can be controlled in "config.yaml". The default setting parameters are provided in config_def.yaml in source directory.

The commands for configuration are listed below.

3.2.1 Directory

All tags in directory define the path of directories used in AMP^2. If there is no directory in the path for Output, Done and ERROR, AMP^2 makes new directories.

- **Submit:** submit tag should be set to be the path for target materials. In AMP^2, user can designate a specific material or a bunch of materials as target materials. To perform the AMP^2 for a specific materials, submit path is set to be the structure file or the directory for continuous calculation. The valid formats for structure file are explained in /Input_and_Output/Input_files. For calculating a bunch of materials, Submit path is set to be the directory where the valid strcture format files and directories for continuous calculation are placed.

  Usage:

  ```
  directory:
    submit: [path of structure file] | [path of directory]
  ```

  Default:

  ```
  directory:
    submit: ./Submit
  ```

- **Output:** Output tag defines the path where the material on calculation is located.

  Usage:

  ```
  directory:
    output: [path of directory]
  ```

Default:

```
directory:
  output: ./Output
```

- **Done:** Done tag defines the path where calculated materials are saved.

  Usage:

  ```
  directory:
    done: [path of directory]
  ```

  Default:

  ```
  directory:
    done: ./Done
  ```

- **Error:** Output tag defines the path saving the materials in which calculation error broke out.

  Usage:

  ```
  directory:
    error: [path of directory]
  ```

  Default:

  ```
  directory:
    error: ./ERROR
  ```

- **src_path:** src_path tag should be set to be the directory for AMP^2 source codes.

  Usage:

  ```
  directory:
    src_path: [path of directory]
  ```

  Default:

  ```
  directory:
    src_path: ./src
  ```

- **pot_path_GGA (pot_path_LDA):** pot_path_GGA (pot_path_LDA) should be set to be the directory for pseudopotential provided by VASP.

  Usage:

  ```
  directory:
    pot_path_GGA: [path of directory]
    pot_path_LDA: [path of directory]
  ```

  Default:

  ```
  directory:
    pot_path_GGA: ./PBE
    pot_path_LDA: ./LDA
  ```

3.2.2 Program

The all tags in program determine the path of executable files except mpi_command.

- **vasp_std:** vasp_std tag should be set to be the path for standard version of VASP.

  Usage:

```
Program:
  vasp_std: [path]
```

  Default:

```
Program:
  vasp_std: ./vasp_std
```

- **vasp_gam:** vasp_gam tag should be set to be the path for gamma only version of VASP.

  Usage:

```
Program:
  vasp_gam: [path]
```

  Default:

```
Program:
  vasp_gam: ./vasp_gam
```

- **vasp_ncl:** vasp_ncl tag should be set to be the path for non-collinear version of VASP. Though wrong path is set, most of calculations except spin-orbit coupling calculation can be conducted.

  Usage:

```
Program:
  vasp_ncl: [path]
```

  Default:

```
Program:
  vasp_ncl: ./vasp_ncl
```

- **gnuplot:** gnuplot tag should be set to be the path for gnuplot. Though wrong path is set, most of calculations except drawing images can be conducted.

  Usage:

```
Program:
  gnuplot: [path]
```

  Default:

```
Program:
  gnuplot: /gnuplot
```

- **mpi_command:** mpi_command tag should be set to be the operation command to conduct parallel computing calculation.

  Usage:

```
Program:
  mpi_command: [command]
```

  Default:

```
Program:
  mpi_command: mpirun
```

3.2.3 Calculation

The all tags in calculation determine whether the calculation is performed or not.

- **magnetic_ordering:** magnetic_ordering tag determines whether to identify the most stable magnetic spin ordering or not.

  Usage:

  ```
  Calculation:
    magnetic_ordering: True | False
  ```

  Default:

  ```
  Calculation:
    magnetic_ordering: True
  ```

- **band:** band tag determines whether to estimate the band gap and to draw band structure or not.

  Usage:

  ```
  Calculation:
    band: True | False
  ```

  Default:

  ```
  Calculation:
    band: True
  ```

- **density_of_states:** density_of_states tag determines whether to estimate the density of states or not.

  Usage:

  ```
  Calculation:
    density_of_states: True | False
  ```

  Default:

  ```
  Calculation:
    density_of_states: True
  ```

- **hse_oneshot:** hse_oneshot tag determines whether to perform the hybrid calculation or not. This hybrid calculation is conducted without full band searching and structure optimization. For hybrid calculation band calculation must be conducted.

  Usage:

  ```
  Calculation:
    hse_oneshot: True | False
  ```

  Default:

  ```
  Calculation:
    hse_oneshot: True
  ```

- **dielectric:** dielectric tag determines whether to estimate the dielectric constant or not. Dielectric constant is unphysical in metallic system. Thus, band structure calculation must be conducted to check whether it is metal or not.

  Usage:

```
Calculation:
  dielectric: True | False
```

  Default:

```
Calculation:
  dielectric: True
```

- **effective_mass:** effective_mass tag determines whether to estimate the hole (and/or electron) effective mass or not. For effective mass calculation band calculation must be conducted.

  Usage:

```
Calculation:
  effective_mass: True | False
```

  Default:

```
Calculation:
  effective_mass: True
```

- **potential_type** potential_type tag determines the functional scheme (LDA or GGA) for convergence test. Only one of them should be chosen.

  Usage:

```
Calculation:
  potential_type: GGA | LDA
```

  Default:

```
Calculation:
  potential_type: GGA
```

3.2.4 Vasp_parallel

npar and kpar tags are used to enhance the efficiency of parallel computing calculation of VASP.

- **npar:** napr tag determines the number of bands that are treated in parallel. It is same to NPAR tag in VASP.

  Usage:

```
vasp_parallel:
  npar: [integer]
```

  Default:

```
vasp_parallel:
  npar: 2
```

- **kpar:** kpar tag determines the number of kpoints that are treated in parallel. It is same to NPAR tag in VASP.

  Usage:

```
vasp_parallel:
  kpar: [integer]
```

Default:

```
vasp_parallel:
  kpar: 2
```

3.2.5 cif2vasp

In AMP^2, input files for VASP calculation are automatically generated from structure files. These parameters can control the initial input files for VASP.

- **pot_name:** pot_name tag determines the pseudopotential potential for element. By default, the potential file (POTCAR) is built using the preset pseudopotential. (Preset pseudopotential: /Input_and_Output/Configuration/potential)

  Usage:

```
cif2vasp:
  pot_name:
    GGA:
      [element name]: [type of pseudopotential]
    LDA:
      [element name]: [type of pseudopotential]
```

- **soc_target:** soc_target tag determines the elements to carry out spin-orbit coupling calculation. In AMP^2, spin-orbit coupling calculation is performed only for band structure and density of states.

  Usage:

```
cif2vasp:
  soc_target:
    - [element name]
    - Bi
```

  Default:

```
cif2vasp:
  soc_target:
```

- **u_value:** u_value tag controls U values for PBE + Hubbard U method. By default, AMP^2 imposes U parameters for 3d transition metal. If all tag is used instead of element name, every U value is set to be the target value.

  Usage:

```
cif2vasp:
  u_value:
    - [element name]: real
```

  Default:

```
cif2vasp:
  u_value:
    V: 3.1
```

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```
    Cr: 3.5
    Mn: 4
    Fe: 4
    Co: 3.3
    Ni: 6.4
    Cu: 4
    Zn: 7.5
```

3.2.6 Hybrid_oneshot

Conventional density functional theory calculation like LDA and PBE underestimates band gap and somtimes it gives wrong results for small gap materials such as Ge and InAs. Thus, AMP^2 performs hybrid calculation for accurate band gap. In the previous study, it is shown that accurate band gap can be obtained using extremum points (valence band maximum and conduction band minimum) and optimized structure in PBE scheme. Since hybrid calculation demands high computational cost, this approach is imposed in AMP^2.

For the small gap materials with metallic band structure in PBE functionals, DOS (density of states) based correction scheme is applied in AMP^2. (See /Input_and_Output/Configuration/small_gap_correction)

Finally, AMP^2 provides a method to select mixing parameter using permittivity since there is an inverse correlation between mixing parameter and permittivity.

- **alpha:** alpha tag determines a mixing parameter for hybrid calculation. As we mentioned above, mixing parameter in PBE0 has a inverse correlation with permittivity. If alpha: auto is used, the mixing parameter is determined as one of permittivity.

  Usage:

  ```
  hybrid_oneshot:
    alpha: [real] | Auto
  ```

  Default:

  ```
  hybrid_oneshot:
    alpha: 0.25
  ```

- **cutoff_df_dvb:** cutoff_df_dvb tag controls $D_{\mathrm{VB}}/D_{\mathrm{F}}$ used to classify semiconductor candidates.

  Usage:

  ```
  hybrid_oneshot:
    cutoff_df_dvb: [real]
  ```

  Default:

  ```
  hybrid_oneshot:
    cutoff_df_dvb: 0.3
  ```

- **band_structure_correction:** band_structure_correction determines whether to conduct scissor-correction for band structure or not.

  Usage:

  ```
  hybrid_oneshot:
    band_structure_correction: True | False
  ```

  Default:

```
hybrid_oneshot:
  band_structure_correction: True
```

3.2.7 Effective_mass

In AMP^2, effective mass tensor is estimated using semiclassical transport theory. The details are explained in the paper.

- **carrier_type:** carrier_type tag determines the type of carrier (hole or electron) to be estimated.

  Usage:

```
effective_mass:
  carrier_type:
    - hole | electron
```

  Default:

```
effective_mass:
  carrier_type:
    - hole
    - electron
```

CHAPTER 4

Output

4.1 Output files

AMP[2] makes directory for each configuration file as its name (from name.cif or POSCAR_name). When the calculation is on progress, the directory is placed in output path in the configuration. If calculation is well finished, the calculation directory is moved to done path. If any error breaks out, it is move to error path.

Each directory includes several sub-directory as follow;

4.1.1 INPUT0

Directory for input files for VASP calculation.

- **POSCAR_rlx_POT:** Optimized structure file with POT functional.
- **KPOINTS:** Converged k-points file
- **INCAR:** VASP input file with converged cutoff energy and ground-state magnetic ordering

4.1.2 kptest

Directory for k-point convergence test.

- **kpoint.log:** Calculation log for k-points convergence test

4.1.3 encut

Directory for cutoff energy convergence test.

- **cutoff.log:** Calculation log for cutoff energy convergence test

4.1.4 relax_POT (POT = GGA or LDA)

Directory for structure relaxation.

4.1.5 magnetic_ordering

Directory for identifying magnetic spin ordering.

4.1.6 band_POT (POT = GGA or LDA)

Directory for band structure and band gap calculation.

4.1.7 dos_POT (POT = GGA or LDA)

Directory for density of states calculation.

4.1.8 dielectric_POT (POT = GGA or LDA)

Directory for dielectric constant calculation.

4.1.9 hybrid_POT1_POT2 (POT = GGA or LDA)

Directory for band gap calculation with hybrid oneshot scheme.

4.1.10 effm_POT (POT = GGA or LDA)

Directory for effective mass calculation.

4.1.11 Results

Directory for calculation results.

- **POSCAR_GGA:** Optimized structure
- **Band_gap_GGA.log:** Information of band gap
- **band_GGA.png (band_GGA.pdf):** Band structure image
- **band_corrected.png (band_corrected.pdf):** Corrected band structure image
- **Band_gap_hybrid_GGA.log:** Information of band gap with HSE@PBE scheme
- **dos_GGA.pnd (dos_GGA.pdf):** Density of states image
- **dielectric_GGA.log:** Information of dielectric constant
- **effective_mass_hole_GGA.log:** Information of effective mass of hole
- **effective_mass_electron_GGA.log:** Information of effective mass of electron
- **Properties.json:** Summarized material properties

4.1.12 INPUT0_old

Directory for input files for VASP calculation with ferromagnetic ordering. If more stable magnetic spin ordering is obsevred, this directory is made.

4.1.13 relax_POT_old (POT = GGA or LDA)

Directory for structure relaxation with ferromagnetic ordering. If more stable magnetic spin ordering is obsevred, this directory is made.

4.1.14 name_with_U

Directory for AMP^2 calculation with DFT+U calculation. If the material is metallic and DFT+U calculation has been conducted, all of results move to this directory.

Additionally, AMP^2 provides log file as amp2.log for tracing the calculation.

CHAPTER 5

Examples

5.1 Introduction

AMP^{2}includes several examples (for Si, Ge and NiO) in *AMP2/examples/*.

5.2 Execute AMP^2

Before running examples, please set the configuration to be suitable for your system. (See *Installation and execution*) Then, you can execute AMP^2 using shell script as following.

```
sh run.sh
```

5.3 Calculation results

When the calculation is finished, Sub-directory is generated in Done path. (Ex. */Done/Si*) In the *Sub-directory/Results*, you can obtain optimized structure, band gap, band structure, density of states, dielectric constant and effective mass of hole and electron.

5.3.1 Si

Si is a typical example of semiconductor. Therefore, we calculate all properties supported by AMP^{2}in this example.

Optimized structure (/Results/POSCAR_rlx_GGA)

```
relaxed poscar
1.000000000
    0.0    2.73243086189    2.73243086189
    2.73243086189    -0.0    2.73243086189
```

(continues on next page)

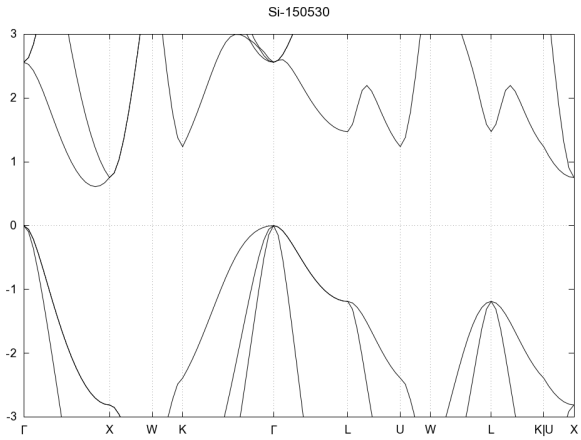
(continued from previous page)

```
    2.73243086189    2.73243086189    0.0
    Si
    2
Selective dynamics
Direct
    0.5    0.5    0.5  T  T  T ! Si1
    0.75    0.75    0.75  T  T  T ! Si1
```

Band gap (/Results/band_gap_GGA.log)

```
Band gap:      0.612 eV (Indirect)

VBM: 0.0  0.0  0.0   :      5.649 eV
CBM: 0.4166667  0.0  0.4166667   :      6.261 eV

nVBM: 4  spin: 1
nCBM: 5  spin: 1
```

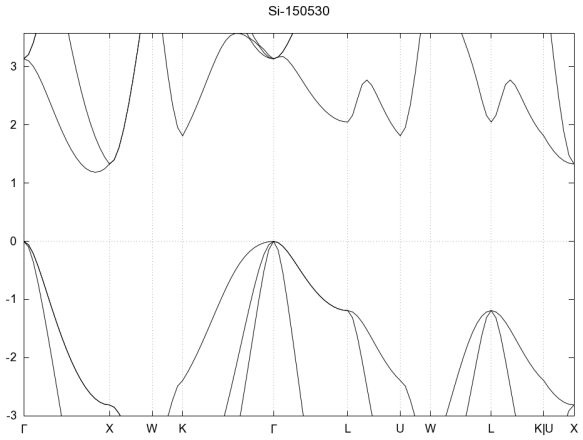
Band structure (/Results/band_GGA.png and /Results/band_GGA.pdf)



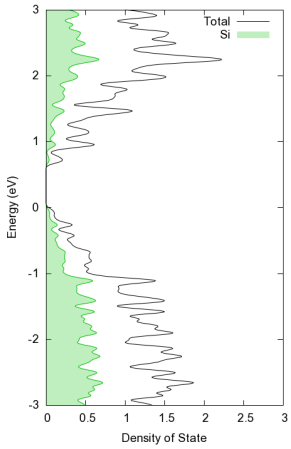
Band gap from HSE@PBE (/Results/band_hybrid_GGA.log)

```
Band gap:      1.187 eV (Indirect)

VBM: 0.0  0.0  0.0   :      5.289 eV
CBM: 0.4166667  0.0  0.4166667   :      6.477 eV

nVBM: 4  spin: 1
nCBM: 5  spin: 1
```

Corrected band structure (/Results/band_GGA_corrected.png and /Results/band_GGA_corrected.pdf)



Density of states (/Results/dos_GGA.log)



Dielectric constant (/Results/dielectric_GGA.log)

```
Dielectric tensor (electronic contribution):
    12.936       0.000      -0.000
    0.000       12.936       0.000
    -0.000       0.000      12.936
Dielectric tensor (ionic contribution):
    0.000        0.000       0.000
    0.000       -0.000      -0.000
    0.000       -0.000       0.000

Dielectric constant diagonalization (electronic):     12.936     12.936
↪12.936
Dielectric constant diagonalization (ionic):      0.000     -0.000      0.000

Averaged static dielectric constant:     12.936
```

Effective mass of hole (/effective_mass_hole_GGA.log)

```
hole
    -0.266     -0.000     -0.000
    -0.000     -0.266     -0.000
    -0.000     -0.000     -0.266
Diagonalized effective mass:     -0.266     -0.266     -0.266
```

Effective mass of electron (/Results/effective_mass_hole_GGA.log)

```
electron
    0.287       0.000       0.000
    0.000       0.287       0.000
    0.000       0.000       0.287
Diagonalized effective mass:       0.287       0.287       0.287
```

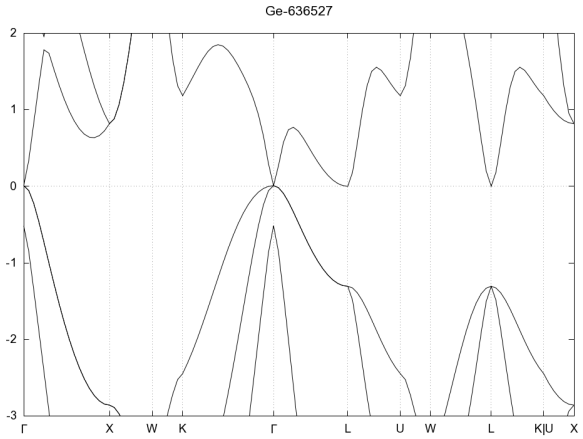
5.3.2 Ge

Ge is a well-known semiconductor with metallic band structure in conventional DFT schemes like LDA and PBE. In AMP^2, however, we can obtain the reliable band gap and band structure due to the band gap correction scheme. In this example, we calculate corrected band structure.

Band gap (/Results/band_gap_GGA.log)

```
This system is metallic.
! If it is not hybrid calculation, additional search is required for hybrid␣
↪calculation.
```

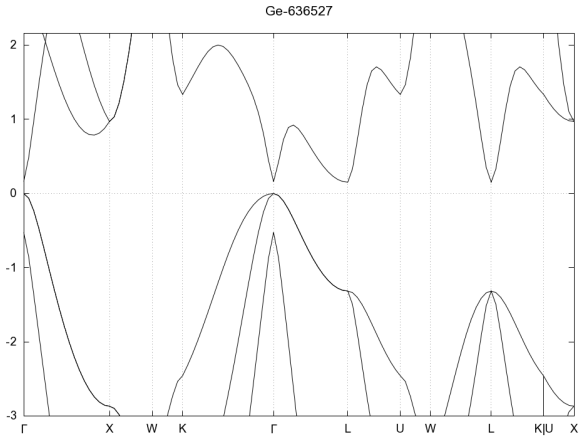
Band structure (/Results/band_GGA.png and /Results/band_GGA.pdf)



Band gap from HSE@PBE (/Results/band_hybrid_GGA.log)

```
Band gap:       0.161 eV (Direct)

VBM: 0.0  0.0  0.0   :       2.875 eV
CBM: 0.0  0.0  0.0   :       3.036 eV

nVBM: 4  spin: 1
nCBM: 5  spin: 1
```

Corrected band structure (/Results/band_GGA_corrected.png and /Results/band_GGA_corrected.pdf)



5.3.3 NiO

NiO is one of the antiferromagnetic materials. In this example, we show the most stable magnetic spin ordering for NiO and its electronic configurations (band strucrue and density of states).

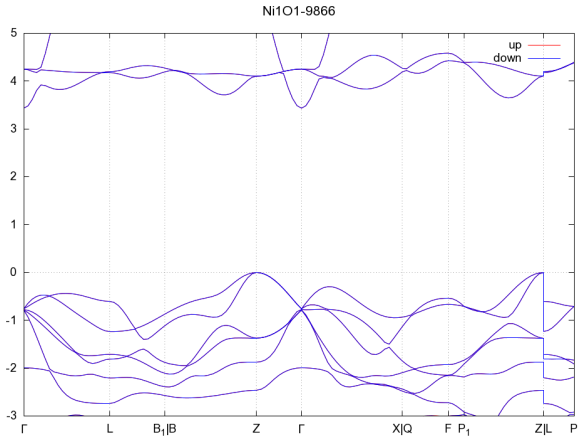
Optimized structure (/Results/POSCAR_rlx_GGA)

```
relaxed poscar
1.000000000
    1.47786935879    0.853248272122    4.82278497551
    -1.47786935879    0.853248272122    4.82278497551
    0.0    -1.70649654425    4.82278497551
    Ni    O
    2    2
Selective dynamics
Direct
    0.5    0.5    0.5  T  T  T ! Ni1_up
    -0.0    -0.0    0.0  T  T  T ! Ni1_down
    0.750000037602    0.750000037602    0.750000037602  T  T  T ! O1
    0.249999962398    0.249999962398    0.249999962398  T  T  T ! O1
```

Band gap (/Results/band_gap_GGA.log)

```
Band gap:      3.433 eV (Indirect)

VBM: 0.5  0.5  0.5   :      6.242 eV
CBM: 0.0  0.0  0.0   :      9.675 eV

nVBM: 16  spin: 1
nCBM: 17  spin: 2
```

Band structure (/Results/band_GGA.png and /Results/band_GGA.pdf)



Density of states (/Results/dos_GGA.log)