AMP^2 Manual

0.9.6

Yong Youn
Miso Lee
Changho Hong
Doyeon Kim
Sangtae Kim
Jisu Jung
Kanghoon Yim
Seungwu Han

Aug 25, 2023

Contents:

CHAPTER 1

Installation and execution

1.1 Installation AMP^2

1.1.1 System requirements

AMP^2 supports Python 2.7 and 3. Currently, the package is not compatible with lower 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]
- PyYAML [https://pypi.org/project/PyYAML]

These modules should be pre-installed. In addition, AMP^2 needs gnuplot supporting 'pngcairo' and 'pdfcairo' 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 Essential setting

1.2.1 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 AMP^2

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 such as PBS_nodefile in Portable Batch System (PBS) and HOSTNAME in Sun Grid Engine (SGE). In the PBS system, we recommand to use the command, "echo $PBS_nodefile > nodefile". Also, users can save an arbitrary text by writing in the nodefile.
- [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 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: ./pot/PBE            # the path of directory for GGA␣
↪pseudopotential
  pot_path_lda: ./pot/LDA            # the path of directory for LDA␣
↪pseudopotential

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

(continues on next page)

(continued from previous page)

```
  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 AMP²

You can execute AMP² using shell script as following.

```
sh run.sh
```

The details for shell script are mentioned in the section, "Execution AMP²" 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
```

(continues on next page)

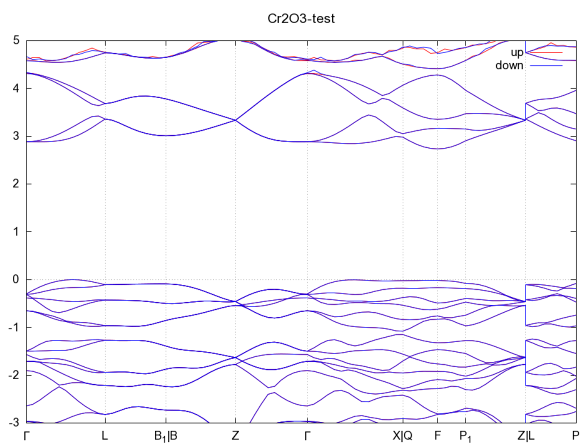
(continued from previous page)

```
    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
```

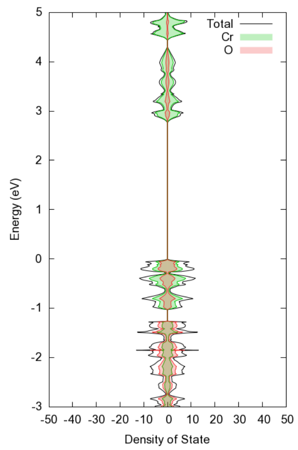
Band_gap_GGA.log:

```
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:



2.4 List of source codes

AMP² consists of several python codes as follows:

- **main.py:** This is main code to run AMP².
- **amp2_input.py:** This is for generating input files for VASP from structure file.
- **kpoint.py:** This is for conducting a convergence test of k-points.
- **cutoff.py:** This is for conducting a convergence test of cutoff energy.
- **relax.py:** This is for conducting structure optimization.
- **magnetic_ordering.py:** This is for identifying the most stable magnetic spin ordering.
- **band.py:** This is for drawing band structure and estimating band gap.
- **dos.py:** This is for drawing density of states.
- **hse_gap.py:** This is for estimating band gap with PBE@HSE scheme.
- **effm.py:** This is for estimating effective masses of hole and electron.
- **dielectric.py:** This is for estimating dielectric tensor.
- **get_result.py:** This is for summarizing the calculation results.
- **input_conf.py:** This is for handling YAML type configuration.
- **rerun_for_metal.py:** This is a code to restart the all calculations without the on-site U term if the material was found to be metallic and U was applied.
- **genetic_algorithm.py:** This is for performing genetic algorithm to find the most stable magnetic spin ordering.
- **genetic_operator.py:** This is a package of modules for performing genetic algorithm.
- **make_supercell.py:** This is a code to build supercell to find magnetic primitive cell.
- **mk_suprecell.py:** This is a code to build supercell for the Ising coefficient.
- **module_subr.py:** This is a package of modules for 'mk_supercell.py'.
- **module_amp2_input.py:** This is a package of modules for generating input files for VASP from structure file.
- **module_converge.py:** This is a package of modules for convergence test.
- **module_relax.py:** This is a package of modules for structure optimization.
- **module_AF.py:** This is a package of modules for identifying the most stable magnetic spin ordering.
- **module_GA.py:** This is a package of modules for genetic algorithm.
- **module_band.py:** This is a package of modules for drawing band structure and calculating band gap.
- **module_dos.py:** This is a package of modules for drawing density of states.
- **module_hse.py:** This is a package of modules for calculating band gap with HSE@PBE scheme.
- **module_effm.py:** This is a package of modules for calculating effective mass.
- **module_dielectric.py:** This is a package of modules for calculating dielectric tensor.
- **module_vasprun.py:** This is a package of modules to run VASP.
- **module_log.py:** This is a package of modules to record log.
- **module_vector.py:** This is a package of modules to calculate several properties such as distance between two points and angle.

Additionally, there are files for predefined variables.

- **INCAR0:** This is for default configuration for 'INCAR'.
- **U_table.yaml:** This is for default *U* parameters.
- **pot_table.yaml:** This is for default potential files.
- **config_def.yaml:** This is default configuration for 'config.yaml'.

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: ./pot/PBE              # the path of directory for GGA␣
↪pseudopotential
  pot_path_lda: ./pot/LDA              # the path of directory for LDA␣
↪pseudopotential

program:
  vasp_std: ./vasp_std                 # the path of standard version of␣
↪VASP
  vasp_gam: ./vasp_gam                 # the path of gamma-only version of␣
↪VASP
  vasp_ncl: ./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)
```

(continues on next page)

(continued from previous page)

```
  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

AMP² uses YAML style configuration file. All configurations for AMP² 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 AMP². If there is no directory in the path for Output, Done and ERROR, AMP² makes new directories.

- **Submit:** submit tag should be set to be the path for target materials. In AMP², user can designate a specific material or a bunch of materials as target materials. To perform the AMP² 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: ./pot/PBE
    pot_path_LDA: ./pot/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: /usr/local/bin/gnuplot
```

- **mpi_command:** mpi_command tag should be set to be the operation command to conduct parallel computing calculation. The predefined commands are ’mpirun’, ’jsrun’, ’srun’, ’mpiexec’, ’mpiexec.hydra’, ’mpich’. Except for the predefined commands, the command should include a flag to specify the number of processors like ’mpirun -np’.

  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 KPAR 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
    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 AMP², 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
  ```

- **temperature_for_fermi:** It controls the temperature to estimate the hole or electron distribution based on the Fermi-Dirac function.

  Usage:

  ```
  effective_mass:
    temperature_for_fermi: [real]
  ```

  Default:

  ```
  effective_mass:
    temperature_for_fermi: 300
  ```

3.3 Advanced configuration

For advanced users, AMP² provides some additional configuration parameters written in the default configuration file ('/src/cpnfig_def.yaml').

config_def.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
```

(continues on next page)

(continued from previous page)

```
  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: ./pot/PBE                 # the path of directory for GGA␣
↪pseudopotential
  pot_path_lda: ./pot/LDA                 # the path of directory for LDA␣
↪pseudopotential

program:
  vasp_std: ./vasp_std                    # the path of standard version of VASP
  vasp_gam: ./vasp_gam                    # the path of gamma-only version of VASP
  vasp_ncl: ./vasp_ncl                    # the path of noncollinear version of VASP
  gnuplot: /usr/local/bin/gnuplot         # the path of executable file for gnuplot
  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.

calculation:
  kp_test: T                              # On/Off for convergence test of k-points
  encut_test: T                           # On/Off for convergence test of cutoff energy
  relaxation: T                           # On/Off for structure optimization
  magnetic_ordering: T                    # On/Off for calculation to identify 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)

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)
  u_value:                                # U values for PBE+U calculation (Ex. u_
↪value:\n    La: 7.5\n    Ce: 8.5)
  max_nelm: 100                           # the maximum number of iteration for␣
↪structure optimization.

convergence_test:
  enconv: 0.01                            # convergence condition for energy (eV/atom).␣
↪Negative value indicates that energy is not used as the condition.
  prconv: 10                              # convergence condition for pressure (bar).␣
↪Negative value indicates that pressure is not used as the condition.
  foconv: -1                              # convergence condition for force (eV/angst).␣
↪Negative value indicates that force is not used as the condition.
```

(continues on next page)

(continued from previous page)

```
  initial_kpl: 1                          # Minimum value for the convergence test of k-
↪points. It corresponds to the largest mesh grid in the three directions.
  max_kpl: 20                             # Maximum value for the convergence test of k-
↪points. It corresponds to the largest mesh grid in the three directions.
  enstart: 200                            # Minimum value for the convergence test of␣
↪cutoff energy
  enstep: 50                              # Interval for the convergence test of cutoff␣
↪energy
  enmax: 1000                             # Maximum value for the convergence test of␣
↪cutoff energy
  potential_type: GGA                     # Calculation scheme for convergence test.␣
↪User have to choose one potential among the GGA, LDA and HSE.

relaxation:
  potential_type:                          # Calculation scheme for structure␣
↪optimization. User can choose one or more potential among the GGA, LDA and HSE.
    - GGA
  max_iteration: 10                       # The maximum iteration number from␣
↪previously optimized structure
  converged_ionic_step: -1                # The tolerance of steps for iteration. Until␣
↪the relaxation finishes within the tolerance, we iterate the structure relaxation␣
↪from previously optimized structure. In negative value, it is neglected.
  length_tolerance: 0.002                 # The tolerance of length (ratio). Until the␣
↪relaxation finishes within the tolerance, we iterate the structure relaxation from␣
↪previously optimized structure. In negative value, it is neglected.
  angle_tolerance: 0.01                   # The tolerance of angle (degrees). Until the␣
↪relaxation finishes within the tolerance, we iterate the structure relaxation from␣
↪previously optimized structure. In negative value, it is neglected.
  energy: -1                              # The energy tolerance (eV) to break the loop␣
↪for structure optimization in VASP. In negative value, it is neglected.
  pressure: 10                            # The pressure tolerance (bar) to break the␣
↪loop for structure optimization in VASP. In negative value, it is neglected.
  force: 0.02                             # The force tolerance (eV/angst) to break the␣
↪loop for structure optimization in VASP. In negative value, it is neglected.

band_calculation:
  kspacing_for_band: 0.01                 # The distance between adjacent points in the␣
↪band structure (2pi/ang).
  type_of_kpt: all                        # Set the lines to calculate the band gap. In␣
↪the 'all', AMP2 calculates the eigenvalues along the lines connecting every␣
↪combination of high symmetric k-points. In the 'band', AMP2 calculates the␣
↪eigenvalue along the line to draw band structure.
  y_min: 3                                # The minimum energy range for band structure.
  y_max: 2                                # The maximum energy range from conduction␣
↪band minimum for band structure.
  potential_type:                         # Calculation scheme for band structure. User␣
↪can choose one or more potential among the GGA, LDA and HSE.
    - GGA

density_of_states:
  kp_multiplier: all                      # Multiplier for k-points for smooth figure.
  y_min: 3                                # The minimum energy range for density of␣
↪states.
  y_max: 2                                # The maximum energy range from conduction␣
↪band minimum for density of states.
  potential_type:                         # Calculation scheme for density of states.␣
↪User can choose one or more potential among the GGA, LDA and HSE.
```

(continues on next page)

(continued from previous page)

```
    - GGA

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.
  fermi_width: 0.3                      # The energy range for DF
  vb_dos_min: 1                         # The energy range for DVB
  vb_dos_max: 3                         # The energy range for DVB
  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
  potential_type:                       # The potential used for lattice parameter␣
↪optimization and for identifying the points at VBM and VBM. If one variable is␣
↪inserted, AMP2 uses the lattice parameter and the points of VBM and CBM with that␣
↪potential. If two variables are inserted, AMP2 uses the lattice parameter with␣
↪above potential and the points of VBM and CBM with below potential. (Ex. potential_
↪type:\n     - - HSE\n       - GGA)
    - GGA

dielectric:
  kp_multiplier: all                    # Multiplier for k-points for dielectric␣
↪constant.
  potential_type:                       # Calculation scheme for dielectric constant.␣
↪User can choose one or more potential among the GGA and LDA
    - GGA

effective_mass:
  carrier_type:                         # carrier type of effective mass to be␣
↪estimated
    - hole
    - electron
  temperature_for_fermi: 300            # The temperature to estimate the Fermi␣
↪distribution
  fermi_for_cutoff: 0.99                # Boundary condition for valid Fermi␣
↪distribution (1-f)
```

3.3.1 To get more accurate band gap

We suggest two approaches to get more accurate band gap.

- Band calculation with hybrid functional

  In the basic version, the band calculation is performed using PBE scheme. However, users can add the tags below to use hybrid functional for structure optimization and band calculation.

```
relaxation:
  potential_type:
    - HSE
band_calculation:
  potential_type:
    - HSE
```

- Using HSE@PBE scheme with hybrid structure

  Second approach is still using HSE@PBE method but the optimized structure is calculated using hybrid functional. Since the band calculation with hybrid functional is too expensive, the k-points corresponding to the

VBM and CBM are determined by using GGA method. For this calculation, users can use the commands below. Here, if potential_type in hybrid_oneshot is the main category, the method tags (HSE and GGA) are child subcategory not parent subcategory. Please be careful.

```
relaxation:
  potential_type:
    - GGA
    - HSE
hybrid_oneshot:
  potential_type:
    - - HSE
      - GGA
```

3.3.2 Organic crystal

Organic crystals usually have lower Young's modulus than inorganic materials. Thus, the error in the structural parameters can be substantial and they require high precision for calculation. The tags below can control the precision of calculation.

```
cif2vasp:
  INCAR:
    EDIFF: 1e-08

convergence_test:
  enconv: 0.001
  prconv: 1

relaxation:
  pressure: 1
  force: 0.002
```

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.png (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)

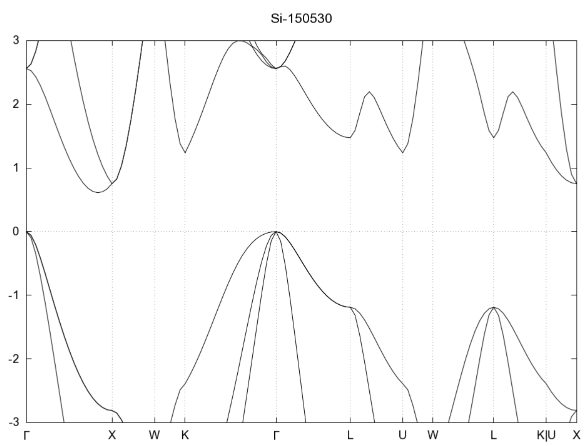
(continued from previous page)

```
    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
```

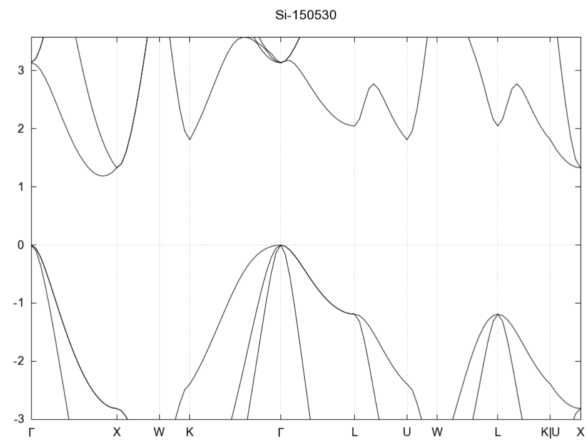
Band structure (/Results/band_GGA.png and /Results/band_GGA.pdf)



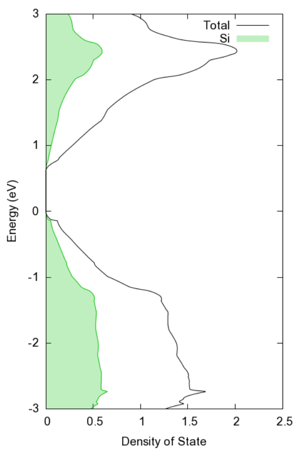
Band gap from HSE@PBE (/Results/band_hybrid_GGA.log)

```
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
```

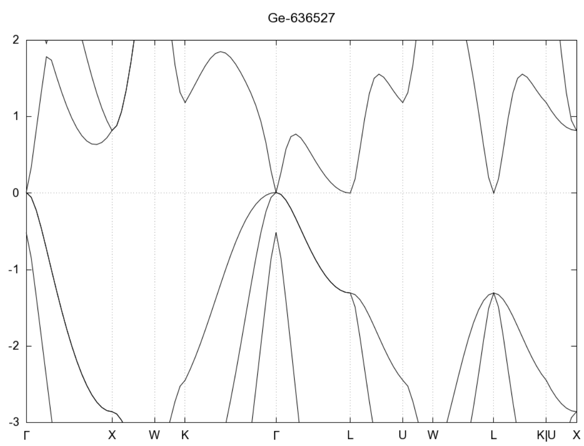
5.3.2 Ge

Ge is a well-known semiconductor with metallic band structure in conventional DFT schemes like LDA and PBE. In AMP², 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.
```

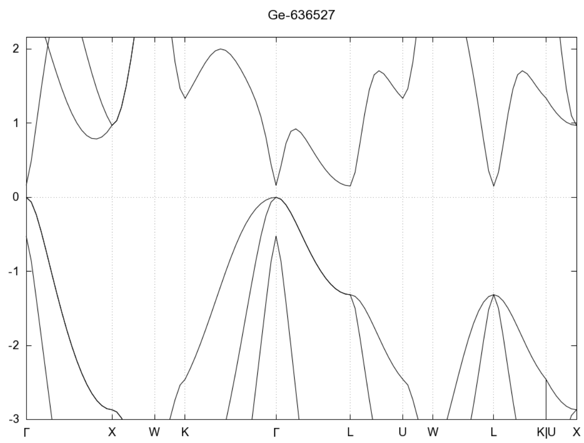
Band structure (/Results/band_GGA.png and /Results/band_GGA.pdf)



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).

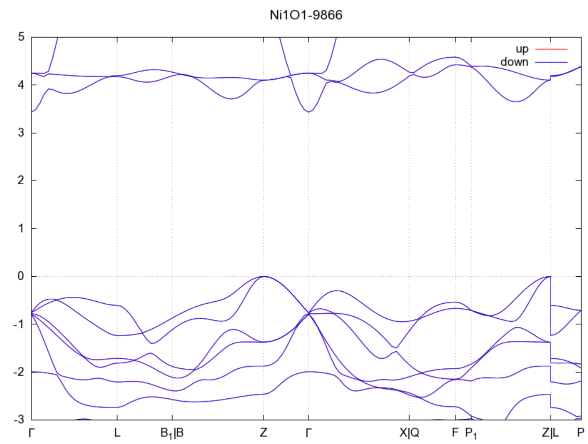
Optimized structure (/Results/POSCAR_rlx_GGA)

```
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
```

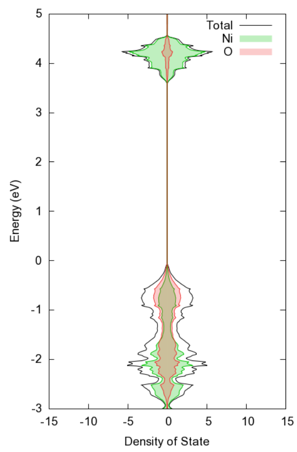
Band gap (/Results/band_gap_GGA.log)

```
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)



CHAPTER 6

Test

6.1 Test_list