SPaMD Auto Series User Manual

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Catalog

1 Open SPaMD Auto Series sub-function screen

1) Double click SPaMD -> Simulation -> VASP -> Auto Series -> ABAND (different functions can be selected)

2) A graphical login screen pops up and successfully accesses the Auto Series sub-function screen

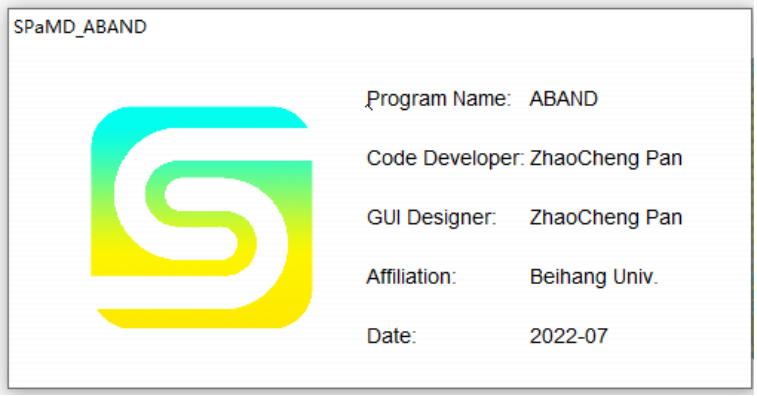

Fig 1.1 Login screen

2 SPaMD Auto Series Sub-Function Interface Introduction

The Auto Series sub-function interface has six functional areas, namely Model, Potential, Setting, Output, Submit, and Download, and each area will be introduced in turn. Selecting different sub-functions in the Auto Series menu will result in different Setting and Output areas, so the details of these two sections are introduced together with the Auto Series sub-functions.

2.1 Model area (Model)

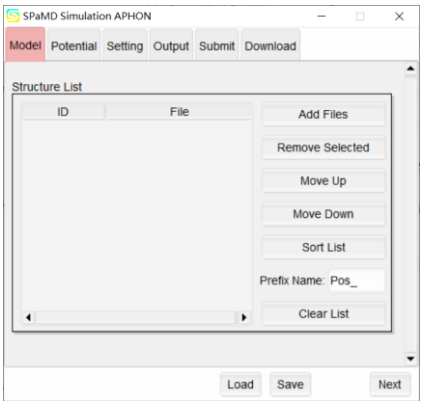

Fig 2.1 SPaMD Auto Series sub-function interface - Model area (Model)

The model area is used to add and adjust the order of structure files, and the para meters can be set as follows

Structure List: the list of structure files added, the ID column shows the file ord er, the File column shows the file location, the added structure files are standard POS CAR files;

Add Files: select the structure files to be added;

Remove Selected: removes the selected file;

Move Up: moves up the order of the selected files;

Move Down: moves down the order of the selected files;

Sort List: organizes the order of the files so that they are arranged in the alphabe tical and numerical order of the file names, which can be converted to reverse order b y clicking again;

Prefix Name: setting of the file name prefix;

Clear List: Clear all the list files.

2.2 Potential function area (Potential)

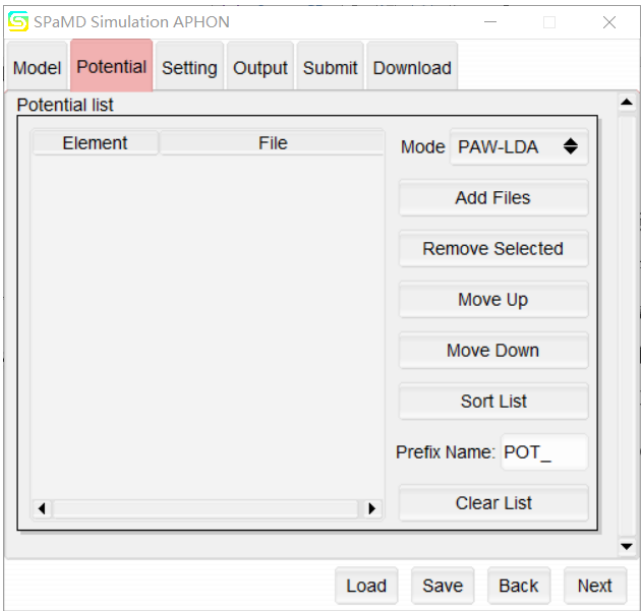

Fig 2.2 SPaMD Auto Series sub-function interface - Potential function area (Potential)

The potential function area is used to add and adjust the potential function file, a nd the parameters can be set as follows

Potential List: the list of added potential function files, the ID column shows th

e file order, the File column shows the file location, the added files are standard POTCAR files;

Mode: selection of pseudopotential types, including PAW-LDA, PAW-PW91, PAW-PBE, USPP-LDA, USPP-GGA;

Add Files: select the potential function files to be added;

Remove Selected: removes the selected file;

Move Up: moves up the order of the selected files;

Move Down: moves down the order of the selected files;

Sort List: organizes the order of the files so that they are arranged in the alphabetical and numerical order of the file names, which can be converted to reverse order by clicking again;

Prefix Name: setting of the file name prefix;

Clear List: Clear all the list files.

2.3 Setting area (Setting)

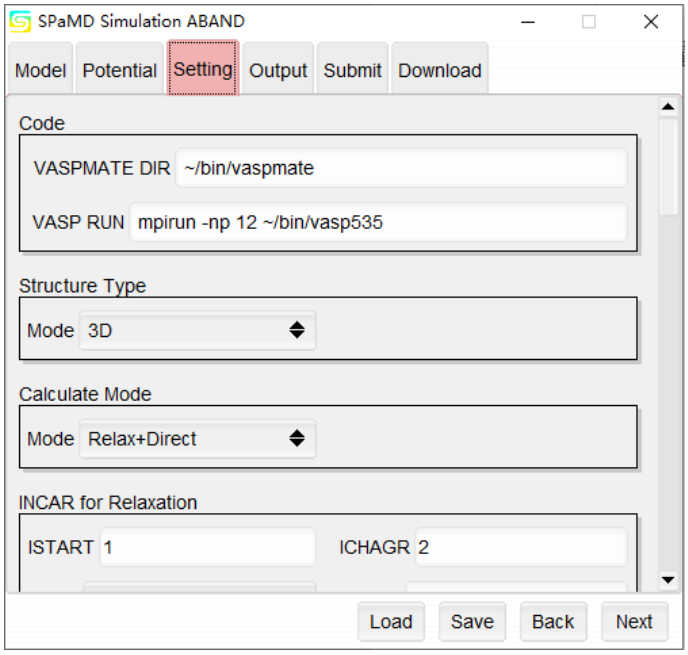

Fig 2.3 SPaMD Auto Series sub-function screen - Setting area (Setting)

The setup area is used to set the commands of VASPMATE, VASP and other third-party programs to run; and also set the parameters of VASP and other third-party programs input files, such as: INCAR file parameters, KPOINTS file parameters, etc.; s

ome other parameters can also be set. In addition, the setting area is managed by grou ping parameters, which can effectively avoid confusion.

2.4 Output area (Output)

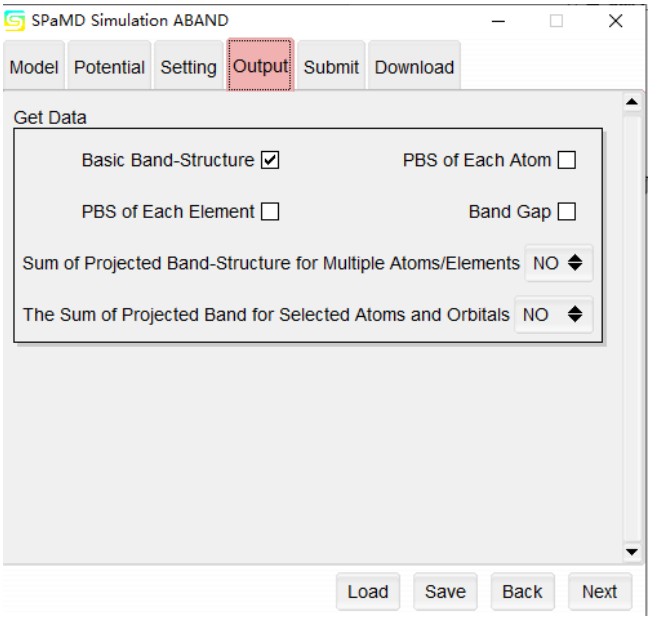

Fig 2.4 SPaMD Auto Series sub-function screen - Output area (Output)

The output area is used to selectively save related files.

2.5 Submission area (Submit)

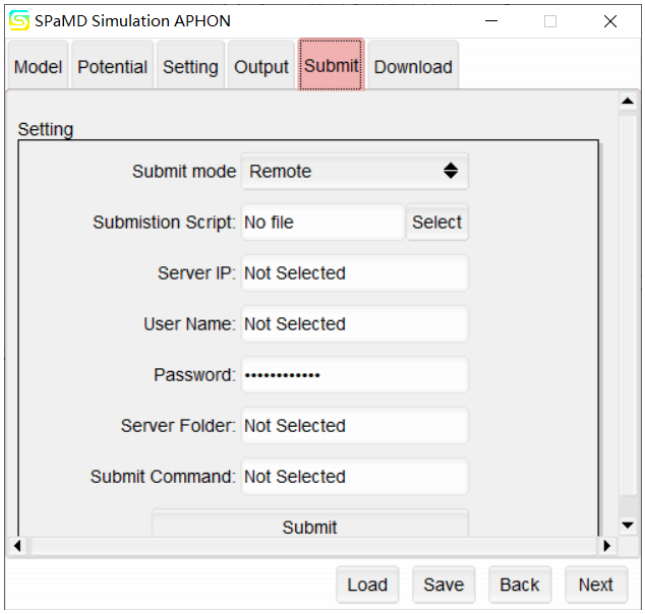

Fig 2.5 SPaMD Auto Series sub-function interface - Submit area (Submit)

The commit area is used to set some parameters of the commit process, which ca n be set as follows:

Submit mode: selection of remote submission of tasks;

Submistion Script: selects the location of the submission script;

Server IP: Enter the server IP;

User Name: enter the user name;

Password: Enter the user name and password;

Server Folder: specifies the path to the submitted task in the server;

Server Command: Enter the submit task command;

Submit: Submit the assignment.

2.6 Download area (Download)

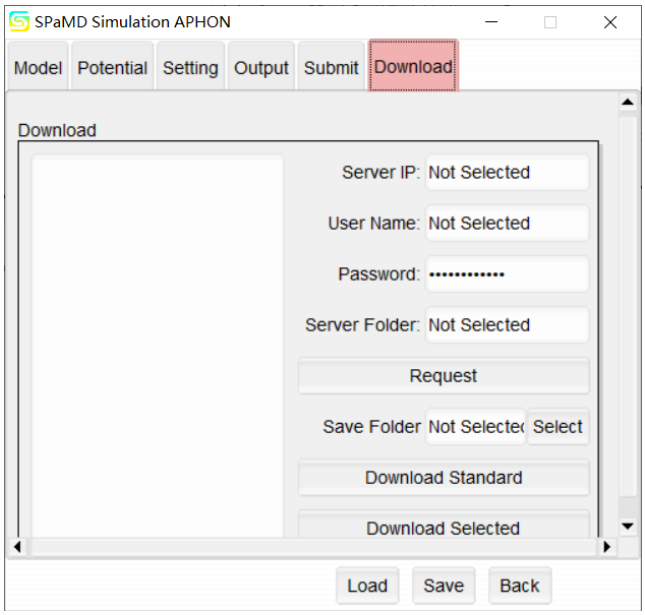

Fig 2.5 SPaMD Auto Series sub-function screen - Download area (Download)

The download area is used to set the download file save location and download t he file:

Server IP: Enter the server IP;

User Name: enter the user name;

Password: Enter the user name and password;

Server Folder: the path to the task file on the server;

Request: View the contents of the task folder on the server

Save Folder: select the location where the downloaded file is saved;

Download Standard: Download standard files;

Download Seleceted: Downloads the selected file.

2.7 SPaMD Auto Series sub-function interface task submission

The general order of task submission is as follows: first, select the structure file o f the material in the Model area; set the potential function mode in the Potential area a nd provide the potential function file; set the VASP run command, input file parameter s and related analysis parameters in the Setting area; set the file submission location a nd output file download location, etc., after which the software will After that, the soft ware will automatically analyze and organize the parameters and generate the submiss ion folder, upload the submission folder to the server, and use the server-side program for calculation, then the corresponding calculation can be performed until the end of t he run.

3 ABAND

3.1 A brief introduction to ABAND

SPaMD ABAND is an efficient open-source program for first-principles calculati ons of material energy band structure and other related properties. The overall calculat ion flow is organized by the VASPMATE program, which is divided into structure opt imization, first Brillouin zone high symmetry path generation, INCAR parameter setti ng, pseudopotential merging, energy band information extraction, band gap calculatio n, energy band mapping, etc. The computational flow is shown in the following Fig:

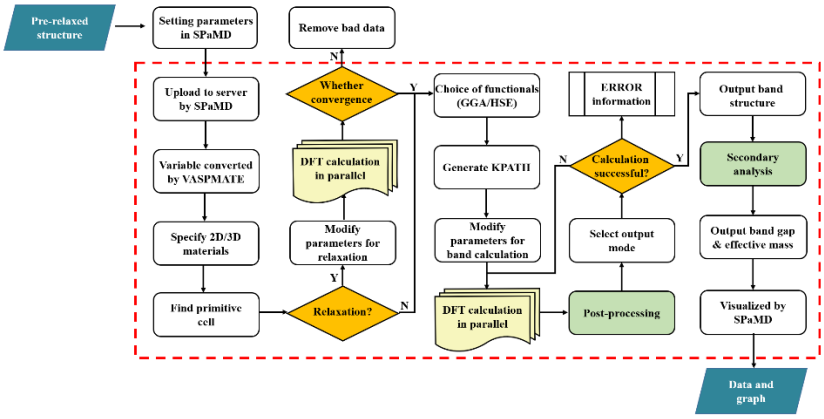

Fig 3.1 Flow chart of ABAND calculation

3.2 ABAND setting area (Setting)

3.2.1 Structure file import

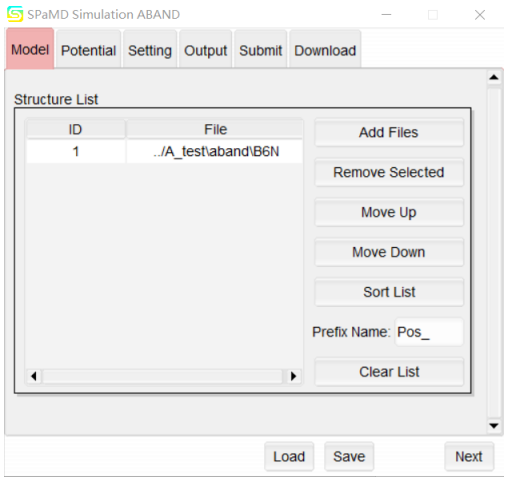

Fig 3.2 SPaMD Auto Series sub-function ABAND interface-Model

Select Add Files to import the structure.

3.2.2 Pseudopotential file import

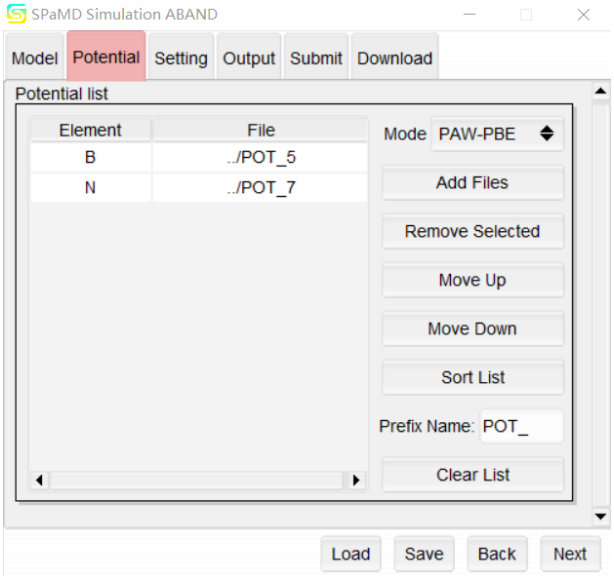

Fig 3.3 SPaMD Auto Series sub-function ABAND interface-Potential

Select Add Files to import the pseudopotential file, and select the pseudopotential typ e in Mode to match the file type, in this case PAW-PBE.

3.2.3 VASP input file parameter adjustment

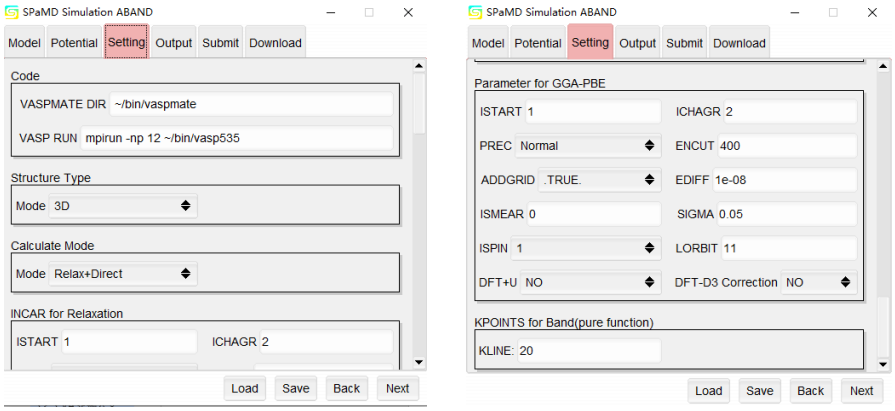

Fig 3.4 SPaMD Auto Series sub-function ABAND interface-Setting

VASPMATE DIR and VASP RUN in Code are the storage paths for the programs VA SPMATE and VASP, respectively.

Structure Type: Structure type, divided into 1D, 2D, 3D (currently only support 3D str ucture).

Calculate Mode: Calculate Mode 1. Relax + Direct Optimize first and then calculate t he energy band 2. Direct Calculate the energy band directly.

INCAR for Relaxation: INCAR parameters for structural optimization, which generat es the file incar_rlx.

KPOINTS for Relaxation: structure-optimized KPOINTS parameters, generating the f ile NEWKPT.

Three scattering point models: 1). KPPRA recommended value 4000-8000 2). KSPAC recommended value 0.5 3). Kmesh manual setting of specific scattering points

Functional Mode: Generalized mode selection 1. GGA-PBE 2. HSE-PBE

Parameter for GGA-PBE: The INCAR parameter when selecting the GGA-PBE gener alization, corresponding to the Parameter for HSE-PBE.

KPOINTS for Band (pure function): selects the number of points to be scattered on th e high symmetry path of the GGA-PBE generalization function.

KPOINTS for Band (HSE): KPOINTS parameters when selecting HSE-PBE. The firs t three are the general scattering accuracy settings for SCF calculation, and KPRA (De nsity of PATH) is the density of scattering points on the energy band path.

3.3 ABAND output area (Output)

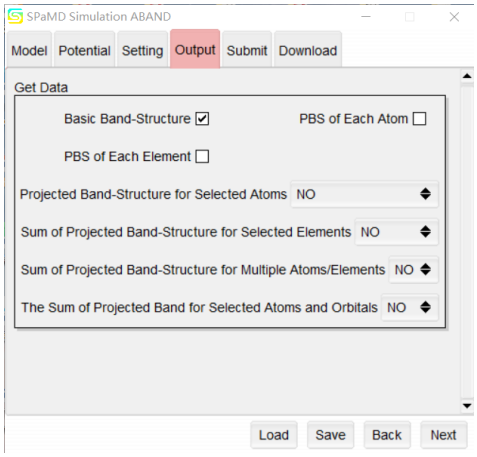

Fig 3.5 SPaMD Auto Series sub-function ABAND interface - Output

The output module has 7 mode options.

1）Basic Band-Structure

VASPMATE command: VASPMATE --band -b

Obtain the basic energy band structure for plotting.

2）Projected Band-Structure of Each Atom

VASPMATE command: VASPMATE --band -a

Obtain the projection of each atom on the energy band.

3）Projected Band-Structure of each element

VASPMATE command: VASPMATE --band -e

Get the projection of each element on the energy band.

4）Projected Band-Structure for Selected Atoms

VASPMATE command: VASPMATE --band -sa <atom-index>

The projections of the selected atoms on the energy band are obtained separately.

5）Projected Band-Structure for Selected Elements

VASPMATE command: VASPMATE --band -se <element-index>

Get the projection of the selected elements on the energy band respectively.

6）Sum of Projected Band-Structure for Multiple Atoms/Elements

VASPMATE command: VASPMATE --band -m/-ma/-me <atom/element-index>

Obtain the sum of the projections of the selected atom or element on the energy ba

nd.

7）The Sum of Projected Band for Selected Atoms and Orbitals

VASPMATE command: VASPMATE --band -o <atom&orbit-list>

Obtain the sum of the projections of the selected atoms on the selected orbitals.

All the above data have been set to 0 for the Fermi energy level.

3.4 Example of ABAND

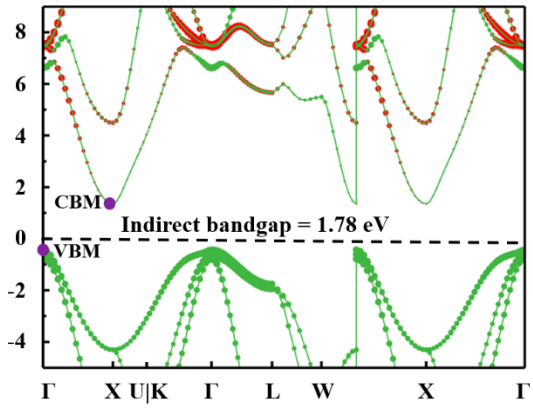

Fig 3.6 SPaMD Auto Series SiC-3C energy band structure

4 AEDOS

4.1 Brief introduction of AEDOS

SPaMD AEDOS is an efficient open-source program for first-principles calculations of density of states and other related properties of materials. The overall calculation process is organized by the VASPMATE program, which is divided into structure optimization, automatic generation of k points in the Brillouin zone, INCAR parameter setting, pseudopotential merging, density of states information extraction, Fermi energy level extraction, density of states mapping, etc.

4.2 AEDOS setting area (Setting)

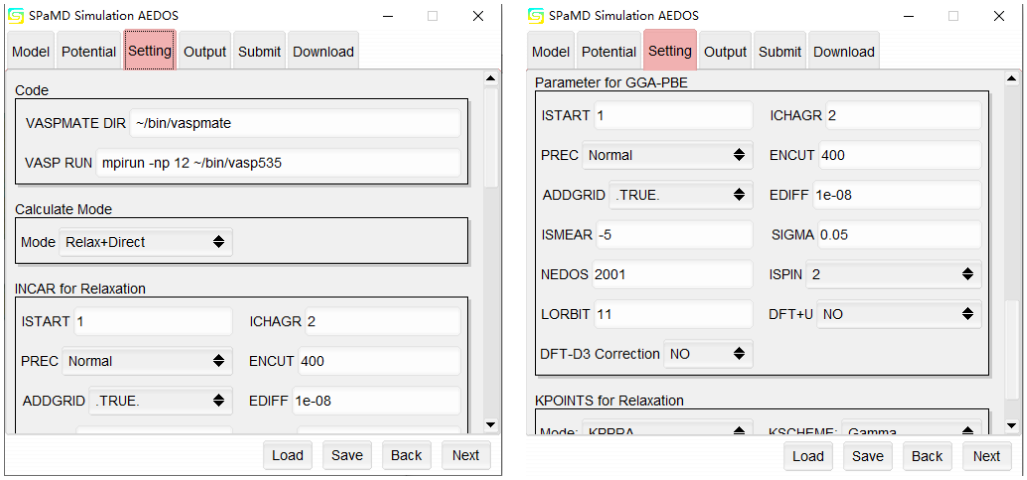

Fig 4.1 SPaMD Auto Series sub-function AEDOS interface - Setting

Refer to ABND.

4.3 AEDOS output area (Output)

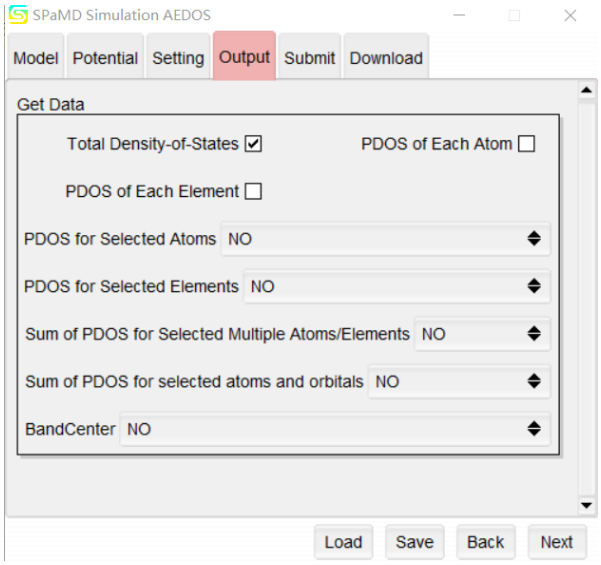

Fig 4.2 SPaMD Auto Series sub-function AEDOS interface - Output

1) Total Density-of-states

VASPMATE command: VASPMATE --dos -t

Get the total DOS.

Usage: Check the box.

2) PDOS of Each Atom

VASPMATE command: VASPMATE --dos -a

Obtain the PDOS of each atom.

Usage: Check the box.

3) PDOS of Each Element

VASPMATE command: VASPMATE --dos -e

Obtain the PDOS for each element.

Usage: Check the box.

4) PDOS of Selected Atoms

VASPMATE command: VASPMATE --dos -sa <atom-index>

Obtain the PDOS of the selected atom.

Usage: Check the box and enter the atomic number in the input field.

5) PDOS of Selected Elements

VASPMATE command: VASPMATE --dos -se <element-index>

Get the PDOS of the selected element.

Usage: Check the box and enter the element symbol in the input field.

6) Sum of Projected Band-Structure for Multiple Atoms/Elements

VASPMATE command: VASPMATE --band -m/-ma/-me <atom/element-index>

Obtain the sum of the projections of the selected atoms or elements.

How to use: Check the box and enter the atomic number or element symbol in the inp ut field.

7) PDOS of Selected Atoms and Orbitals

VASPMATE command: VASPMATE --dos -o <atom&orbit-list>

Selected atoms and the sum of projections of the orbitals.

How to use: Check the box and enter the atomic number plus the corresponding atomi c track (free format) in the input field.

8) BandCenter

VASPMATE command: VASPMATE --dos -bc <atom/element-index>

Calculate the band centers of s, p, d, and f.

Usage: Check the box and enter the atomic number or the element symbol in the input

field.

All the above data have been set to 0 for the Fermi energy level.

4.4 Example of AEDOS

SiC-3C energy band and density of states.

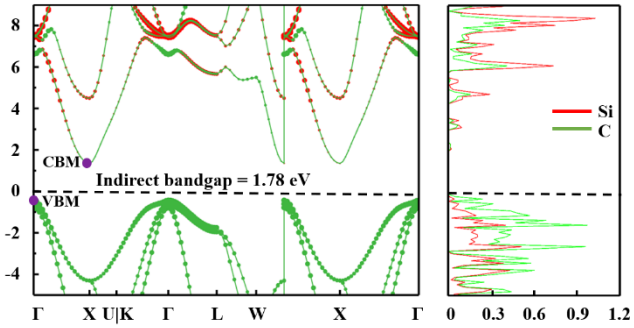

Fig 4.3 band structure, and density of states for bulk 3C-SiC respectively.

5 AHULL

5.1 Brief introduction of AEDOS

AHULL is mainly used to calculate the convex envelope map of binary compoun ds by performing structural relaxation and static self-consistency of the cell with suita ble computational parameters and obtaining the enthalpy of formation by pre-defined individual atomic energy calculations. VASPMATE gives the convex hull diagram by counting all structural components and enthalpies of formation and visualized by SPa MD.

5.2 AHULL setting area (Setting)

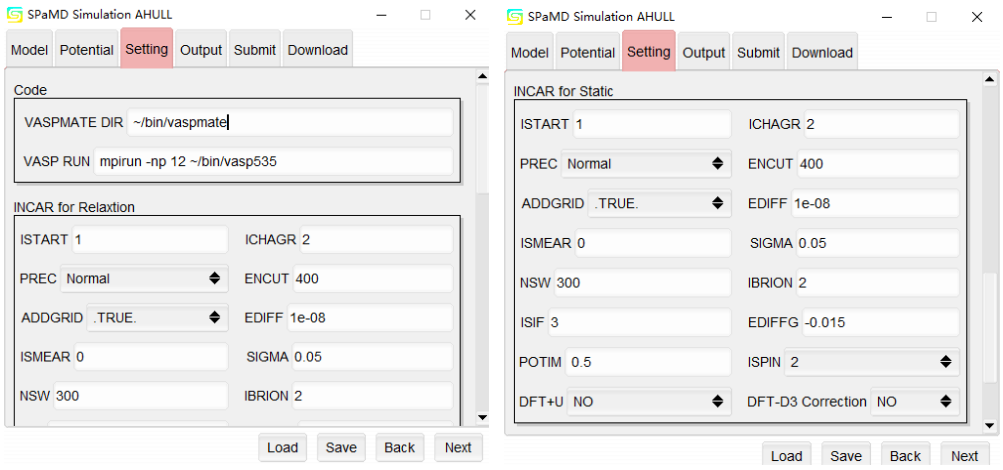

Fig 5.1 SPaMD Auto Series sub-function AHULL interface - Setting

Refer to ABND.

5.3 AHULL setting area (Setting)

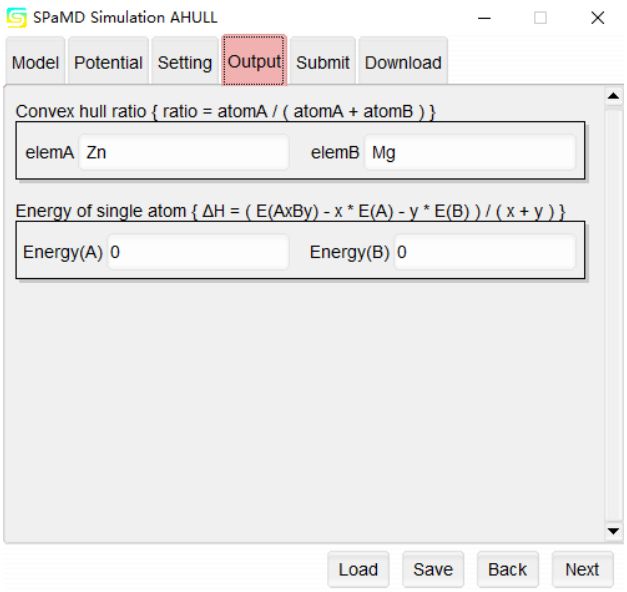

Fig 5.2 SPaMD Auto Series sub-function AHULL interface - Output

Since the convex hull diagram is mainly for the enthalpy of formation of binary c ompounds, we need to provide in advance the individual atomic masses of the constit uent elements, which correspond to Energy(A) and Energy(B) in the diagram. In addit ion to this, we need to determine the composition of the component ratios in the conve x packet diagram, i.e., the way the ratio parameter is calculated. The user needs to surf ace which elements correspond to elemA and elemB, respectively, and VASPMATE w

ill match them one by one with the elements in POSCAR.

5.4 Example of AHULL

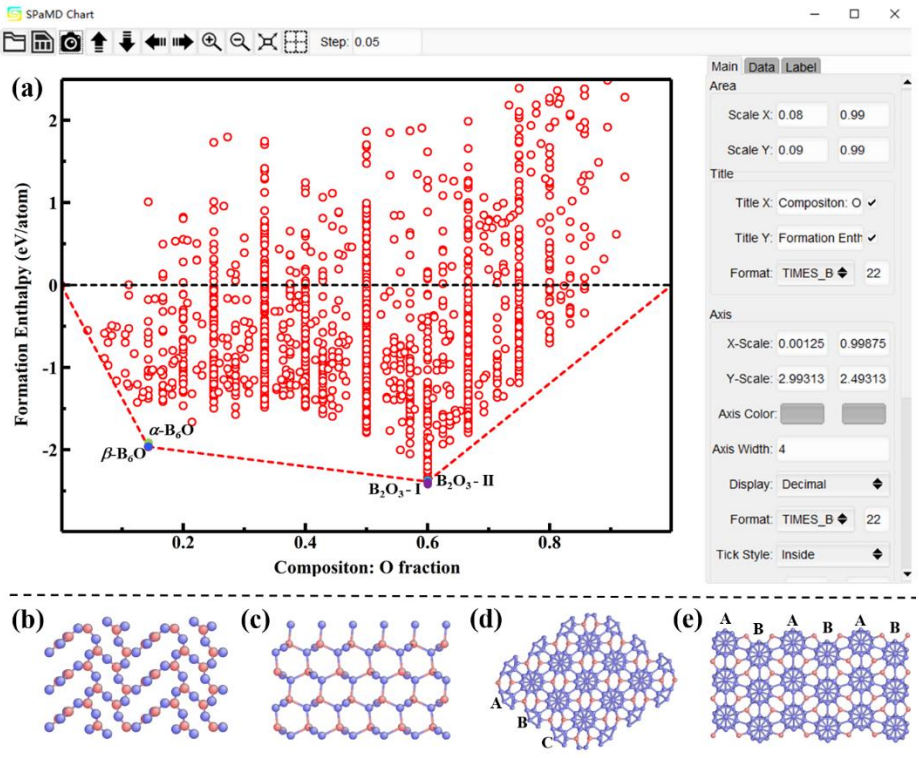

Fig 5.3 (a) Convex hull of the B-O system at ambient pressure. (b) B_2O_3-I, (c) B_2O_3-II, (d) α-B_6O and (e) β-B_6O crystal structures visualized by SPaMD.