MATSDP

The materials simulation and data processing toolkit

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Contents

Chapter 1

Introduction

MATSDP is a materials simulation and data processing toolkit. The Vienna ab-initio simulation package (VASP) and the Three-dimensional atom probe tomography (APT) analyzing and data processing tools are included.

1.1 Functions

VASP analyzing and data processing tools:

- vasp_build: Build model by atom substitution or atom selection based on a POSCAR file.
- vasp_read: Read DOSCAR, OUTCAR, POSCAR, and OSZICAR
- vasp_plot.plot_poscar: Plot POSCAR/CONTCAR model (also support color mapping of atom properties), Required files: POSCAR/-CONTCAR or POSCAR with data of atom properties
- vasp_plot.plot_dos: Plot DOS (PDOS, LDOS, TDOS) information. Required input: DOSCAR, OUTCAR, POSCAR
- vasp_analyze.nn_map: Calculate the nearest neighbor information. Required input: POSCAR
- vasp_analyze.simple_cna: Perform simple common neighbor analysis
- vasp_analyze.estruct: Calculate structural energy (E_{struct}). Required files: CONTCAR, OUTCAR, POSCAR

- vasp_write.write_poscar_with_force: Write atom force information into the POSCAR

APT postprocessing tools:

- apt_read.read_proxigram_csv: Read the concentration profile *.csv file
- apt_plot.plot_proxigram_csv: Plot the concentration profile

The matsdp package contains the vasp and apt modules as shown in Figure 1.1. The structures of the vasp module and the apt module are shown in Figure 1.2 and Figure 1.3.

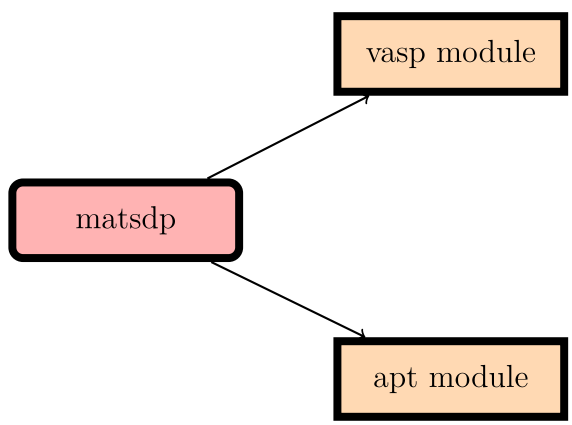


Figure 1.1: subpackages of the matsdp program.

1.2 Requirements

- numpy
- scipy
- scikit-learn
- matplotlib

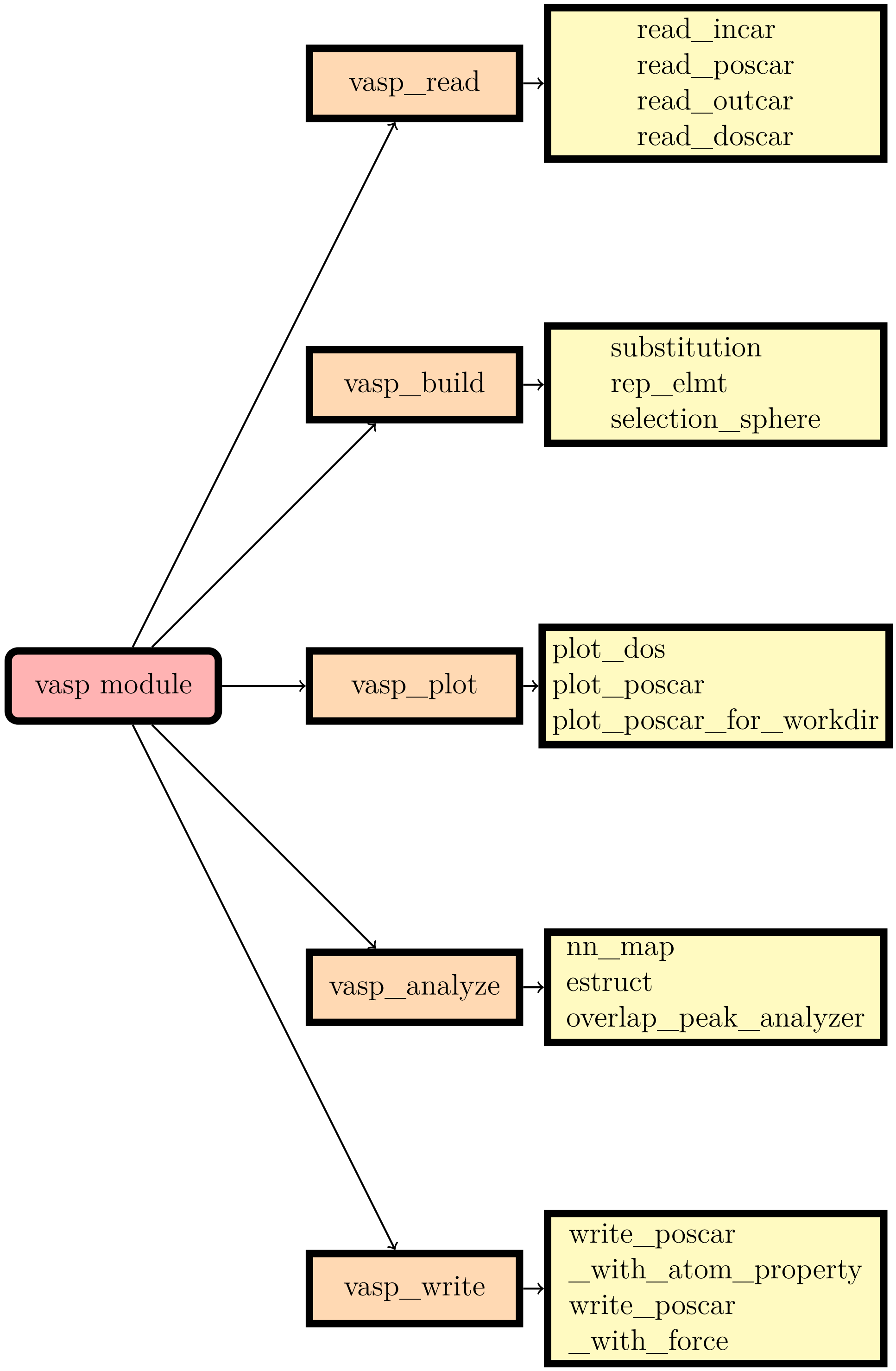


Figure 1.2: vasp module.

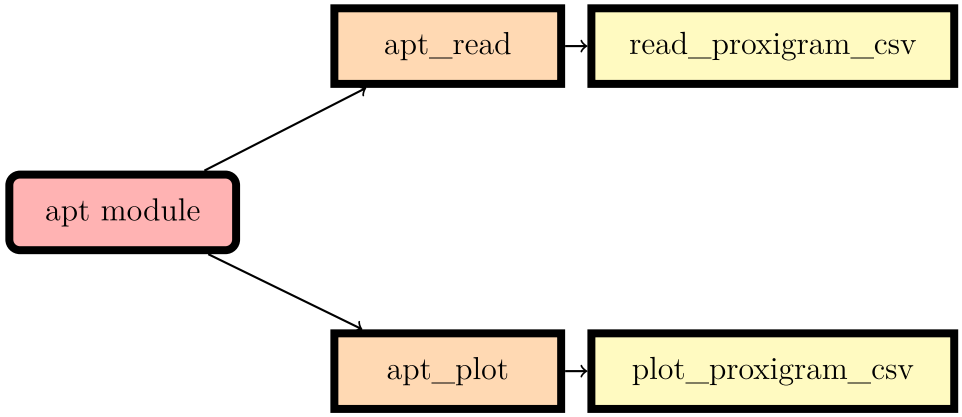


Figure 1.3: apt module.

1.3 Installation

For the Python users, the package can be retrieved by the following command.

```
pip install matsdp
```

For the GUI users, please run the matsdp_gui.exe directly.

1.4 Usage

1.4.1 Running with Python environment

After installing the matsdp package, the program can be used by importing the modules and call the related functions.

1.4.2 Running Graphical User Interface (GUI) application

The program provides a graphical user interface (matsdp_gui.exe). The GUI is shown in the Figure 1.4:

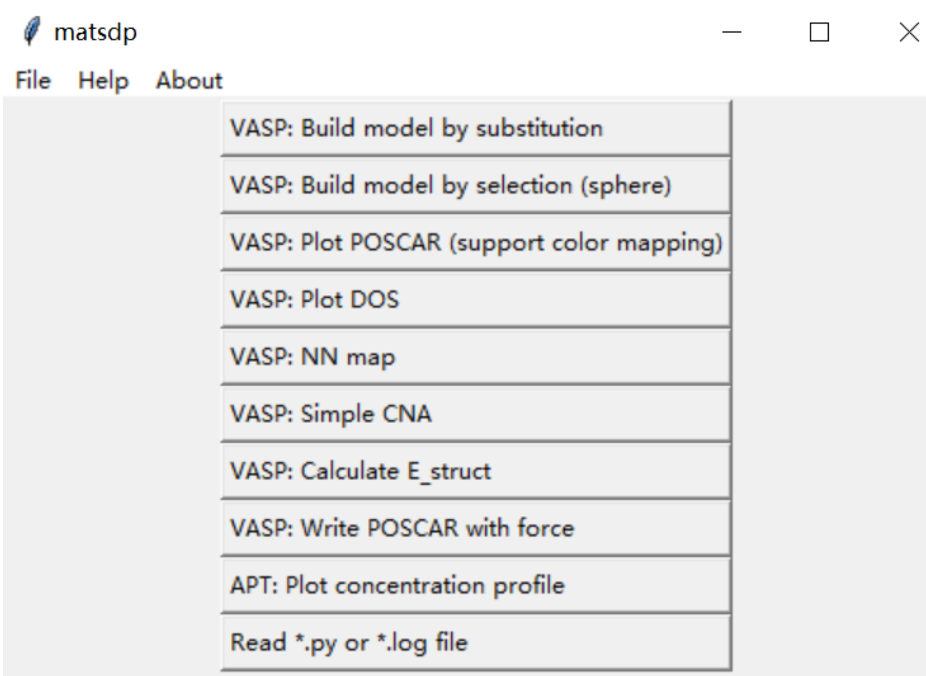


Figure 1.4: GUI for the main program

1.5 Notes

Note that for the module that requires POSCAR/CONTCAR, OUTCAR and DOSCAR files, these files need to be in the same folder.

The following sections will introduce the settings of the parameters in the GUI.

Chapter 2

subpackage: vasp

Modules to import before using the vasp package

- from matsdp.vasp import vasp_read
- from matsdp.vasp import vasp_build
- from matsdp.vasp import vasp_plot
- from matsdp.vasp import vasp_analyze
- from matsdp.vasp import vasp_write

2.1 vasp_build module

2.1.1 vasp_build.substitution

Descriptions

Building models by substitution of atoms

Syntax

```
from matsdp.vasp import vasp_build
vasp_build.substitution(
    substitution_list_file = './example/vasp/example/
    vasp.subst',
    poscar_dir = './example/vasp/POSCAR_NoDope',
```

```
)
```

Arguments

- substitution_list_file: String format. It specifies the directory of the .subst file (substitution list file)
- poscar_dir: String format. The directory of the POSCAR file which is to be subsituted. It can either be full path or relative path.

.subst file

Descriptions

- The .subst file (substitution list file) is required and should consists of system entries.
- A system corresponds to a specific model configuration.
- System entries specifies how atoms are substituted in different systems.
- A system entry is a block of successive lines without line breaks.
- Each system entries must be separated by blank lines.

File formats. A typical system entry has the following format:

```
n_subst
elment_name_to_be_substituted new_element_name
elment_name_to_be_substituted new_element_name
...
(n_subst lines of elment_name_to_be_substituted
elment_subindx new_element_name)
```

where, elment_name_to_be_substituted is he name of the element which is to be substituted. new_element_name is the name of the new element which take the place of the substituted atom. If new_element_name = Va, then a vacancy is added. As shown above, each system should start with a line which specifies a number: n_subst. n_subst is the number of atoms to be substituted in the system. Then each of the following n_subst lines specifies the element(s) to be substituted and the element(s) which take its/their place(s).

A specific example .subst file is as follow:

```
1
Ni244 W

2
Ni244  Re
Al12  Re

...
```

GUI

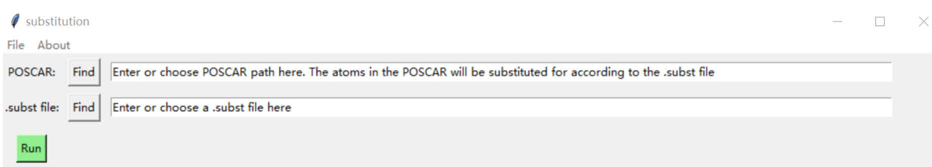


Figure 2.1: GUI for Substitution

Outputs

Outputs: The final system name is L(line_number)_composition_D(duplicate)

2.1.2 vasp_build.selection_sphere

Descriptions

Building models by selection of atoms. The atoms within a sphere will be selected.

Syntax

```
from matsdp.vasp import vasp_build
vasp_build.selection_sphere(
    poscar_dir = './tests/vasp/CONTCAR',
    origin_atom_name = 'Re1',
    radius = 7,
    include_mirror_atoms = False,
    output_file_name = 'example'
    )
```

Arguments

- poscar_dir: String format. The directory of the POSCAR file. It can either be full path or relative path.
- origin_atom_name: String type. It defines the origin atom of the sphere
- radius: Float type. The atoms within a distance "radius" from the original atom are selected (units in Angstroms);
- include_mirror_atoms: Logical value. Whether to include the mirror atoms or not;
- output_file_name: user-defined output file name.

GUI

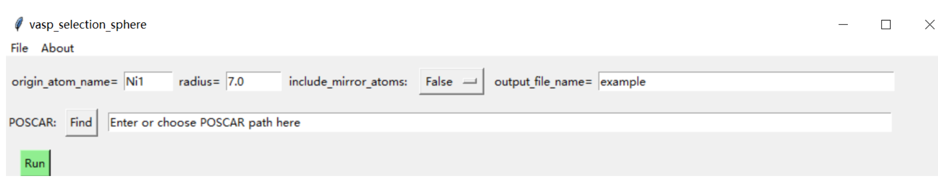


Figure 2.2: GUI for selection_sphere

Outputs

Outputs: *.vasp, *.xyz, and *.incar files. The *.incar file can be used as the input file for the DVM program.

2.2 vasp_plot module

2.2.1 vasp_plot.plot_poscar

Descriptions

- Visualization of POSCAR model. Euler angles are used to rotate the view of the model.
- Viewer direction is in x direction. The original orientation: x direction is perpendicular to the paper, z direction is in the paper and point to upper direction
- Reference for Eulerian angles: Herbert Goldstein, Charles P. Poole Jr. and John L. Safko, Classical Mechanics (3rd Edition). Goldstein Poole & Safko, 2001.
- This module can also show the atom properties by color mapping. The POSCAR file with additional data columns used to save the data of the atom properties.

Syntax

```
from matsdp.vasp import vasp_plot
vasp_plot.plot_poscar(
    poscar_dir = './example/vasp/POSCAR',
    euler_angle_type = 'zyz',
    phi = -3,
    theta = 4,
    psi = 0,
    elmt_color = {'Ni':'red','Re':'blue'},
    draw_mirror_atom = True,
    box_on = True,
    axis_indicator =True,
    plot_cell_basis_vector_label = True,
    plot_atom_label = True,
    fig_format = 'png',
    fig_dpi = 100,
    draw_colormap = False,
```

```
    colormap_column_indx = 1,
    colormap_vmin = None,
    colormap_vmax = None,
    vmin_color = 'blue',
    vmax_color = 'red',
    colorbar_alignment = 'vertical'
        )
```

Arguments

- poscar_dir: String format. Directory of the POSCAR file which you want to plot
- euler_angle_type: string of length 3. It specify the type of rotations based on Eulerian angles. Choices are 'zyz', 'zxz', 'zyx', etc.. Usually the 'zyz' type is used.

  'zyz' : proper Euler angle, y-convention. Perform consecutive rotations at axes counter-clockwisely. z-y-z rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate y axis of atoms by an angle theta, finally rotate the final z axis of atoms by an angle psi

  'zxz' : proper Euler angle, x-convention. Perform consecutive rotations at axes counter-clockwisely. z-x-z rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate x axis of atoms by an angle theta, finally rotate the final z axis of atoms by an angle psi

  'zyx' : Tait-Bryan angles. z-y-x rotation. Perform consecutive rotations at axes counter-clockwisely. z-y-x rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate y axis of atoms by an angle theta, finally rotate the final x axis of atoms by an angle psi
- phi, theta, psi: float formats. The first, second, and third rotation Eulerian angles, units in degrees.
- elmt_color: dictionary formats. this dictionary sepcifies the color for each element. For example elmt_color = {'Ni':'black','Al':'magenta'}
- draw_mirror_atom: Logical value. Whether to plot the mirror atoms at the periodic boundary

- box_on: Logical value. Whether to plot the box or not
- axis_indicator: Logic value. Whether to plot the axis indicator
- plot_cell_basis_vector_label: Logical value. Whether to plot the cell basis vector labels(i.e., to label the three basis vectors of the cell as a, b, and c)
- plot_atom_label: Logical value. If true, then plot the atom name of each atom.
- fig_format: String format. fig_format is a string that defines output figure format. Supported fig_format: 'png', 'eps', 'pdf', 'tif', 'tiff', 'jpg', 'jpeg', 'svg', 'svgz', 'pgf', 'ps', 'raw', 'rgba'
- fig_dpi: float format. The DPI for non-vector graphics.
- draw_colormap: Logical value. If true, the color mapping of atom properties will be Performed. Default: False.
- colormap_column_indx: Integer value. Define which column of the atom property columns will be color mapped. Default: 1.
- colormap_vmin: Float value. Define the minimum value of the color map. If colormap_vmin=None, the minimum value of the original data will be used. Default: None.
- colormap_vmax: Float value. Define the maximum value of the color map. If colormap_vmax=None, the maximum value of the original data will be used. Default: None.
- vmin_color = 'blue': String type. Define the color for the smallest value of the atom properties in the color map. Default: 'blue'.
- vmax_color = 'red': String type. Define the color for the largest value of the atom properties in the color map. Default: 'red'.
- colorbar_alignment: String type. Defines the alignment of the color bar in the figure of the color map. The value can be either 'vertical' or 'horizontal'. Default: 'vertical'.

GUI

The GUI of the plot_poscar module is shown in the Figure 2.3

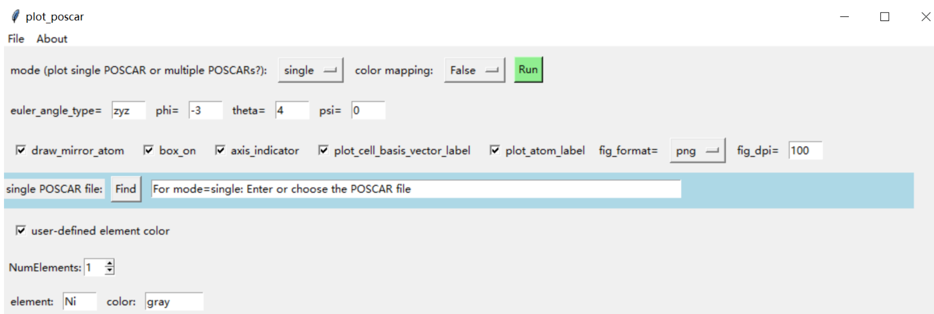


Figure 2.3: GUI for matsdp.vasp.vasp_plot.plot_poscar

Outputs

Figures of POSCAR models.

Examples

The examples are shown in the Figure 2.4, Figure 2.5, Figure 2.6 and Figure 2.7.

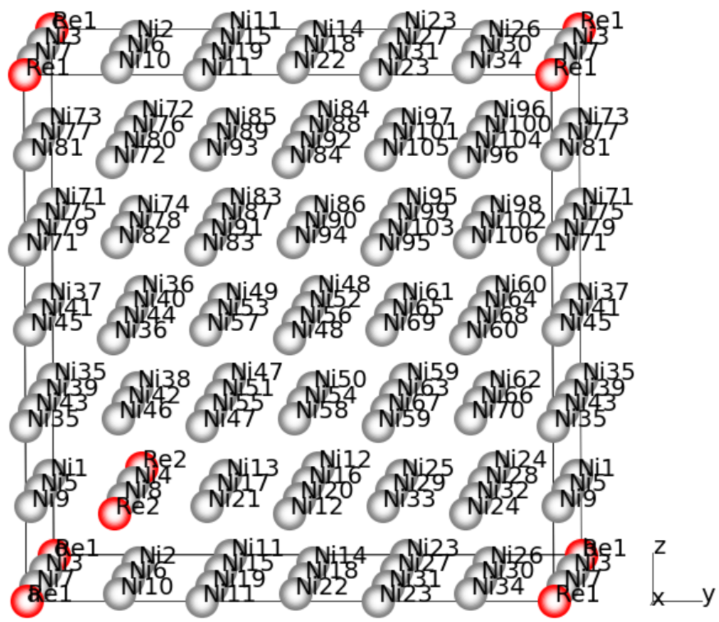


Figure 2.4: Result of the plot_poscar module. The atom label is added.

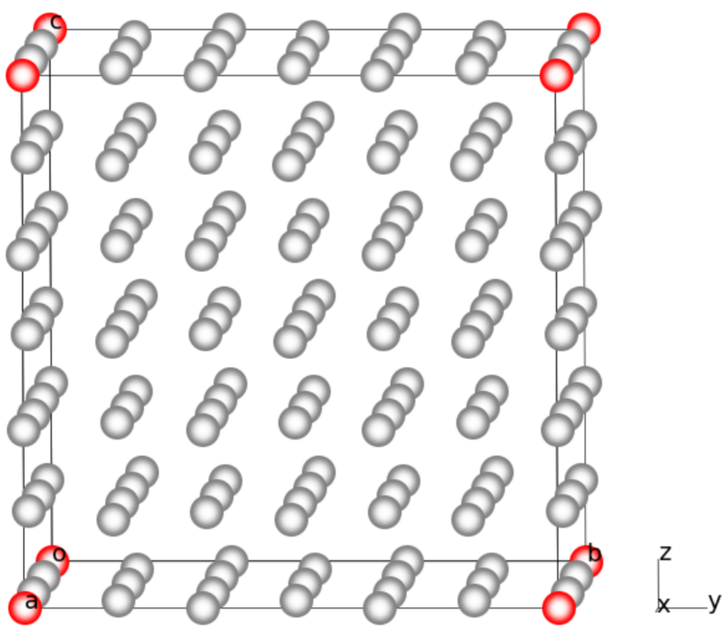


Figure 2.5: Result of the plot_poscar module. The atom label is removed.

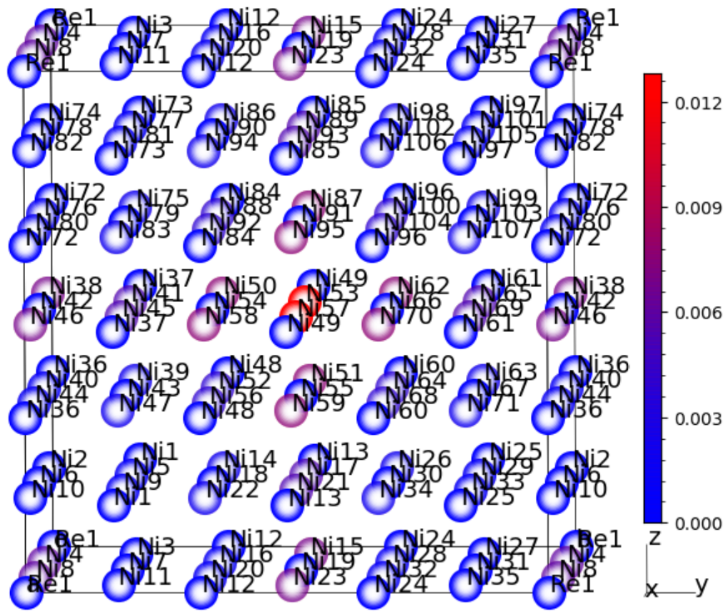


Figure 2.6: Result of the plot_poscar module: color mapping of atom properties. The color bar is vertically aligned.

2.2.2 vasp_plot.plot_poscar_for_workdir

Descriptions

- Visualization of POSCARs.
- The mother folder needs to be specified which contains the folders with POSCARs
- Euler angles are used to rotate the view of the model
- This module can also show the atom properties by color mapping. The POSCAR file with additional data columns used to save the data of the atom properties.

Syntax

```
from matsdp.vasp import vasp_plot
vasp_plot.plot_poscar_for_workdir(
```

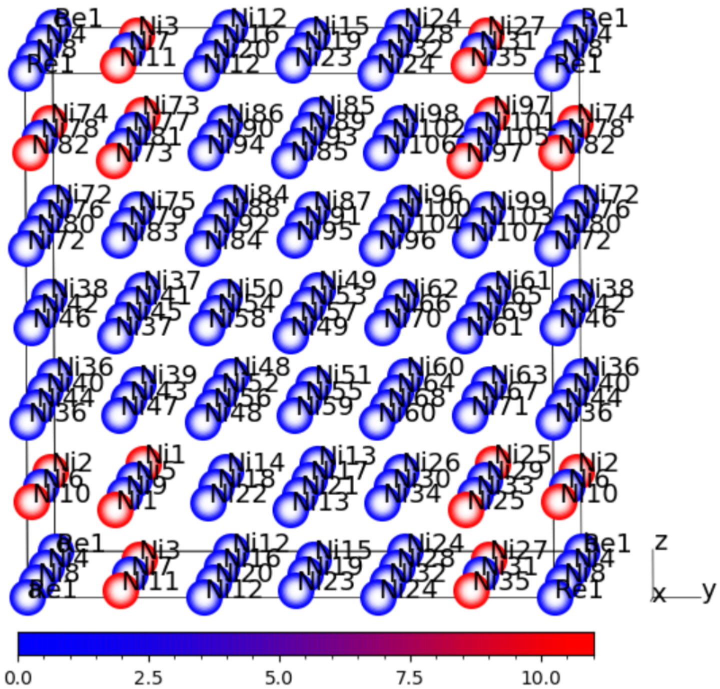


Figure 2.7: Result of the plot_poscar module: color mapping of atom properties. The color bar is horizontally aligned.

```
    workdir = './tests/vasp/',
    euler_angle_type = 'zyx',
    phi = -3,
    theta = 4,
    psi = 0,
    elmt_color = None,
    draw_mirror_atom = True,
    box_on = True,
    axis_indicator =True,
    plot_cell_basis_vector_label = True,
    plot_atom_label = True,
    poscar_or_contcar = 'POSCAR',
    fig_format = 'png',
    fig_dpi = 100,
    draw_colormap = False,
    colormap_column_indx = 1,
    colormap_vmin = None,
    colormap_vmax = None,
    vmin_color = 'blue',
    vmax_color = 'red',
    colorbar_alignment = 'vertical'
    )
```

Arguments

- workdir: String format. The mother folder which contains the folders with POSCARs

- euler_angle_type: string of length 3. It specify the type of rotations based on Eulerian angles. Choices are 'zyz', 'zxz', 'zyx', etc.. Usually the 'zyz' type is used.

  'zyz' : proper Euler angle, y-convention. Perform consecutive rotations at axes counter-clockwisely. z-y-z rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate y axis of atoms by an angle theta, finally rotate the final z axis of atoms by an angle psi

  'zxz' : proper Euler angle, x-convention. Perform consecutive rotations at axes counter-clockwisely. z-x-z rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate x axis of atoms by an angle theta, finally rotate the final z axis of atoms by an angle psi

'zyx' : Tait-Bryan angles. z-y-x rotation. Perform consecutive rotations at axes counter-clockwisely. z-y-x rotation. First rotate the z axes of atoms by an angle phi, then rotate the intermediate y axis of atoms by an angle theta, finally rotate the final x axis of atoms by an angle psi

- phi, theta, psi: float formats. The first, second, and third rotation Eulerian angles, units in degrees.
- elmt_color: dictionary formats. this dictionary sepcifies the color for each element. For example elmt_color = {'Ni':'black','Al':'magenta'}
- draw_mirror_atom: Logical value. Whether to plot the mirror atoms at the periodic boundary
- box_on: Logical value. Whether to plot the box or not
- axis_indicator: Logic value. Whether to plot the axis indicator
- plot_cell_basis_vector_label: Logical value. Whether to plot the cell basis vector labels(i.e., to label the three basis vectors of the cell as a, b, and c)
- plot_atom_label: Logical value. If true, then plot the atom name of each atom.
- poscar_or_contcar: String format. Determine whether to plot POSCAR or CONTCAR. Either 'POSCAR' or 'CONTCAR' can be used.
- fig_format: String format. fig_format is a string that defines output figure format. Supported fig_format: 'png', 'eps', 'pdf', 'tif', 'tiff', 'jpg', 'jpeg', 'svg', 'svgz', 'pgf', 'ps', 'raw', 'rgba'
- fig_dpi: float format. The DPI for non-vector graphics.
- draw_colormap: Logical value. If true, the color mapping of atom properties will be Performed. Default: False.
- colormap_column_indx: Integer value. Define which column of the atom property columns will be color mapped. Default: 1.

- colormap_vmin: Float value. Define the minimum value of the color map. If colormap_vmin=None, the minimum value of the original data will be used. Default: None.
- colormap_vmax: Float value. Define the maximum value of the color map. If colormap_vmax=None, the maximum value of the original data will be used. Default: None.
- vmin_color = 'blue': String type. Define the color for the smallest value of the atom properties in the color map. Default: 'blue'.
- vmax_color = 'red': String type. Define the color for the largest value of the atom properties in the color map. Default: 'red'.
- colorbar_alignment: String type. Defines the alignment of the color bar in the figure of the color map. The value can be either 'vertical' or 'horizontal'. Default: 'vertical'.

Outputs

Figures of POSCAR models.

2.2.3 vasp_plot.plot_dos

Descriptions

* Plot PDOS, LDOS, TDOS, now only available for LORBIT = 11. * There are three types of input arguments: atom related input arguments, subplot related input arguments, and others

Syntax

```
from matsdp.vasp import vasp_plot
DOS1_Dir = './tests/vasp/DOSCAR'
vasp_plot.plot_dos(
    atom_doscar_dir_list = [DOS1_Dir],
    atom_sysname_list = ['C5'],
    atom_indx_list = ['Ni1'],
    atom_palette_list = ['black'],
    atom_subplot_arg_list = [111],
```

```
    subplot_arg_list = [111],
    subplot_xlo_list = [-6.5],
    subplot_xhi_list = [4.0],
    subplot_ylo_list = [None],
    subplot_yhi_list = [None],
    subplot_xtick_list = [True],
    subplot_ytick_list = [True],
    subplot_xlabel_list = [False],
    subplot_ylable_list = [False],
    subplot_share_xy_list = [False, False],
    mainplot_axis_label_list = [True, True],
    dos_mode = None,
    fermi_shift_zero = True,
    peak_analyzer = False,
    fig_format = 'png',
    fig_size = [13.0, 9.5],
    fig_dpi = 600,
    )
vasp_plot.plot_dos(
    atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir],
    atom_sysname_list = ['C1', 'C1'],
    atom_indx_list = ['Ni1', 'Re1'],
    atom_palette_list = ['black', 'red'],
    atom_subplot_arg_list = [111, 111],
    subplot_arg_list = [111],
    subplot_xlo_list = [-6.5],
    subplot_xhi_list = [4.0],
    subplot_ylo_list = [None],
    subplot_yhi_list = [None],
    subplot_xtick_list = [True],
    subplot_ytick_list = [True],
    subplot_xlabel_list = [False],
    subplot_ylable_list = [False],
    subplot_share_xy_list = [False, False],
    mainplot_axis_label_list = [True, True],
    dos_mode = {'Ni':['d'], 'Re':['d']},
    fermi_shift_zero = True,
    peak_analyzer = False,
```

```
    fig_format = 'png',
    fig_size = [11.0, 9.5],
    fig_dpi = 600,
    )
```

Arguments

Atom related Args

- atom_doscar_dir_list: list format. Contains DOSCAR files for each atom. The directory of DOSCAR files can either be full path or relative path
- atom_sysname_list: system name for each atom, it corresponds to the atoms in the atom_doscar_dir_list. This is for the purpose of labeling the DOS curves in the legend.

  If sysnameList = None, then the label of system name will not shown in the legend

  For example, sysnameList = ['System1', 'System1', 'System2']
- atom_indx_list: list format. Atom index list, it corresponding to the atoms in atom_doscar_dir_list. If it is integer type then it denotes the atom index, if it is string type then it denotes the atom name

  atom_indx_list = [1,2,45] denotes the 1st, 2nd, and the 45th atoms in the POSCAR

  atom_indx_list = ['Ni1','Al3','Re3'] denotes Ni1, Al3, and Re3 in the POSCAR

  atom_indx_list = ['TDOS'] and atom_indx_list = [0] denotes the total dos
- atom_palette_list: list format. Color for DOS curves of each atom.
- atom_subplot_arg_list: list format. Defines the DOS curves of the atom are in which subplot. For example, atom_subplot_arg_list = [221, 222] denotes that the DOS curves of the first and the second atoms are in the subplot(221) and subplot(222) subplots, respectively.

Subplot related Args

- subplot_arg_list: list format. The subplot argument list, for example subplot_arg_list=[221,222] corresponds to subplot(221) and subplot(222)

- subplot_xlo_list: list format. Low boundary of the x axis for each subplots. If None value is given, the low boundary of x axis in the data set will be chosen.

- subplot_xhi_list: list format. High boundary of the x axis for each subplots. If None value is given, the high boundary of x axis in the data set will be chosen.

- subplot_ylo_list: list format. Low boundary of the y axis for each subplots. If None value is given, the low boundary of y axis in the data set will be chosen.

- subplot_yhi_list: list format. High boundary of the y axis for each subplots. If None value is given, the high boundary of y axis in the data set will be chosen.

- subplot_xtick_list: list of logical values. If the list element is True (False), then the tick of the x axis will be shown (removed).

- subplot_ytick_list: list of logical values. If the list element is True (False), then the tick of the x axis will be shown (removed).

- subplot_xlabel_list: list of logical values. Defines whether the x-label of each subplots are shown, it won't work for subplot=(111) figure.

- subplot_xlabel_list: list of logical values. Defines whether the y-label of each subplots are shown, it won't work for subplot=(111) figure.

- subplot_share_xy_list: list of logical values of length two. Defines whether the x or y axis will be shared or not. [False, False] denotes both x and y axes will not be shared.

Other Args

- mainplot_axis_label_list: list of logical values of length two. Defines whether the x or y labels of the main figure will be shown or not. [False, False] denotes both x and y labels of the main figure will not be shown.

- dos_mode is a dictionary that defines which partial DOS or whether LDOS is plotted for different element type. e.g.: dos_mode = {'Ni':['s','p','d'], 'Al':['s','p']} or dos_mode = {'Ni':['dxy','dx2']}, or dos_mode = {'Ni':['LDOS']}.
- fermi_shift_zero is a logical value which determines whether to shift Fermi energy level to zero.
- peak_analyzer:logical value. Determines whether to analyze peaks in DOS. if True, the peaks will be labeled
- fig_format: String format. Defines output figure format. Supported fig_format: 'png', 'eps', 'pdf', 'tif', 'tiff', 'jpg', 'jpeg', 'svg', 'svgz', 'pgf', 'ps', 'raw', 'rgba'
- fig_size: list of floats. Defines the size of the figure, e.g. fig_size = (7.0,6.0)
- fig_dpi: float format. The DPI for non-vector graphics.

GUI

The GUI is shown in Figure 2.8. The panel can be devided into several control regions and the several control regions are shown in Figure 2.9. The settings for the plot_dos function is shown in Figure 2.10. The subplot layout is shown in Figure 2.11

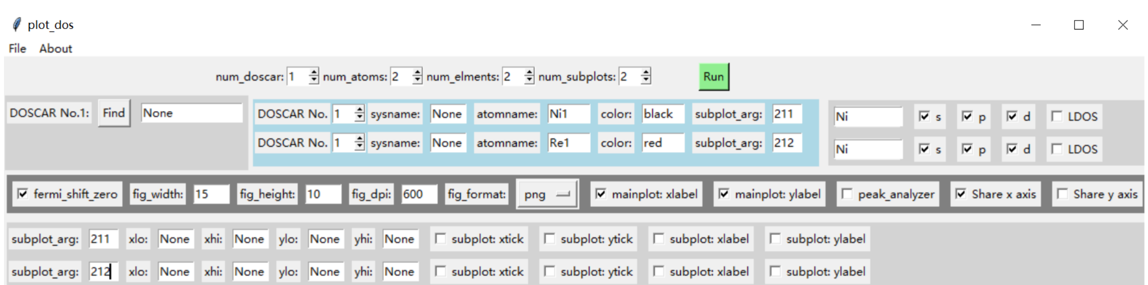


Figure 2.8: GUI for plot_dos

Some of the parameters are listed below:

- num_doscar: Number of DOSCAR files, this region can be used to import different DOSCAR

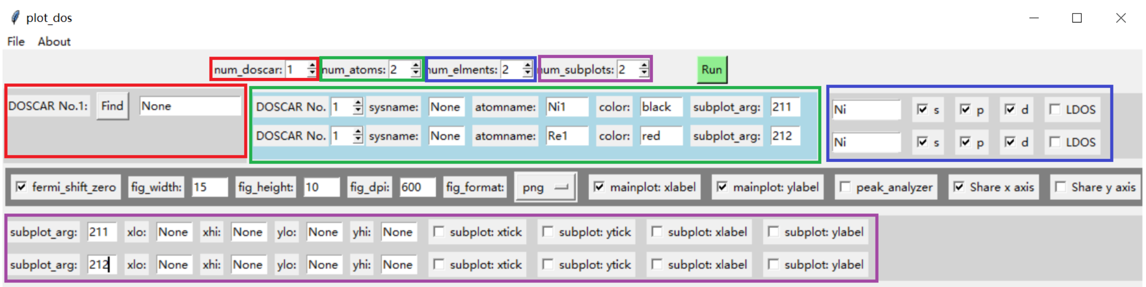
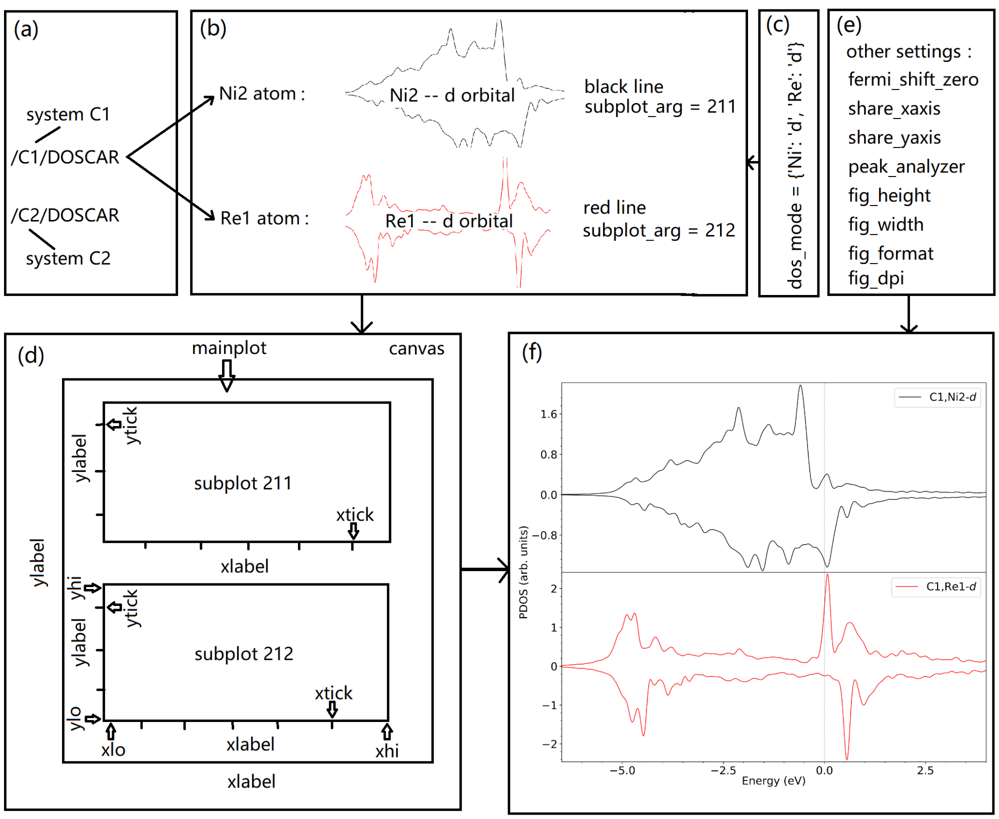


Figure 2.9: Control regions in the plot_dos panel



(a) DOSCAR related settings; (b) atom related settings; (c) element related settings;
(d) subplot related settings; (e) other settings; (f) figure output

Figure 2.10: plot_dos settings

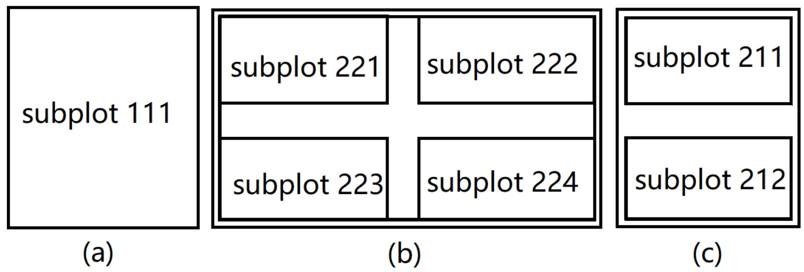


Figure 2.11: Subplot layout

- num_atoms: Number of atoms for plotting the DOSs
- num_elements: Number of elements
- num_subplots: Number of subplots
- subplot_arg: The position of the subplot. The illustration of the subplot is shown in Fig. 2.11

If only one DOS curve will be plotted, then set num_doscar=1 and num_atom=1. The value of subplot_arg then can be subplot_arg=111. For example, if the PDOSs of "Ni1" and "A2" are to be compared, the parameter num_atom should be taken as num_atom=2.

Output

Figures of DOS curves

Examples

The examples are shown in the Figure 2.12 and Figure 2.13.

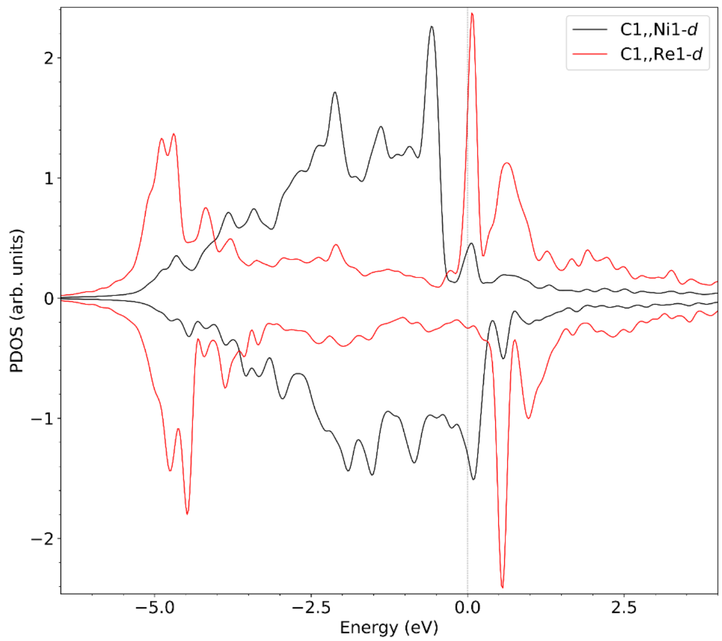


Figure 2.12: Result of the plot_doscar module.

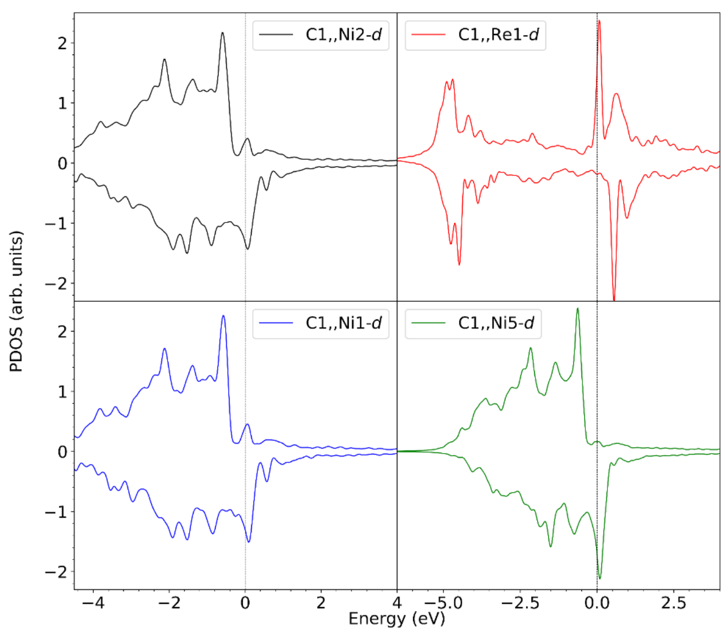


Figure 2.13: Result of the plot_doscar module.

2.3 vasp_read module

2.3.1 vasp_read.read_doscar

Descriptions

Read DOSCAR and dump density of states inoformation file into the folder where the DOSCAR lies

Syntax

```
from matsdp.vasp import vasp_read
vasp_read.read_doscar(
    doscar_dir = './tests/vasp/DOSCAR',
    atom_indx = 2,
    save_dos_arr = True,
    )
```

Arguments

- doscar_dir: String format. The directory of the DOSCAR file. It can either be full path or relative path
- atom_indx: Integer format. The real atom index in the POSCAR. If there are N atoms then the atom indices are frim 1 to N. Note that atom_indx = 0 means to extract TDOS inoformation
- save_dos_arr: logical format. If save_dos_arr = True, the density of states inoformation will be saved to files. If save_dos_arr = False, the density of states inoformation will not be saved to files

Outputs

DOS information file for the specified atom

2.4 vasp_analyze module

2.4.1 vasp_analyze.nn_map

Calculate the nearest neighbor (NN) map.

Descriptions

Calculate the nearest neighbor (NN) map.

Syntax

```
from matsdp.vasp import vasp_analyze
vasp_analyze.nn_map(
    poscar_dir = './tests/vasp/POSCAR',
    a0 = 3.545,
    n_shell = 2,
    )
```

Args

- poscar_dir: String format. It specifies the directory of the POSCAR file
- a0: Float format. The lattice constant of the model. Unit in Angstrom
- n_shell: Integer format. It determines up to which crystallographic shell the nearest neighbour map calculates

GUI

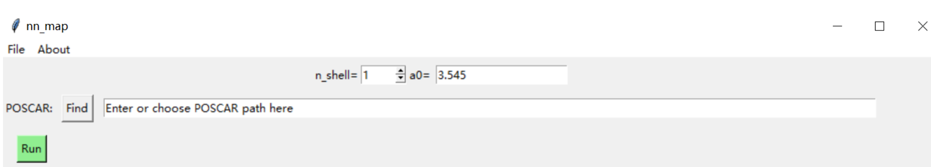


Figure 2.14: GUI for nn_map

2.4.2 vasp_analyze.simple_cna

Peform simple common neighbor analysis (CNA).

Descriptions

Peform simple common neighbor analysis (CNA). Atom A is the common neighbor of element E1 and E2, this module will count the times that A appeared as the common neighbor of E1 and E2.

Syntax

```
from matsdp.vasp import vasp_analyze
vasp_analyze.simple_cna(
    poscar_dir = './tests/vasp/POSCAR',
    a0 = 3.545,
    common_neighbor_elmt_list = ['Re', 'W', 'Ta','Ni']
    )
```

Args

- poscar_dir: String format. It specifies the directory of the POSCAR file
- a0: Float format. The lattice constant of the model. Unit in Angstrom
- common_neighbor_elmt_list: List format. It determines what elements are taken into account in the common neighbor analysis. If common_neighbor_elmt_list = ['Re', 'W', 'Ta'], then the common neighbor to Re-Re, Re-W, Re-Ta, W-W, W-Ta, Ta-Ta will be counted and printed.

GUI

2.4.3 vasp_analyze.estruct

Descriptions

- Calculates the structural energies at each atomic site

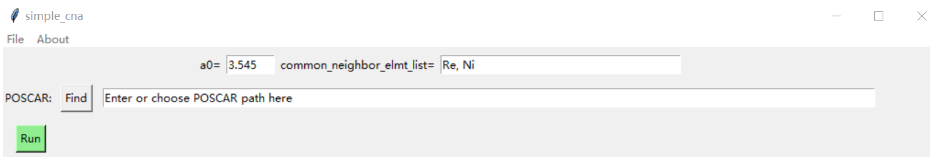


Figure 2.15: GUI for simple_cna

- The definition of E_{struct} can be found in the literature of the author Chongyu Wang [2, 3]

Syntax

```
from matsdp.vasp import vasp_analyze
vasp_analyze.estruct(
    doscar_dir = './tests/vasp/DOSCAR',
    sysname = 'DOS1',
    )
```

Arguments

- dOSCAR_dir: String format. It specifies the directory of the DOSCAR
- sysname: String format. User defined system name

GUI

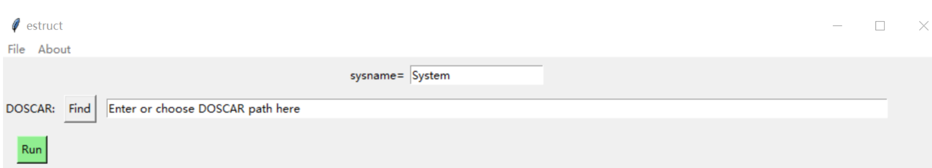


Figure 2.16: GUI for estruct

Output

The first column is the atom name, the second column is E_{struct} for each atom

2.4.4 vasp_analyze.overlap_peak_analyzer

Descriptions

- Finding the overlapped orbitals of two neighboring atoms in the DOS analysis.
- DOS peak analyses for selected atoms with their neighboring atoms.
- Find the overlapped orbitals and their corresponding energy levels.

Syntax

```
from matsdp.vasp import vasp_analyze
vasp_analyze.overlap_peak_analyzer(
    doscar_dir = './tests/vasp/DOSCAR',
    sysname = 'DOS1',
    atom_indx_list = ['Ni1','Re1'],
    n_shell = 2,
    a0 = 3.52,
    dos_mode = {'Ni':['d'],'Re':['d']},
    fermi_shift_zero = True,
    )
```

Arguments

- doscar_dir: String format. The directory which contains the DOSCAR file, abstract path can be accepted
- sysname: String format. A string character which specifies the name of the system, this string will be used as part of the output file name
- atom_indx_list: List of strings. Specifies the list of selected atoms.
- n_shell: float format. Up to which crystallographic shell(up to which nearest neighbor) of the selected atom will be considered
- a0: float format. The approximate lattice constant of the crystal
- dos_mode: dictionary format. Determines which orbital will be considered, f, d, p, s, dxy, dyz, ... can be used

- fermi_shift_zero: A logical value determining whether the energy levels of the DOS will be shifted to zero

Outputs

overlapped peak files

2.5 vasp_write module

2.5.1 vasp_write.write_poscar_with_force

Descriptions

write atom force data into the POSCAR file.

Syntax

```
from matsdp.vasp import vasp_write
vasp_write.write_poscar_with_force(
    outcar_dir = './tests/vasp/OUTCAR',
    ionic_step = 'last',
    output_poscar_file_name = None
    )
```

Arguments

- outcar_dir: String format. It specifies the directory of the OUTCAR
- ionic_step: String format or interger type. If string type value is taken, either ionic_step='last' or ionic_step='first' can be taken. If integer type value is taken, ionic_step defines the ionic step number. ionic_step = 3 denotes that the force of each atom for the third ionic step will be written to the POSCAR file.
- output_poscar_file_name: String type or None. If string type is taken, this parameter lets the user define the POSCAR file name which contains the atom force information. If output_poscar_file_name=None, the program determines the name of the output POSCAR file.

GUI

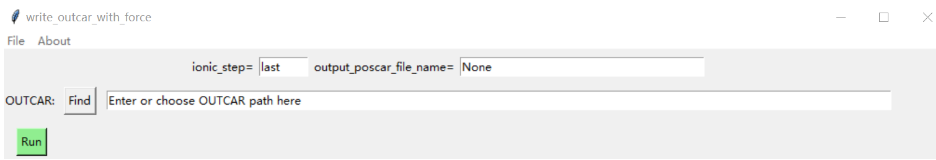


Figure 2.17: GUI for write_poscar_with_force

Output

The POSCAR file which contains the force on each atom.

Chapter 3

subpackage: apt

Modules to import before using the apt package

- from matsdp.apt import apt_read
- from matsdp.apt import apt_plot

3.1 apt_read module

3.1.1 apt_read.read_proxigram_csv

Descriptions

- Read the concentration profile file (*.csv file)

Syntax

```
from matsdp.apt import apt_read
apt_read.read_proxigram_csv(proxigram_csv_dir)
```

Arguments

- proxigram_csv_dir: string type. The concentration profile file.

Outputs

- data_set: numpy array type. The original data of the concentration profile file
- elmtname_list: List type. The elements contained in the concentration profile file

3.2 apt_plot module

3.2.1 apt_plot.plot_proxigram_csv

Descriptions

- Plot the concentration profile based on the proxigram *.csv file

Syntax

```
from matsdp.apt import apt_plot
apt_plot.plot_proxigram_csv(
    proxigram_csv_dir = './tests/apt/profile-
    interface0.csv',
    sysname = 'M2',
    visible_elmt_list = ['Ni','Al'],
    interplation_on = False,
    fig_width = 6,
    fig_height = 5,
    fig_dpi = 600,
    fig_format = 'png',
    )
```

Arguments

- proxigram_csv_dir: string type. The concentration profile file.
- sysname: string type. The system name.
- visible_elmt_list: List type. The elements which are to be plotted. For example, ['Ni','Al'].

- interpolation_on: logical type. whether to interpolate the concentration profile or not.
- fig_width: float type. Figure width.
- fig_height: float type. Figure height.
- fig_dpi: float format. The DPI for non-vector graphics.
- fig_format: String format. fig_format is a string that defines output figure format. Supported fig_format: 'png', 'eps', 'pdf', 'tif', 'tiff', 'jpg', 'jpeg', 'svg', 'svgz', 'pgf', 'ps', 'raw', 'rgba'

GUI

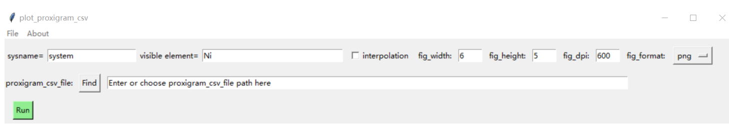


Figure 3.1: GUI for plot_concentration_profile

Examples

The example is shown in the Figure 2.12.

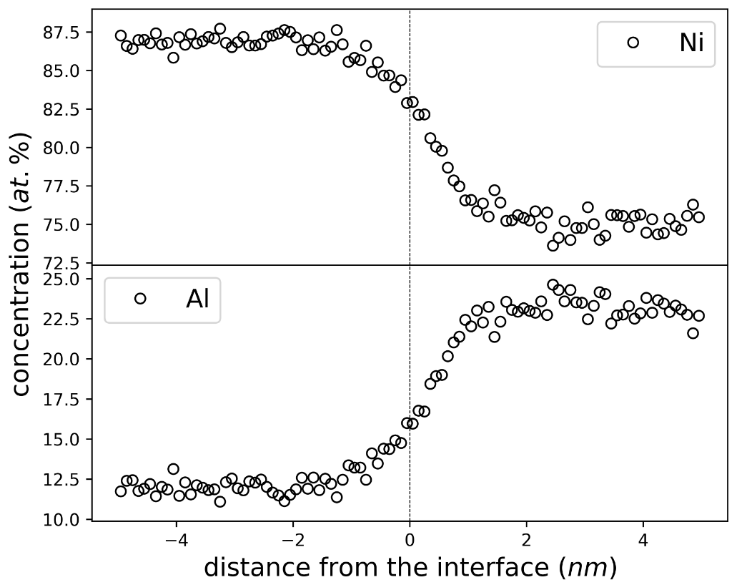


Figure 3.2: Result of the plot_proxigram_csv module.

Chapter 4

tests

4.1 example .py test file

The example.py test file is provided as runtests.py. Its content is listed below. The parameter “package_path” is used to define the matsdp package directory and can be modified by the users.

```
# -*- coding: utf-8 -*-
import os
import sys
package_path = './'
sys.path.insert(0, os.path.abspath(package_path))

from matsdp.vasp import vasp_read
from matsdp.vasp import vasp_plot
from matsdp.vasp import vasp_analyze
from matsdp.vasp import vasp_build
from matsdp.vasp import vasp_write
from matsdp.apt import apt_read
from matsdp.apt import apt_plot

run_nn_map = True
run_simple_cna = True
run_substitute = True
run_replace_elmt = True
run_selection_sphere = True
```

```
run_get_doscar = True
run_plot_dos = True
run_plot_poscar = True
run_plot_poscar_for_workdir = True
run_overlap_peak_analyzer = True
run_estruct = True
run_write_poscar_with_force = True
run_plot_concentration_profile = True

###############
# nn_map_Calc
###############
if run_nn_map == True:
    vasp_analyze.nn_map(
        poscar_dir = './tests/vasp/POSCAR',
        a0 = 3.545,
        n_shell = 2,
        )
########################
# simple_common_neighbor
########################
if run_simple_cna == True:
    vasp_analyze.simple_cna(
        poscar_dir = './tests/vasp/POSCAR',
        a0 = 3.545,
        common_neighbor_elmt_list = ['Re', 'W', 'Ta','
        Ni']
        )
    vasp_plot.plot_poscar(
        poscar_dir = './outputs/
        POSCAR_simple_common_neighbor_pair_count_ReNi'
        ,
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
```

```
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = True,
        colormap_column_indx = 2,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )
    vasp_plot.plot_poscar(
        poscar_dir = './outputs/
        POSCAR_simple_common_neighbor_pair_count_ReNi'
        ,
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = True,
        colormap_column_indx = 2,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'horizontal'
        )
```

```
###################
# run_substitute
###################
if run_substitute == True:
    vasp_build.substitution(
        substitution_list_file = './tests/vasp/example
        .subst',
        poscar_dir = './tests/vasp/POSCAR_NoDope',
        )
#####################
# run_replace_elmt
#####################
if run_replace_elmt == True:
    vasp_build.rep_elmt(
        substitution_list_file = './tests/vasp/example
        .subst',
        poscar_dir = './tests/vasp/POSCAR_NoDope',
        old_elmt= 'Re',
        elmt_group = ['W','Cr'],
        )
####################################
# atom selection -- sphere
####################################
if run_selection_sphere == True:
    vasp_build.selection_sphere(
        poscar_dir = './tests/vasp/CONTCAR',
        origin_atom_name = 'Re1',
        radius = 7,
        include_mirror_atoms = False,
        output_file_name = 'example'
        )
############
#plot_dos
############
if run_plot_dos == True:
    DOS1_Dir = './tests/vasp/DOSCAR'
    vasp_plot.plot_dos(
```

```
        atom_doscar_dir_list = [DOS1_Dir],
        atom_sysname_list = ['C5'],
        atom_indx_list = ['Ni1'],
        atom_palette_list = ['black'],
        atom_subplot_arg_list = [111],
        subplot_arg_list = [111],
        subplot_xlo_list = [-6.5],
        subplot_xhi_list = [4.0],
        subplot_ylo_list = [None],
        subplot_yhi_list = [None],
        subplot_xtick_list = [True],
        subplot_ytick_list = [True],
        subplot_xlabel_list = [False],
        subplot_ylabel_list = [False],
        subplot_share_xy_list = [False, False],
        mainplot_axis_label_list = [True, True],
        dos_mode = None,
        fermi_shift_zero = True,
        peak_analyzer = False,
        fig_format = 'png',
        fig_size = [13.0, 9.5],
        fig_dpi = 600,
        )
    vasp_plot.plot_dos(
        atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir],
        atom_sysname_list = ['C1', 'C1'],
        atom_indx_list = ['Ni1', 'Re1'],
        atom_palette_list = ['black', 'red'],
        atom_subplot_arg_list = [111, 111],
        subplot_arg_list = [111],
        subplot_xlo_list = [-6.5],
        subplot_xhi_list = [4.0],
        subplot_ylo_list = [None],
        subplot_yhi_list = [None],
        subplot_xtick_list = [True],
        subplot_ytick_list = [True],
        subplot_xlabel_list = [False],
        subplot_ylabel_list = [False],
```

```
        subplot_share_xy_list = [False, False],
        mainplot_axis_label_list = [True, True],
        dos_mode = {'Ni':['d'], 'Re':['d']},
        fermi_shift_zero = True,
        peak_analyzer = False,
        fig_format = 'png',
        fig_size = [11.0, 9.5],
        fig_dpi = 600,
        )

    vasp_plot.plot_dos(
        atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir],
        atom_sysname_list = ['C1', 'C1'],
        atom_indx_list = ['Ni2', 'Re1'],
        atom_palette_list = ['black', 'red'],
        atom_subplot_arg_list = [211, 212],
        subplot_arg_list = [211, 212],
        subplot_xlo_list = [-6.5, -6.5],
        subplot_xhi_list = [4.0, 4.0],
        subplot_ylo_list = [None, None],
        subplot_yhi_list = [None, None],
        subplot_xtick_list = [True, True],
        subplot_ytick_list = [True, True],
        subplot_xlabel_list = [False, False],
        subplot_ylabel_list = [False, False],
        subplot_share_xy_list = [False, False],
        mainplot_axis_label_list = [True, True],
        dos_mode = {'Ni':['d'], 'Re':['d']},
        fermi_shift_zero = True,
        peak_analyzer = False,
        fig_format = 'png',
        fig_size = [11.0, 9.5],
        fig_dpi = 600,
        )

    vasp_plot.plot_dos(
        atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir],
        atom_sysname_list = ['C1', 'C1'],
```

```
        atom_indx_list = ['Ni2', 'Re1'],
        atom_palette_list = ['black', 'red'],
        atom_subplot_arg_list = [211, 212],
        subplot_arg_list = [211, 212],
        subplot_xlo_list = [-6.5, -6.5],
        subplot_xhi_list = [4.0, 4.0],
        subplot_ylo_list = [None, None],
        subplot_yhi_list = [None, None],
        subplot_xtick_list = [False, True],
        subplot_ytick_list = [True, True],
        subplot_xlabel_list = [False, False],
        subplot_ylabel_list = [False, False],
        subplot_share_xy_list = [True, False],
        mainplot_axis_label_list = [True, True],
        dos_mode = {'Ni':['d'], 'Re':['d']},
        fermi_shift_zero = True,
        peak_analyzer = False,
        fig_format = 'png',
        fig_size = [11.0, 9.5],
        fig_dpi = 600,
        )


    vasp_plot.plot_dos(
        atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir,
        DOS1_Dir, DOS1_Dir],
        atom_sysname_list = ['C1', 'C1', 'C1', 'C1'],
        atom_indx_list = ['Ni2', 'Re1', 'Ni1', 'Ni5'],
        atom_palette_list = ['black', 'red', 'blue', '
        green'],
        atom_subplot_arg_list = [221, 222, 223, 224],
        subplot_arg_list = [221, 222, 223, 224],
        subplot_xlo_list = [-4.5, -6.5, -4.5, -6.5],
        subplot_xhi_list = [4.0, 4.0, 4.0, 4.0],
        subplot_ylo_list = [None, None, None, None],
        subplot_yhi_list = [None, None, None, None],
        subplot_xtick_list = [True, True, True, True],
        subplot_ytick_list = [True, True, True, True],
```

```
        subplot_xlabel_list = [False, False, False,
        False],
        subplot_ylabel_list = [False, False, False,
        False],
        subplot_share_xy_list = [False, False],
        mainplot_axis_label_list = [True, True],
        dos_mode = {'Ni':['d'], 'Re':['d']},
        fermi_shift_zero = True,
        peak_analyzer = False,
        fig_format = 'png',
        fig_size = [11.0, 9.5],
        fig_dpi = 600,
        )
    vasp_plot.plot_dos(
        atom_doscar_dir_list = [DOS1_Dir, DOS1_Dir,
        DOS1_Dir, DOS1_Dir],
        atom_sysname_list = ['C1', 'C1', 'C1', 'C1'],
        atom_indx_list = ['Ni2', 'Re1', 'Ni1', 'Ni5'],
        atom_palette_list = ['black', 'red', 'blue', '
        green'],
        atom_subplot_arg_list = [221, 222, 223, 224],
        subplot_arg_list = [221, 222, 223, 224],
        subplot_xlo_list = [-4.5, -6.5, -4.5, -6.5],
        subplot_xhi_list = [4.0, 4.0, 4.0, 4.0],
        subplot_ylo_list = [-2.3, -2.3, -2.3, -2.3],
        subplot_yhi_list = [2.5, 2.5, 2.5, 2.5],
        subplot_xtick_list = [False, False, True, True
        ],
        subplot_ytick_list = [True, False, True, False
        ],
        subplot_xlabel_list = [False, False, False,
        False],
        subplot_ylabel_list = [False, False, False,
        False],
        subplot_share_xy_list = [True, True],
        mainplot_axis_label_list = [True, True],
        dos_mode = {'Ni':['d'], 'Re':['d']},
        fermi_shift_zero = True,
```

```
            peak_analyzer = False,
            fig_format = 'png',
            fig_size = [11.0, 9.5],
            fig_dpi = 600,
            )
############################
# overlap_peak_analyzer
############################
if run_overlap_peak_analyzer == True:
    vasp_analyze.overlap_peak_analyzer(
        doscar_dir = './tests/vasp/DOSCAR',
        sysname = 'DOS1',
        atom_indx_list = ['Ni1','Re1'],
        n_shell = 2,
        a0 = 3.52,
        dos_mode = {'Ni':['d'],'Re':['d']},
        fermi_shift_zero = True,
        )
#################################
#Get DOS files with DOS info
#################################
if run_get_doscar == True:
    poscar_dir = './tests/vasp/POSCAR'
    poscar_dict = vasp_read.read_poscar(poscar_dir)
    for atom_indx in range(0, len(poscar_dict['
    atom_species_arr']) + 1):
        vasp_read.read_doscar(
            doscar_dir = './tests/vasp/DOSCAR',
            atom_indx = atom_indx,
            save_dos_arr = True,
            )

############################
#Visualization of POSCAR
############################
if run_plot_poscar == True:
    vasp_plot.plot_poscar(
        poscar_dir = './tests/vasp/POSCAR',
```

```
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = False,
        colormap_column_indx = 1,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )

###########################
# write_poscar_with_force
###########################
if run_write_poscar_with_force == True:
    # write_poscar_with_force
    vasp_write.write_poscar_with_force(
        outcar_dir = './tests/vasp/OUTCAR',
        ionic_step = 'last',
        output_poscar_file_name = None
        )
    vasp_plot.plot_poscar(
        poscar_dir = './outputs/
        POSCAR_with_force_step_1',
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
```

```
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = True,
        colormap_column_indx = 1,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )
    vasp_plot.plot_poscar(
        poscar_dir = './outputs/
        POSCAR_with_force_step_1_absforce',
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = True,
        colormap_column_indx = 1,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
```

```
        )

#####################################################
#run_plot_poscar for the POSCARs in a directory
#####################################################
if run_plot_poscar_for_workdir == True:
    vasp_plot.plot_poscar_for_workdir(
        workdir = './outputs/example/',
        euler_angle_type = 'zyx',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = None,
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        poscar_or_contcar = 'POSCAR',
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = False,
        colormap_column_indx = 1,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )
###############
# run_estruct
###############
if run_estruct == True:
    vasp_analyze.estruct(
        doscar_dir = './tests/vasp/DOSCAR',
        sysname = 'DOS1',
        )
    vasp_plot.plot_poscar(
```

```
        poscar_dir = './outputs/POSCAR_estruct_DOS1_Ef
        -7.0888',
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
        draw_colormap = True,
        colormap_column_indx = 1,
        colormap_vmin = None,
        colormap_vmax = None,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )

    vasp_plot.plot_poscar(
        poscar_dir = './outputs/POSCAR_estruct_DOS1_Ef
        -7.0888',
        euler_angle_type = 'zyz',
        phi = -3,
        theta = 5,
        psi = 0,
        elmt_color = {'Ni':'red','Re':'blue'},
        draw_mirror_atom = True,
        box_on = True,
        axis_indicator =True,
        plot_cell_basis_vector_label = True,
        plot_atom_label = True,
        fig_format = 'png',
        fig_dpi = 100,
```

```
        draw_colormap = True,
        colormap_column_indx = 1,
        colormap_vmin = -80,
        colormap_vmax = -40,
        vmin_color = 'blue',
        vmax_color = 'red',
        colorbar_alignment = 'vertical'
        )

####################################
#apt- plot concentration profile
####################################
if run_plot_concentration_profile == True:
    apt_plot.plot_proxigram_csv(
        proxigram_csv_dir = './tests/apt/profile-
        interface0.csv',
        sysname = 'M2',
        visible_elmt_list = ['Ni','Al'],
        interplation_on = False,
        fig_width = 6,
        fig_height = 5,
        fig_dpi = 600,
        fig_format = 'png',
        )
```

Appendix A

Other plotting settings

A.1 Named colors in the program

The named colors which can be used by the program is listed in Figure A.1[1].

[1] https://matplotlib.org/3.1.0/gallery/color/named_colors.html

Figure A.1: The named colors supported by the current program

Bibliography

[1] Herbert Goldstein, Charles P. Poole Jr. and John L. Safko, Classical Mechanics (3rd Edition). Goldstein Poole & Safko, 2001.

[2] Chongyu Wang and Feng An and Binglin Gu and Liu Fusui and Ying Chen, Electronic structure of the light-impurity (boron)–vacancy complex in iron. Physical Review B, 1988: 3905–3912.

[3] Chong-yu Wang, Sen-ying Liu and Lin-guang Han, Electronic structure of impurity (oxygen)–stacking-fault complex in nickel. Physical Review B, 1990: 1359–1367.