Masci-tools Documentation

Release 0.7.1

The JuDFT team

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CONTENTS

This package was developed in the process of developing the AiiDA-FLEUR and AiiDA_KKR plugins to AiiDA. It contains helper functions that can help with common pre- and postprocessing steps of the FLEUR and KKR codes developed at the Forschungszentrum Jülich (see also the juDFT website for more information).

If you use this package please cite: …

CHAPTER

ONE

REQUIREMENTS TO USE THIS CODE:

- lxml
- h5py
- ase
- pymatgen
- numpy
- scipy
- more_itertools

CHAPTER

TWO

INSTALLATION INSTRUCTIONS:

Install from pypi the latest release:

```
$ pip install masci-tools
```

or from the masci-tools source folder any branch:

```
$ pip install .
# or which is very useful to keep track of the changes (developers)
$ pip install -e .
```

CHAPTER

THREE

ACKNOWLEDGMENTS:

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CHAPTER

FOUR

USER'S GUIDE

4.1 User guide

This is the masci-tools user's guide.

4.1.1 Using the Fleur input/output parsers

Contents

4.1.1.1 Parser for the Fleur inp.xml file

The fleur `inp.xml` contains all the information about the setup of a fleur calculation. To use this information in external scripts or aiida-fleur, the information needs to be parsed from the `.xml` format somehow.

For this purpose the *inpxml_parser()* is implemented. The usage is shown below. The input file is parsed recursively and all information is put into the dictionary.

```
from masci_tools.io.parsers.fleur import inpxml_parser

input_dict = inpxml_parser('/path/to/random/inp.xml')

#The call below will output warnings about failed conversions in the warnings dictionary
warnings = {'parser_warnings': []}
input_dict = inpxml_parser('/path/to/random/inp.xml', parser_info_out=warnings)
```

The conversion of each attribute or text is done according to the FleurInputSchema for the same version, which is stored in this repository for versions from `0.27` to `0.34`. The following table shows the version compatibility of the input parser.

File version	Compatible?
0.27 - 0.34	
0.35 -	

4.1.1.2 Parser for the Fleur out.xml file

For the `out.xml` file a similar parser is implemented. However, since the output file contains a lot more information, which is not always useful the *outxml_parser()* is defined a lot more selectively. But the usage is almost completely identical to the input file.

```
from masci_tools.io.parsers.fleur import outxml_parser

#The default is that only the last stable iteration is parsed
output_dict = outxml_parser('/path/to/random/out.xml')

#Here all iterations are parsed
output_dict = outxml_parser('/path/to/random/out.xml', iteration_to_parse='all')

#Or the 5.
output_dict = outxml_parser('/path/to/random/out.xml', iteration_to_parse=5)

#The call below will output warnings about failed conversions in the warnings dictionary
warnings = {'parser_warnings': []}
output_dict = outxml_parser('/path/to/random/out.xml', parser_info_out=warnings)
```

For each iteration the parser decides based on the type of fleur calculation, what things should be parsed. For a more detailed explanation refer to the *Developers Guide*.

The following table shows the version compatibility of the output parser. For versions before *0.34* the file version corresponds to the input version, since the output version is *0.27* for all versions before this point.

File version	Compatible?
0.27 - 0.29	
0.30 - 0.31	
0.32	
0.33	
0.34	
0.35 -	

4.1.1.3 XML getter functions

There are a number of functions for extracting specific parts of the XML files in the *xml_getters* module. The following are available:

- *get_fleur_modes()*: Get information about the mode of the fleur calculation
- *get_nkpts()*: Get the (for older versions approximate if not *kPointList* is used) number of kpoints to be used in the calculation
- *get_cell()*: Get the Bravais matrix of the system
- *get_parameter_data()*: Get the information about the calculation parameters needed to reproduce a calculation starting from the inpgen
- *get_structure_data()*: Get the structure from the xml file (atom positions + unit cell)
- *get_kpoints_data()*: Get the defined kpoint sets (single/multiple) from the xml file (kpoints + weights + unit cell)
- *get_relaxation_information()*: Get the relaxation history and current displacements
- *get_symmetry_information()*: Get the symmetry operations used in the calculation

All of these are used in the same way:

```
from masci_tools.io.io_fleurxml import load_inpxml
from masci_tools.util.xml.xml_getters import get_fleur_modes

xmltree, schema_dict = load_inpxml('/path/to/inp.xml')

fleur_modes = get_fleur_modes(xmltree, schema_dict)
print(fleur_modes)
```

4.1.1.4 Using the schema_dict_util functions

If only a small amount of information is required from the input or output files of fleur the full parsers might be overkill. But there are a number of utility functions allowing easy access to information from the `.xml` files without knowing the exact xpath expressions for each version of the input/output. A code example extracting information from a input file is given below.

```
from masci_tools.io.io_fleurxml import load_inpxml
from masci_tools.util.schema_dict_util import evaluate_attribute, eval_simple_xpath

#First we create a xml-tree from the input file and load the desired input schema␣
↪dictionary
xmltree, schema_dict = load_inpxml('/path/to/inp.xml')
root = xmltree.getroot()

#Here an example of extracting some attributes. The interface to all functions in
#schema_dict_util is the same

#Number of spins
spins = evaluate_attribute(root, schema_dict, 'jspins')

#Planewave cutoff (notice the names are case-insensitive, 'KMAX' would work as well)
kmax = evaluate_attribute(root, schema_dict, 'kmax')
```

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```
#Some attributes need to be specified further for a distinct path
#`radius` exists both for atom species and atom groups so we give a phrase to distinguish␣
↪them
mt_radii = evaluate_attribute(root, schema_dict, 'radius', contains='species')

#But we can also make implicit constraints
# 1. Get some element in the xml tree, where the path is more specified. In the example␣
↪lets
#    get the element containing all species
# 2. If we evaluate the `radius` attribute now on the species elements, we do not need
#    the contains parameter, since from the point of the species element there is only␣
↪one possibility
#    for the `radius` attribute

species = eval_simple_xpath(root, schema_dict, 'atomSpecies')
mt_radii = evaluate_attribute(species, schema_dict, 'radius')
```

4.1.2 FleurXMLModifier

4.1.2.1 Description

The *FleurXMLModifier* class can be used if you want to change anything in a *inp.xml* file in an easy and robust way. It will validate all the changes you wish to do and apply all these changes to a given *inp.xml* and produce a new xmltree.

4.1.2.2 Usage

To modify an existing *inp.xml*, a *FleurXMLModifier* instance has to be initialised. After that, a user should register certain modifications which will be cached. They will be applied on a given *inp.xml*. However, the provided *inp.xml* will not be changed but only a modified xmltree is returned, which you can store in a new *.xml* file.

```
from masci_tools.io.fleurxmlmodifier import  FleurXMLModifier

fm = FleurXMLModifier()                                          # Initialise␣
↪FleurXMLModifier class
fm.set_inpchanges({'dos' : True, 'Kmax': 3.9 })                  # Add changes
new_xmltree = fm.modify_xmlfile('/path/to/original/inp.xml') #Apply
```

4.1.2.3 User Methods

General methods

- *modify_xmlfile()*: Applies the registered changes to a given *inp.xml* (and optional *n_mmp_mat* file)
- *changes()*: Displays the current list of changes.
- *undo()*: Removes the last task or all tasks from the list of changes.

Modification registration methods

The registration methods can be separated into two groups. First of all, there are XML methods that require deeper knowledge about the structure of an `inp.xml` file. All of them require an xpath input and start their method names start with *xml_*:

- *xml_set_attrib_value_no_create()*: Set attributes on the result(s) of the given xpath
- *xml_set_text_no_create()*: Set text on the result(s) of the given xpath
- *xml_create_tag()*: Insert an xml element in the xml tree on the result(s) of the given xpath.
- *xml_delete_tag()*: Delete an xml element in the xml tree on the result(s) of the given xpath.
- *xml_delete_att()*: Delete an attribute in the xml tree on the result(s) of the given xpath.
- *xml_replace_tag()*: Replace an xml element on the result(s) of the given xpath.

On the other hand, there are shortcut methods that already know some paths:

- *set_species()*: Specific user-friendly method to change species parameters.
- *clone_species()*: Method to create a clone of a given species with optional modifications
- *set_atomgroup()*: Specific method to change atom group parameters.
- *set_species_label()*: Specific user-friendly method to change a species of an atom with a certain label.
- *set_atomgroup_label()*: Specific method to change atom group parameters of an atom with a certain label.
- *switch_species()*: user-friendly method for switching the atom species of a atom group
- *switch_species_label()*: user-friendly method for switching the atom species of a atom group with an atom with a certain label.
- *set_nkpts()*: user-friendly method for setting the *kPointCount* (**Only for MaX4 and older**)
- *set_kpath()*: user-friendly method for setting the path for a bandstructure calculations (**Only for MaX4 and older**)
- *set_kpointlist()*: user-friendly method for setting/creating a *kPointlist* from lists
- *switch_kpointset()*: user-friendly method for switching the used kpoint set in a calculation (**Only for MaX5 and newer**)
- *set_inpchanges()*: Specific user-friendly method for easy changes of attribute key value type.
- *shift_value()*: Specific user-friendly method to shift value of an attribute.
- *shift_value_species_label()*: Specific user-friendly method to shift value of an attribute of an atom with a certain label.
- *set_attrib_value()*: user-friendly method for setting attributes in the xml file by specifying their name
- *set_first_attrib_value()*: user-friendly method for setting the first occurrence of an attribute in the xml file by specifying its name
- *add_number_to_attrib()*: user-friendly method for adding to or multiplying values of attributes in the xml file by specifying their name
- *add_number_to_first_attrib()*: user-friendly method for adding to or multiplying values of the first occurrence of the attribute in the xml file by specifying their name
- *set_text()*: user-friendly method for setting text on xml elements in the xml file by specifying their name
- *set_first_text()*: user-friendly method for setting the text on the first occurrence of an xml element in the xml file by specifying its name

- *set_simple_tag()*: user-friendly method for creating and setting attributes on simple xml elements (only attributes) in the xml file by specifying its name
- *set_complex_tag()*: user-friendly method for creating complex tags in the xml file by specifying its name
- *create_tag()*: User-friendly method for inserting a tag in the right place by specifying it's name
- *delete_tag()*: User-friendly method for delete a tag by specifying it's name
- *delete_att()*: User-friendly method for deleting an attribute from a tag by specifying it's name
- *replace_tag()*: User-friendly method for replacing a tag by another by specifying its name
- *set_nmmpmat()*: Specific method for initializing or modifying the density matrix file for a LDA+U calculation (details see below)
- *rotate_nmmpmat()*: Specific method for rotating a block of the density matrix file for a LDA+U calculation (details see below) in real space

4.1.2.4 Modifying the density matrix for LDA+U calculations

The above mentioned *set_nmmpmat()* and *rotate_nmmpmat()* take a special role in the modification registration methods, as the modifications are not done on the `inp.xml` file but the density matrix file `n_mmp_mat` used by Fleur for LDA+U calculations. The resulting new *n_mmp_mat* file is returned next to the new *inp.xml* by the *modify_xmlfile()*.

The code example below shows how to use this method to add a LDA+U procedure to an atom species and provide an initial guess for the density matrix.

```
from masci_tools.io.fleurxmlmodifier import FleurXMLModifier

fm = FleurXMLModifier()                                                    # Initialise␣
↪FleurXMLModifier class
fm.set_species('Nd-1', {'ldaU':                                            # Add LDA+U␣
↪procedure
                        {'l': 3, 'U': 6.76, 'J': 0.76, 'l_amf': 'F'}})
fm.set_nmmpmat('Nd-1', orbital=3, spin=1, occStates=[1,1,1,1,0,0,0]) # Initialize n_mmp_
↪mat file with the states
                                                                           # m = -3 to m = 0␣
↪occupied for spin up
                                                                           # spin down is␣
↪initialized with 0 by default
new_xmltree, nmmp_content = fm.modify_xmlfile('/path/to/original/inp.xml')         #␣
↪Apply
```

Note: The `n_mmp_mat` file is a simple text file with no knowledge of which density matrix block corresponds to which LDA+U procedure. They are read in the same order as they appear in the `inp.xml`. For this reason the `n_mmp_mat` file can become invalid if one adds/removes a LDA+U procedure to the `inp.xml` after the `n_mmp_mat` file was initialized. Therefore any modifications to the *n_mmp_mat* file should be done after adding/removing or modifying the LDA+U configuration.

4.1.3 General HDF5 file reader

Fleur uses the HDF5 library for output files containing large datasets. The masci-tools library provides the *HDF5Reader* class to extract and transform information from these files. The `h5py` library is used to get information from `.hdf` files

4.1.3.1 Basic Usage

The specifications of what to extract and how to transform the data are given in the form of a python dictionary. Let us look at a usage example; extracting data for a bandstructure calculation from the `banddos.hdf` file produced by Fleur.

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurBands

#The HDF5Reader is used with a contextmanager to safely handle
#opening/closing the h5py.File object that is produced to extract information
with HDF5Reader('/path/to/banddos.hdf') as h5reader:
   datasets, attributes = h5reader.read(recipe=FleurBands)
```

The method *read()* produces two python dictionaries. In the case of the `FleurBands` recipe these contain the following information.

- ***datasets***
  - Eigenvalues converted to eV shited to `E_F=0` (if available in the `banddos.hdf`) and split up into spin-up/down and flattened to one dimension
  - The kpath projected to 1D and reshaped to same length as weights/eigenvalues
  - The weights (flattened) of the interstitial region, each atom, each orbital on each atom for all eigenvalues
- ***attributes***
  - The coordinates of the used kpoints
  - Positions, atomic symbols and indices of symmetry equivalent atoms
  - Dimensions of eigenvalues (`nkpts` and `nbands`)
  - Bravais matrix/Reciprocal cell of the system
  - Indices and labels of special k-points
  - Fermi energy
  - Number of spins in the calculation

The following pre-defined recipes are stored in *recipes*:

- Recipe for `banddos.hdf` for bandstructure calculations
- Recipe for `banddos.hdf` for standard density of states calculations
- Different DOS modes are also supported (`jDOS`, `orbcomp`, `mcd`)

If no recipe is provided to the *HDF5Reader*, it will create the `datasets` and `attributes` as two nested dictionaries, exactly mirroring the structure of the `.hdf` file and converting datasets into numpy arrays.

For big datasets it might be useful to keep the dataset as a reference to the file and not load the dataset into memory. To achieve this you can pass `move_to_memory=False`, when initializing the reader. Notice that most of the transformations will still implicitly create numpy arrays and after the hdf file is closed the datasets will no longer be available.

4.1.3.2 Structure of recipes for the `HDF5Reader`

The recipe for extracting bandstructure information form the `banddos.hdf` looks like this:

```

def bands_recipe_format(group: Literal['Local', 'jDOS', 'Orbcomp', 'MCD'], simple: bool = False) -> HDF5Recipe:
    """
    Format for bandstructure calculations retrieving weights from the given group

    :param group: str of the group the weights should be taken from
    :param simple: bool, if True no additional weights are retrieved with the produced recipe

    :returns: dict of the recipe to retrieve a bandstructure calculation
    """

    if group == 'Local':
        atom_prefix = 'MT:'
    elif group == 'jDOS':
        atom_prefix = 'jDOS:'
    elif group == 'Orbcomp':
        atom_prefix = 'ORB:'
    elif group == 'MCD':
        atom_prefix = 'At'
    else:
        raise ValueError(f'Unknown group: {group}')

    recipe = HDF5Recipe({
        'datasets': {
            'eigenvalues': {
                'h5path':
                f'/{group}/BS/eigenvalues',
                'transforms': [
                    AttribTransformation(name='shift_by_attribute',
                                         attrib_name='fermi_energy',
                                         kwargs={
                                             'negative': True,
                                         }),
                    Transformation(name='multiply_scalar', args=(HTR_TO_EV,)),
                    Transformation(name='split_array', kwargs={
                        'suffixes': ['up', 'down'],
                        'name': 'eigenvalues'
                    }),
                    Transformation(name='flatten_array')
                ],
                'unpack_dict':
                True
            },
            'kpath': {
                'h5path':
                '/kpts/coordinates',
```

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```
                'transforms': [
                    AttribTransformation(name='multiply_by_attribute',
                                         attrib_name='reciprocal_cell',
                                         kwargs={'transpose': True}),
                    Transformation(name='calculate_norm', kwargs={'between_neighbours':␣
↪True}),
                    Transformation(name='cumulative_sum'),
                    AttribTransformation(name='repeat_array_by_attribute', attrib_name=
↪'nbands'),
                ]
            },
        },
        'attributes': {
            'group_name': {
                'h5path': f'/{group}',
                'transforms': [
                    Transformation(name='get_name'),
                ],
            },
            'kpoints': {
                'h5path': '/kpts/coordinates',
            },
            'nkpts': {
                'h5path': '/Local/BS/eigenvalues',
                'transforms': [Transformation(name='get_shape'),
                               Transformation(name='index_dataset', args=(1,))]
            },
            'nbands': {
                'h5path': '/Local/BS/eigenvalues',
                'transforms': [Transformation(name='get_shape'),
                               Transformation(name='index_dataset', args=(2,))]
            },
            'atoms_elements': {
                'h5path': '/atoms/atomicNumbers',
                'description': 'Atomic numbers',
                'transforms': [Transformation(name='periodic_elements')]
            },
            'n_types': {
                'h5path':
                '/atoms',
                'description':
                'Number of atom types',
                'transforms':
                [Transformation(name='get_attribute', args=('nTypes',)),
                 Transformation(name='get_first_element')]
            },
            'atoms_position': {
                'h5path': '/atoms/positions',
                'description': 'Atom coordinates per atom',
            },
            'atoms_groups': {
                'h5path': '/atoms/equivAtomsGroup'
```

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```
            },
            'reciprocal_cell': {
                'h5path': '/cell/reciprocalCell'
            },
            'bravais_matrix': {
                'h5path': '/cell/bravaisMatrix',
                'description': 'Coordinate transformation internal to physical for atoms
↪',
                'transforms': [Transformation(name='multiply_scalar', args=(BOHR_A,))]
            },
            'special_kpoint_indices': {
                'h5path': '/kpts/specialPointIndices',
                'transforms': [Transformation(name='shift_dataset', args=(-1,))]
            },
            'special_kpoint_labels': {
                'h5path': '/kpts/specialPointLabels',
                'transforms': [Transformation(name='convert_to_str')]
            },
            'fermi_energy': {
                'h5path':
                '/general',
                'description':
                'fermi_energy of the system',
                'transforms': [
                    Transformation(name='get_attribute', args=('lastFermiEnergy',)),
                    Transformation(name='get_first_element')
                ]
            },
            'spins': {
                'h5path':
                '/general',
                'description':
                'number of distinct spin directions in the system',
                'transforms':
                [Transformation(name='get_attribute', args=('spins',)),
                 Transformation(name='get_first_element')]
            }
        }
    })

    if simple:
        return recipe

    recipe['datasets']['weights'] = {
        'h5path':
        f'/{group}/BS',
        'transforms': [
            Transformation(name='get_all_child_datasets', kwargs={'ignore': ['eigenvalues
↪', 'kpts']}),
            AttribTransformation(name='add_partial_sums',
                                 attrib_name='atoms_groups',
                                 args=(f'{atom_prefix}{{}}'.format,),
```

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```
                                kwargs={'make_set': True}),
            Transformation(name='split_array', kwargs={'suffixes': ['up', 'down']}),
            Transformation(name='flatten_array')
        ],
        'unpack_dict':
        True
    }

    return recipe


def get_fleur_bands_specific_weights(weight_name: str | list[str],
                                     group: Literal['Local', 'jDOS', 'Orbcomp', 'MCD'] =
↪'Local') -> HDF5Recipe:
    """
    Recipe for bandstructure calculations only retrieving one
    additional weight besides the eigenvalues and kpath

    :param weight_name: key or list of keys of the weight(s) to retrieve
    :param group: optional str (default Local) name of the group from where to take the␣
↪weights
```

Each recipe can define the *datasets* and *attributes* entry (if one is not defined, a empty dict is returned in its place). Each entry in these sections has the same strucuture.

```
#Example entry from the FleurBands recipe

'fermi_energy': {
        'h5path':
        '/general',
        'description':
        'fermi_energy of the system',
        'transforms': [
            Transformation(name='get_attribute', args=('lastFermiEnergy',), kwargs={}),
            Transformation(name='get_first_element', args=(), kwargs={})
        ]
    }
```

All entries must define the key `h5path`. This gives the initial dataset for this key, which will be extracted from the given `.hdf` file. The key of the entry corresponds to the key under which the result will be saved to the output dictionary.

If the dataset should be transformed in some way after reading it, there are a number of defined transformations in *transforms*. These are added to an entry by adding a list of namedtuples (*Transformation* for general transformations; *AttribTransformation* for attribute transformations) under the key `transforms`. General Transformations can be used in all entries, while transformations using an attribute value can only be used in the `datasets` entries. Each namedtuple takes the `name` of the transformation function and the positional (`args`), and keyword arguments (`kwargs`) for the transformation. Attribute transformations also take the name of the attribute, whose value should be passed to the transformation in `attrib_name`.

At the moment the following transformation functions are pre-defined:

General Transformations:

- *get_first_element()*: Get the index `0` of the dataset

- *index_dataset()*: Get the index `index` of the dataset
- *slice_dataset()*: Slice the given dataset with the given argument
- *get_shape()*: Get the shape of the dataset
- *tile_array()*: Use np.tile to repeat dataset a given amount of times
- *repeat_array()*: Use np.repeat to repeat each element in the dataset a given amount of times
- *get_all_child_datasets()*: extract all datasets contained in the current hdf group and enter them into a dict
- *merge_subgroup_datasets()*: extract all datasets contained in the subgroups of the current hdf group and enter them into a dict in a list (or one numpy array)
- *stack_datasets()*: Stack the given datasets in the dictionary along a given axis
- *shift_dataset()*: Shift the given dataset with a scalar value
- *multiply_scalar()*: Multiply the given dataset with a scalar value
- *multiply_array()*: Mutiply the given dataset with a given array
- *convert_to_complex_array()*: Convert real dataset to complex array
- *calculate_norm()*: Calculate norm of list of vectors (either absolute or difference between subsequent entries)
- *cumulative_sum()*: Calculative cumulative sum of dataset
- *get_attribute()*: Get the value of one given attribute on the dataset
- *attributes()*: Get all defined attributes on the dataset as a dict
- *move_to_memory()*: Convert dataset to numpy array (if not already done implicitly)
- *flatten_array()*: Create copy of dataset flattened into one dimension
- *split_array()*: Split the given dataset along its first index and store result in a dictionary with keys with suffixes
- *convert_to_str()*: Convert datatype of dataset to string
- *periodic_elements()*: Convert atomic numbers to their atomic symbols

Transformations using an attribute:

- *multiply_by_attribute()*: Multiply dataset by value of attribute (both scalar and matrix)
- *shift_by_attribute()*: Shift the given dataset with the value of an attribute
- *repeat_array_by_attribute()*: Call *repeat_array()* with the value of an attribute as argument
- *tile_array_by_attribute()*: Call *tile_array()* with the value of an attribute as argument
- *add_partial_sums()*: Sum over entries in dictionary datasets with given patterns in the key (Pattern is formatted with given attribute value)

Custom transformation functions can also be defined using the *hdf5_transformation()* decorator. For some transformation, e.g. *get_all_child_datasets()*, the result will be a subdictionary in the `datasets` or `attributes` dictionary. If this is not desired the entry can include `'unpack_dict': True`. With this all keys from the resulting dict will be extracted after all transformations and put into the root dictionary.

4.1.4 Plotting Fleur DOS/bandstructures

This section discusses how to obtain plots of data in the `banddos.hdf` for density of states and bandstructure calculations.

The process here is divided in two parts. First we extract and transform the data in a way to make it easy to plot via the *HDF5Reader*. For a detailed explanation of the capabilities of this tool refer to *General HDF5 file reader*. Here we show the basic usage:

```
#Example: Bandstructure calculation

from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurBands

with HDF5Reader('/path/to/banddos.hdf') as h5reader:
   data, attributes = h5reader.read(recipe=FleurBands)
```

In the following bandstructure and DOS plots are explained. Each section leads with the names of the recipes from the *recipes* module that can be used with the explained visualization function.

All Fleur specific plotting routines are found in *fleur* have implementations for both the matplotlib and bokeh plotting libraries and can be customized heavily. For an explanation on customizing plots refer to *General Plotting routines*.

4.1.4.1 Bandstructures

Compatible Recipes for the *HDF5Reader*:

- `FleurBands`: Default recipe reading in the kpoints, eignevalues and weights for atom and orbital contributions
- `FleurSimpleBands`: Reads in only the kpoints and eigenvalues and now weights
- `FleurOrbcompBands`: In addition to the eigenvalues the weights from an orbital decomposition calculation are read in
- `FleurjDOSBands`: In addition to the eigenvalues the weights from a jDOS calculation are read in
- `FleurMCDBands`: In addition to the eigenvalues the weights from a MCD calculation are read in
- *get_fleur_bands_specific_weights()*: Function to generate a recipe for reading in the eigenvalues+a provided list of weights

The bandstructure visualization *plot_fleur_bands()* can be used to plot

1. Non-spinpolarized/spinpolarized bandstructures
2. Bandstructures with emphasized weights on all eigenvalues (Also non-spinpolarized and spinpolarized)

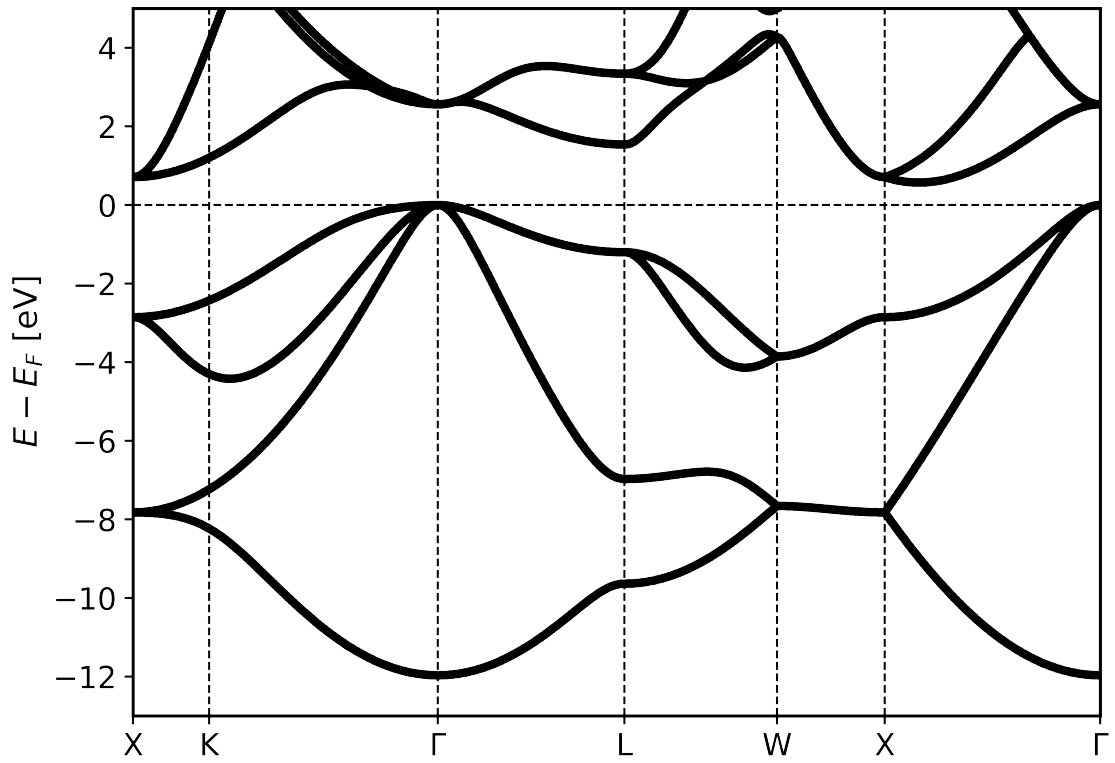
Standard bandstructure

To plot a simple bandstructure without any weighting we just have to pass the data, that the *HDF5Reader* provided to the *plot_fleur_bands()*

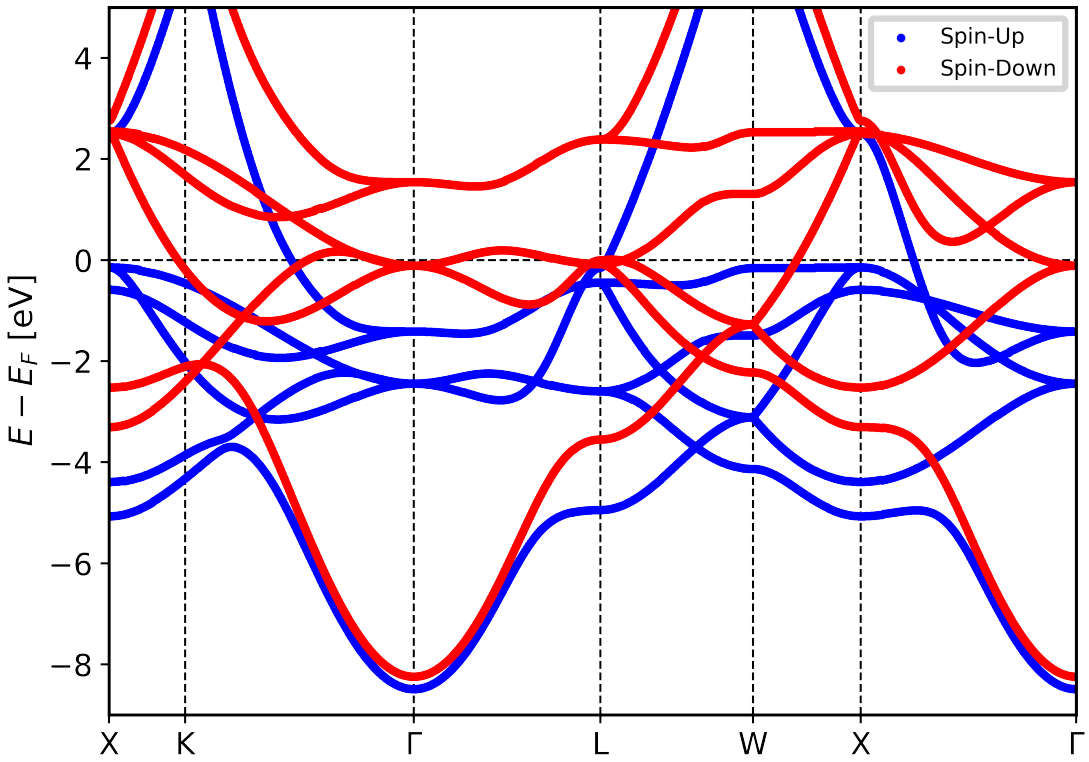
The two exmaples below show the resulting plots for a non-psinpolarized system (bulk Si) and a spin-polarized system (Fe fcc). For both systems the necessary code is exactly the same and is shown above the plots. The shown plots are the ones for the matplotlib plotting backend:

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurBands
from masci_tools.vis.fleur import plot_fleur_bands

#Read in data
with HDF5Reader('/path/to/banddos.hdf') as h5reader:
   data, attributes = h5reader.read(recipe=FleurBands)

#Plot the data
#Notice that you get the axis object of this plot is returned
#if you want to make any special additions
ax = plot_fleur_bands(data, attributes)
```

Non spinpolarized bandstructure



Spinpolarized bandstructure



Bandstructure with weights

To plot a simple bandstructure with weighting we do the same procedure as above, but we pass in the entry we want to use for weights. These correspond to the entries in the `banddos.hdf` file (for example the weight for the s-orbital on the first atom type is called `MT:1s`)

The weights will be used to change the size and color (according to a colormap) to indicate regions of high weight.

The two exmaples below show the resulting plots for a non-psinpolarized system (bulk Si) weighted for the s-orbital on the first atom and a spin-polarized system (Fe fcc) with weights for the d-orbital on the first atom type. For both systems the necessary code is exactly the same and is shown above the plots. The shown plots are the ones for the matplotlib plotting backend:

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurBands
from masci_tools.vis.fleur import plot_fleur_bands

#Read in data
with HDF5Reader('/path/to/banddos.hdf') as h5reader:
   data, attributes = h5reader.read(recipe=FleurBands)
```

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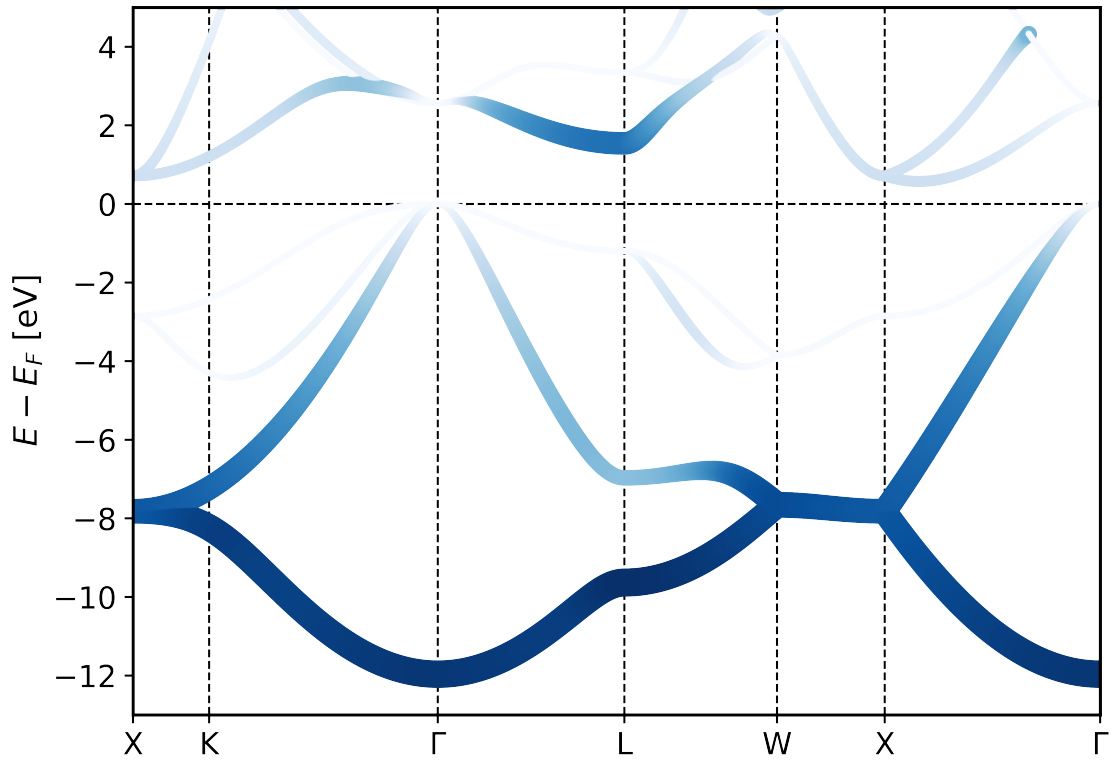
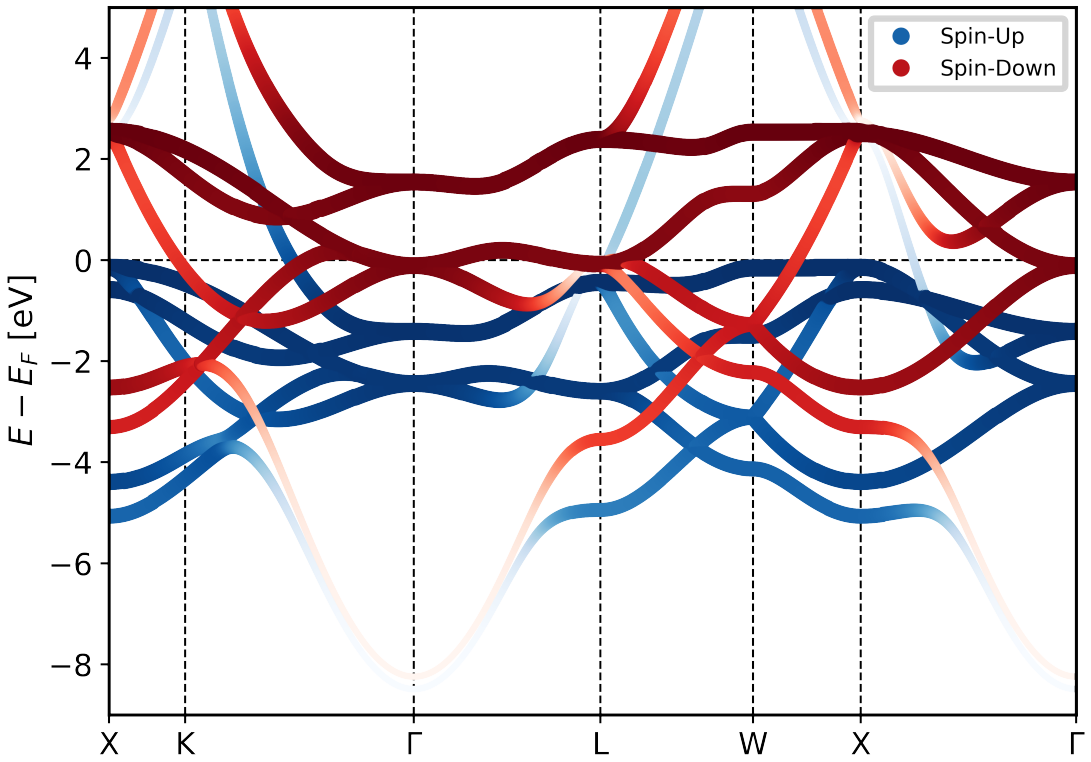
```
#Plot the data
#Notice that you get the axis object of this plot is returned
#if you want to make any special additions
ax = plot_fleur_bands(data, attributes, weight='MT:1s')
```

Non spinpolarized bandstructure (weights for s-orbital)



Spinpolarized bandstructure (weights for d-orbital)



4.1.4.2 Density of States

Compatible Recipes for the *HDF5Reader*:

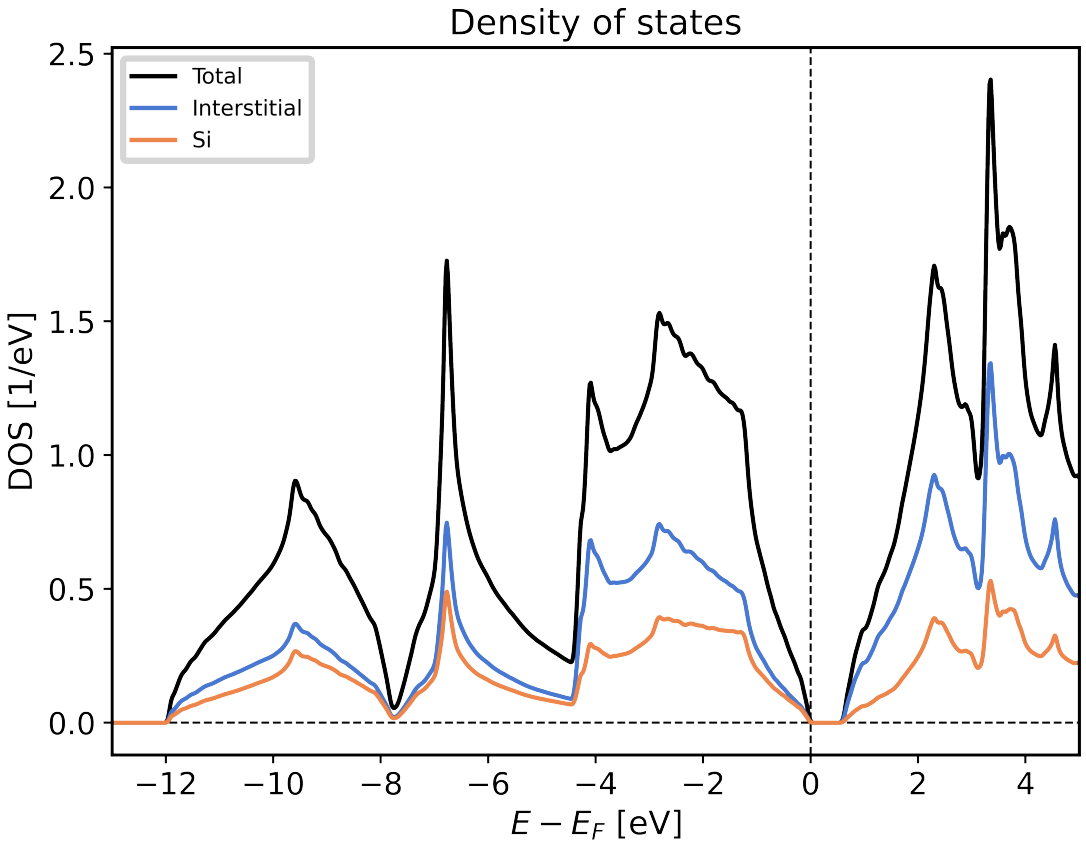
- `FleurDOS`: Default recipe reading in the total, interstitial, vacuum, atom and l-channle resolved DOS
- `FleurORBCOMP`: Read in the DOS from an orbital decomposition calculation
- `FleurJDOS`: Read in the DOS from a jDOS calculation
- `FleurMCD`: Read in the DOS from a MCD calculation

The dos visualization *plot_fleur_dos()* can be used to plot non spinpolarized and spinpolarized DOS, with selection of which components to plot.

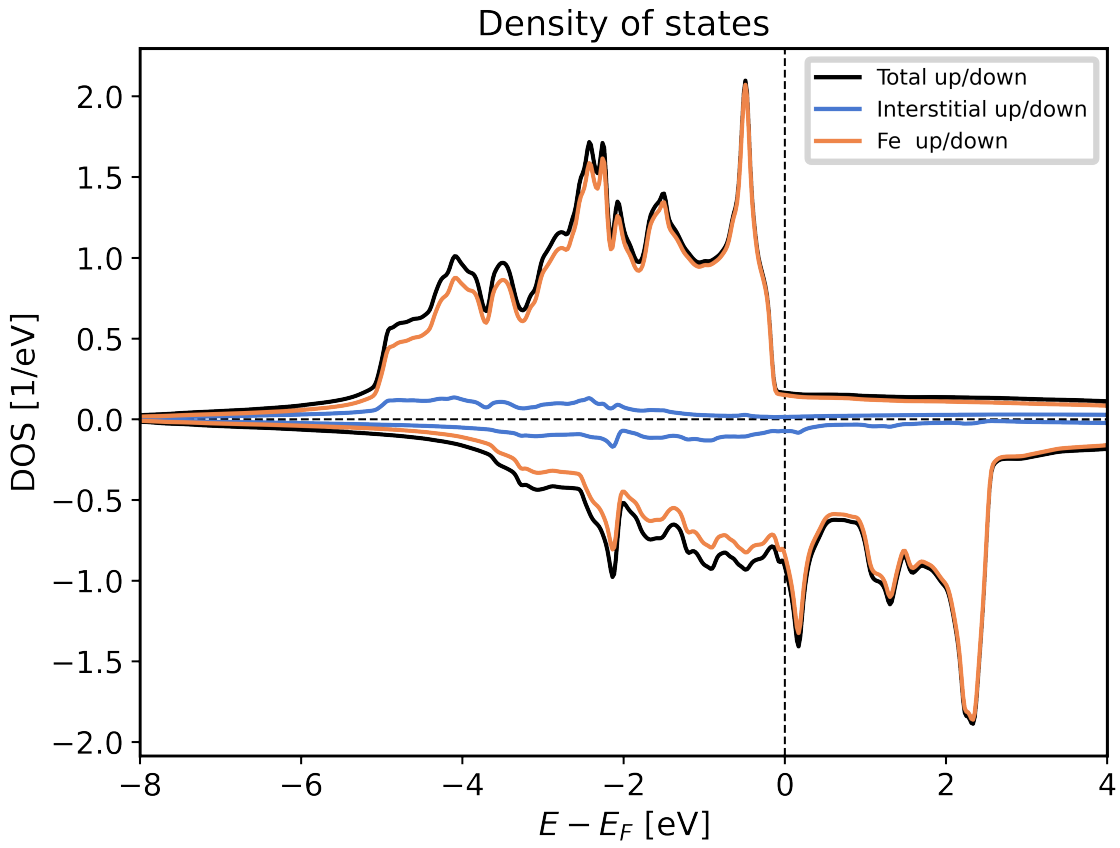
Standard density of states plot

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurDOS
from masci_tools.vis.fleur import plot_fleur_dos

#Read in data
with HDF5Reader('/path/to/banddos.hdf') as h5reader:
   data, attributes = h5reader.read(recipe=FleurDOS)

#Plot the data
#Notice that you get the axis object of this plot is returned
#if you want to make any special additions
ax = plot_fleur_dos(data, attributes)
```

Non spinpolarized DOS



Spinpolarized DOS



Plotting options for DOS plots

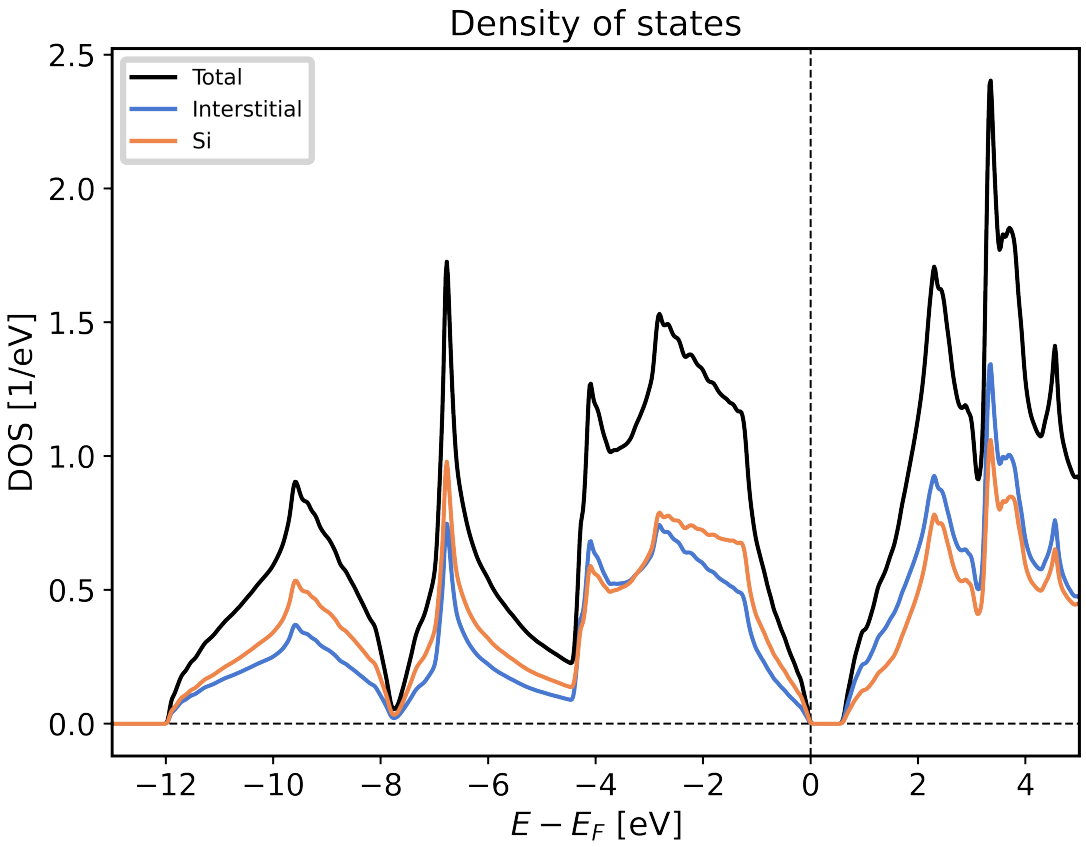
The *plot_fleur_dos()* function has a couple of options to modify, what is being displayed from the `banddos.hdf` file. Below we show a few examples of ways to use these options, together with examples of resulting plots.

DOS with atom components scaled with equivalent atoms

When you look at the example plot for the non spin-polarized DOS, you might notice that the interstitial component and the atom projected components do not add up to the total density of states. This system has two symmetry equivalent *Si* atoms. By default the atom projected density of states corresponds to only one of these atoms.

If you wish to show the atom projected components of the DOS scaled with the number of symmetry equivalent atoms you can provide the option `multiply_by_equiv_atoms=True` option to the plotting function.

```
ax = plot_fleur_dos(data, attributes, multiply_by_equiv_atoms=True)
```



Selecting specific DOS components

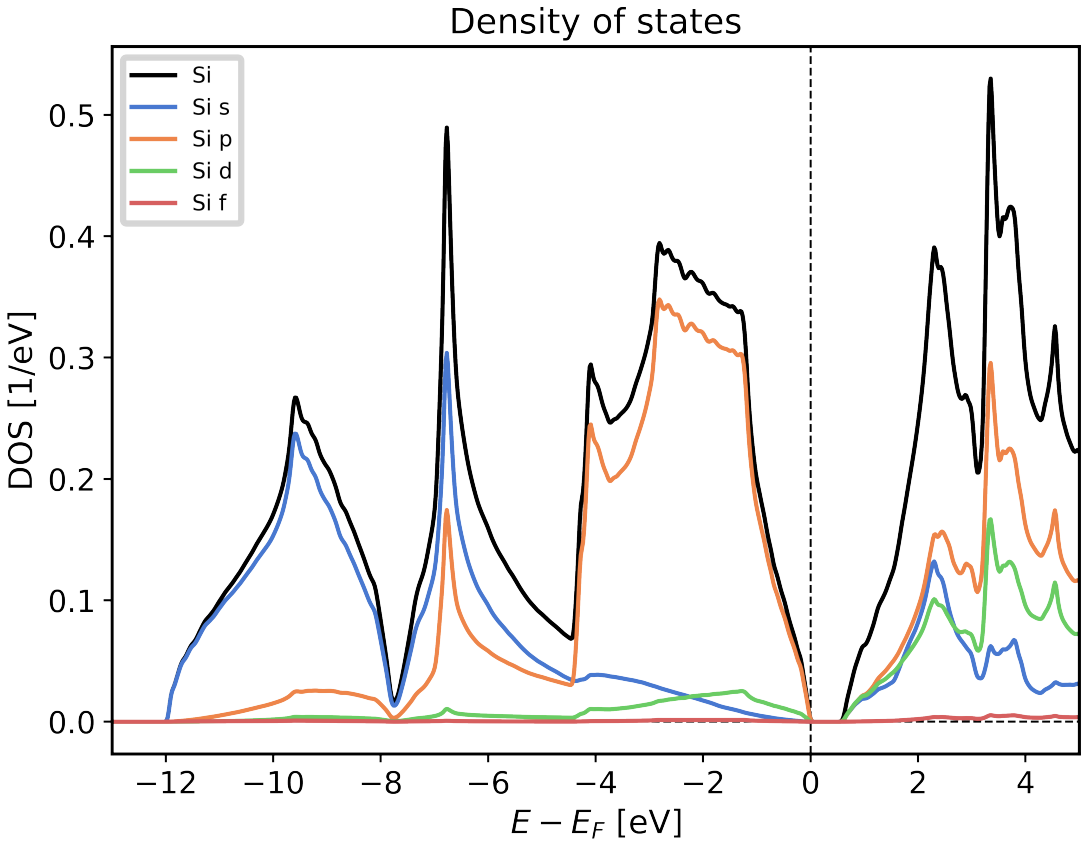
The DOS is made up of a lot of contributions that can be displayed separately.

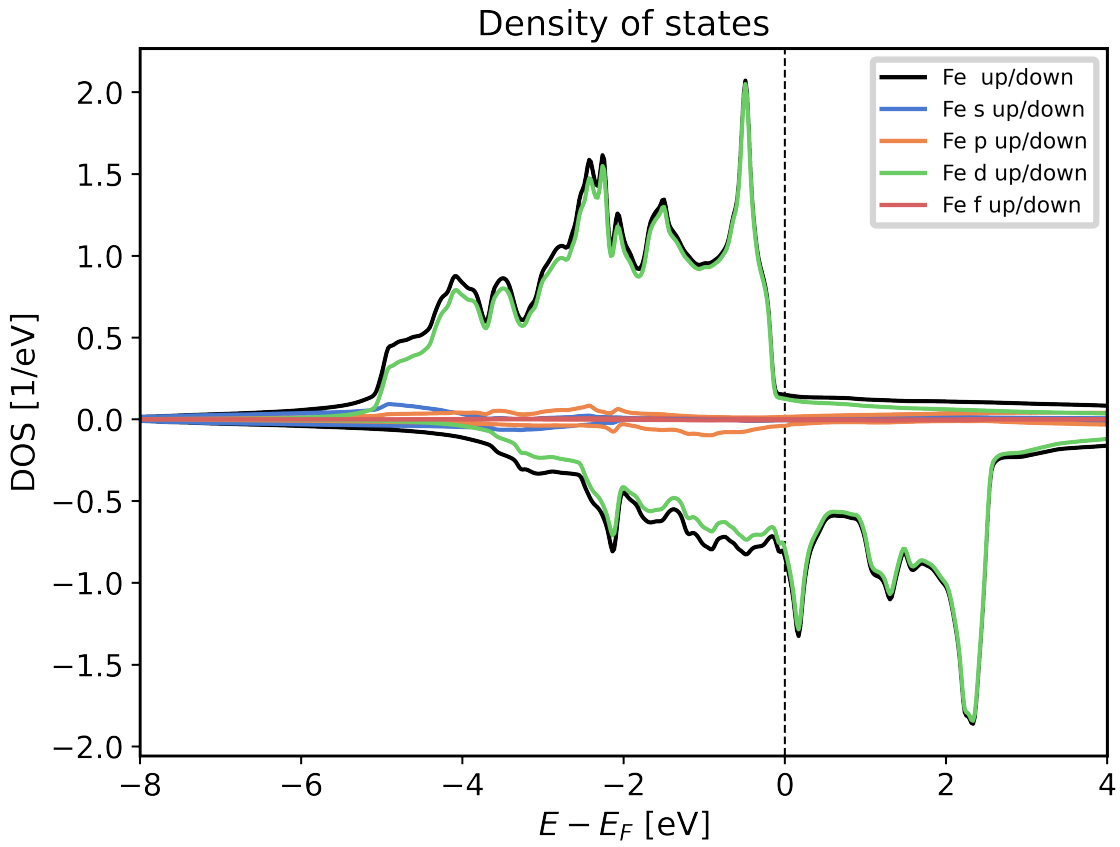
Here we list the options that are available and show exmaple plots for only selecting the atom projected compinents of the density of states

- **plot_keys** Can be used to provide a explicit list of keys you want to display (Same format as in the `banddos.hdf`)
- **show_total** Control, whether to show the total density of states (default `True`)
- **show_interstitial** Control, whether to show the interstitial contribution of the density of states (default `True`)
- **show_atoms** Control, which total atom projected DOS to show. Can be either the string `all` (All components are shown), the value `None` (no components are shown) or a list of the integer indices of the atom types that should be displayed (default `all`)
- **show_lresolved** Control, on which atoms to show the orbital projected DOS. Can be either the string `all` (All components are shown), the value `None` (no components are shown) or a list of the integer indices of the atom types for which to display the orbital components (default `None`)

Below an example of only displaying the atom projected DOS together with their orbital contributions is shown.

```
ax = plot_fleur_dos(data, attributes,
                    show_total=False,
                    show_interstitial=False,
                    show_lresolved='all')
```





4.1.5 General Plotting routines

The plotting of data is always a common task that needs to be performed. However, there is a lot of variation in how someone might want plots to look or be arranged. Some plots might also need to be interactive to be of a real use.

For these reasons the `masci_tools` library provides utility for general plotting and template functions for common plots made wehn working with DFT methods. There are two plotting backends available:

- **matplotlib** Mainly used for non-interactive plots
- **bokeh** Mainly used for interactive plots

4.1.5.1 Available Routines

For both of these there are a lot of plotting routines available (both general or specific to a problem). All of these routines will return the used `Axes` object in the case of matplotlib or the `figure` produced by bokeh for custom modifications.

- ***common*** **(Can be used for both backends):**
  - *`scatter()`*: Make a scatterplot with varying size and color of the points for multiple sets of data
  - *`line()`*: Make a lineplot with multiple sets of data
  - *`dos()`*: Plot a general density of states (non-spinpolarized)
  - *`spinpol_dos()`*: Plot a general density of states (spinpolarized)

  - `bands()`: Plot a general bandstructure (non-spinpolarized)
  - `spinpol_bands()`: Plot a general bandstructure (spinpolarized)

- ***matplotlib*:**
  - `single_scatterplot()`: Make a scatterplot with lines for a single set of data
  - `multiple_scatterplots()`: Make a scatterplot with lines for multiple sets of data
  - `multi_scatter_plot()`: Make a scatterplot with varying size and color fo the points for multiple sets of data
  - `colormesh_plot()`: Make 2D plot with the data represented as color
  - `waterfall_plot()`: Make 3D plot with the *scatter3D* function of matplotlib
  - `surface_plot()`: Make 3D plot with the *plot_surface* function of matplotlib
  - `multiplot_moved()`: Plot multiple sets of data above each other with a configurable shift
  - `histogram()`: Make a histogram plot
  - `barchart()`: Make a barchart plot
  - `multiaxis_scatterplot()`: Make a plot containing multiple sets of data distributed over multiple subplots in a grid
  - `plot_convex_hull2d()`: Make a 2D plot of a convex hull
  - `plot_residuen()`: Make a residual plot for given real and fit data. Can also produce a histogram of the deviations
  - `plot_convergence_results()`: Plot the convergence behaviour of charge density distances and energies of a single calculation
  - `plot_convergence_results_m()`: Plot the convergence behaviour of charge density distances and energies of multiple calculations
  - `plot_lattice_constant()`: Plot the energy curve with changing unit cell volume
  - `plot_dos()`: Plot a general density of states (non-spinpolarized)
  - `plot_spinpol_dos()`: Plot a general density of states (spinpolarized)
  - `plot_bands()`: Plot a general bandstructure (non-spinpolarized)
  - `plot_spinpol_bands()`: Plot a general bandstructure (spinpolarized)

- ***bokeh*:**
  - `bokeh_scatter()`: Make a scatterplot for a single set of data
  - `bokeh_multi_scatter()`: Make a scatterplot for a multiple sets of data
  - `bokeh_line()`: Make a line plot for multiple sets of data
  - `bokeh_dos()`: Plot a general density of states (non-spinpolarized)
  - `bokeh_spinpol_dos()`: Plot a general density of states (spinpolarized)
  - `bokeh_bands()`: Plot a general bandstructure (non-spinpolarized)
  - `bokeh_spinpol_bands()`: Plot a general bandstructure (spinpolarized)
  - `periodic_table_plot()`: Make a interactive plot of data for the periodic table

If you have ideas for new useful and beatiful plotting routines you are welcome to contribute. Refer to the sections *Using the Plotter class* and *Using the PlotData class* for a guide on how to get started.

4.1.5.2 Providing Data

Data can be provided to plotting functions in two main ways:

1. The first arguments and data arguments are given the keys in a mapping, which should be used. The correspinding mapping is provided via the `data` keyword argument
2. The first arguments and data arguments are given the data that should be plotted against each other.

The following two code blocks are equivalent in terms of the provided data.

```
from masci_tools.vis.plot_methods import multiple_scatterplots
import numpy as np

x = np.linspace(-10,10,100)
y1 = x**2
y2 = 20*np.sin(x)

#The data is split up according to fixed rules that the plot function defines.
#The default behaviour is that a list of lists is interpreted as multiple separate plots
ax = multiple_scatterplots(x, [y1, y2])
```

```
from masci_tools.vis.plot_methods import multiple_scatterplots
import numpy as np

x = np.linspace(-10,10,100)
y1 = x**2
y2 = 20*np.sin(x)
data = {'x': x, 'y1': y1, 'y2': y2}

ax = multiple_scatterplots('x', ['y1', 'y2'], data=data)
```

4.1.5.3 Customizing Plots

You might want to change the parameters of your plot. From changing the color, linestyle or shape of the markers there are a million options to tweak.

These can be set by simply passing the keyword arguments with the desired parameters to the plotting function. The names of these parameters mostly correspond to the same names as in the plotting library that is used in the plotting function. However, there are some deviations and also some special keywords that you can use. We will go over the most important ones in this section accompanied with concrete code examples. For a reference of the defaults defined in the `masci_tools` library you can refer to *MatplotlibPlotter* and *BokehPlotter* for a complete reference.

The most important special keywords are listed below. If there are deviating names for these in `matplotlib` and `bokeh` plotting functions both names are written in the order `matplotlib or bokeh`:

- **limits** This is used to set the bounds of the axis specifically. Provided in form of a dictionary. For example passing `limits={'x': (-5,5)}` will set the x-axis limits between `-5` and `5` and `limits={'x': (-5,5), 'y':(0,10)}` will set the y-axis limits in addition
- **scale** Used to set the scaling of the axis in the plots. Also provided in form of a dictionary. For example passing `scale={'x': 'log', 'y': 'log'}` will set both axis to logarithmic scaling `scale={'y': 'log'}` will only to it for the y-axis
- **lines or straight_lines** Easy way to draw help lines into the plot. Provided in form of a dictionary. For example passing `lines={'vertical': 0}` will draw a vertical line at `x=0`

`lines={'horizontal': [1,5,10]}` will draw three horizontal lines at `y=1, 5 or 10` respectively

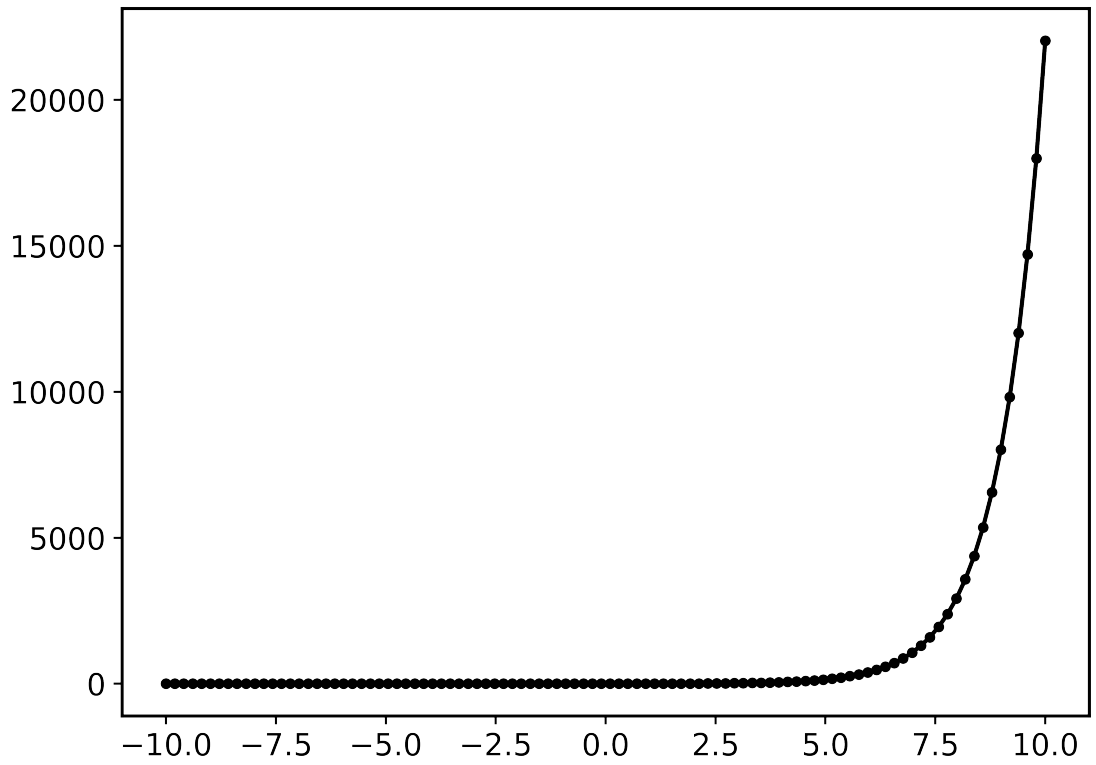
- **plot_labels or legend_labels** Defines labels for the legend of a plot
- **labels for axis** Normally called `xlabel` or `ylabel`, but specialized plot routines might have different names
- **title** Title for the produced plot
- **saving options** `show=True` call the plotting library specific show routines (default). For matplotlib you can also specify `saveas='filename'` and `save_plots=True` to save the plot to file

In the following we will look at examples using the matplotlib plotting functions in *plot_methods*. The options are the same for the bokeh plotting routines in *bokeh_plots*.

Single plots

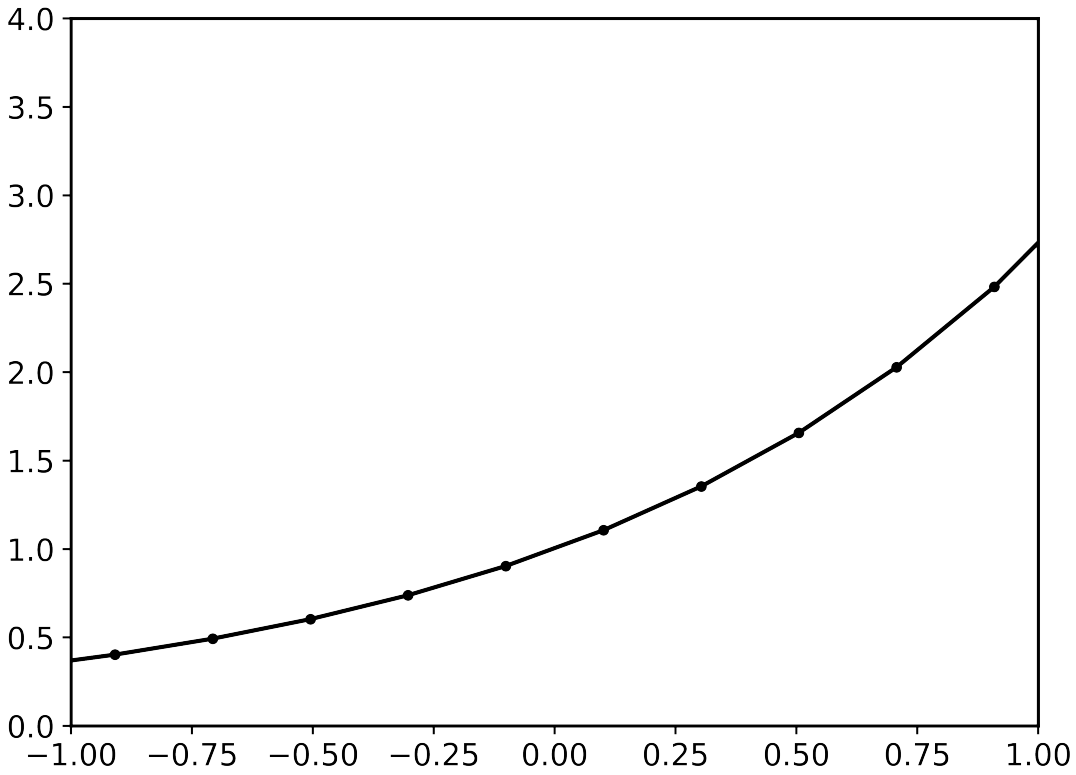
We start from the default result of calling the *single_scatterplot()* function with an exponential function. Afterwards we go through examples of modifying this call in one particular way. All of these can be combined to customize the plot to your desire

```
from masci_tools.vis.plot_methods import single_scatterplot
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

ax = single_scatterplot(x,y)
```



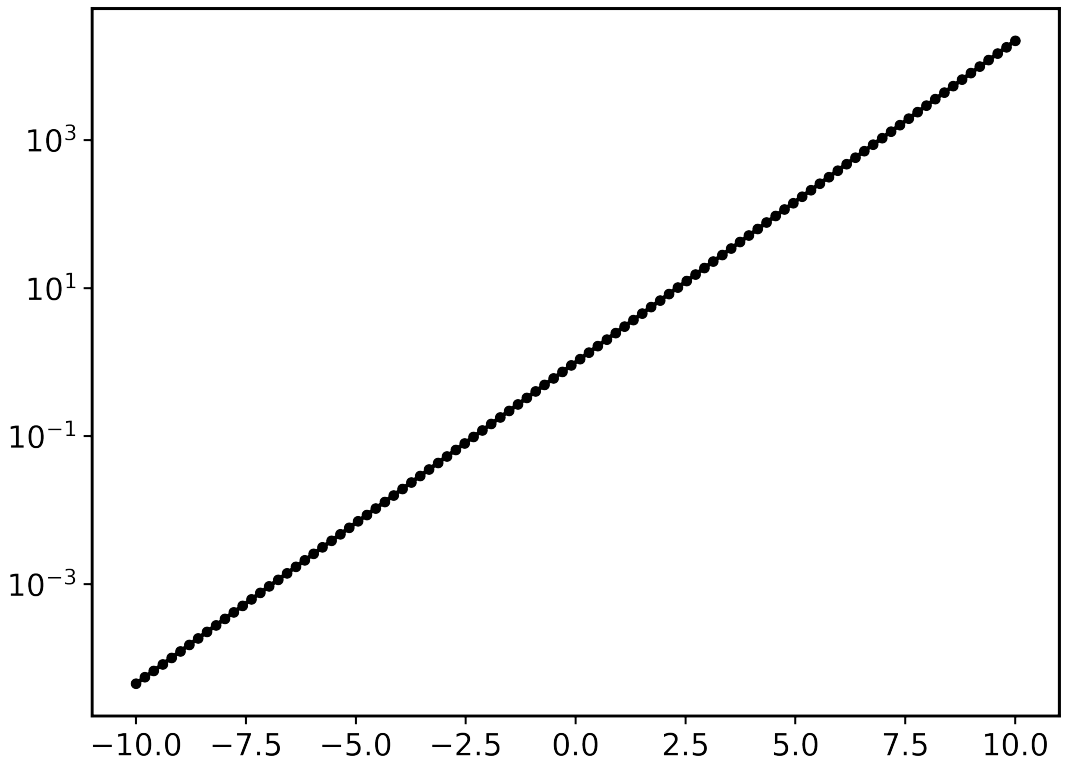
Setting limits

```
from masci_tools.vis.plot_methods import single_scatterplot
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

ax = single_scatterplot(x,y, limits={'x': (-1,1), 'y': (0,4)})
```



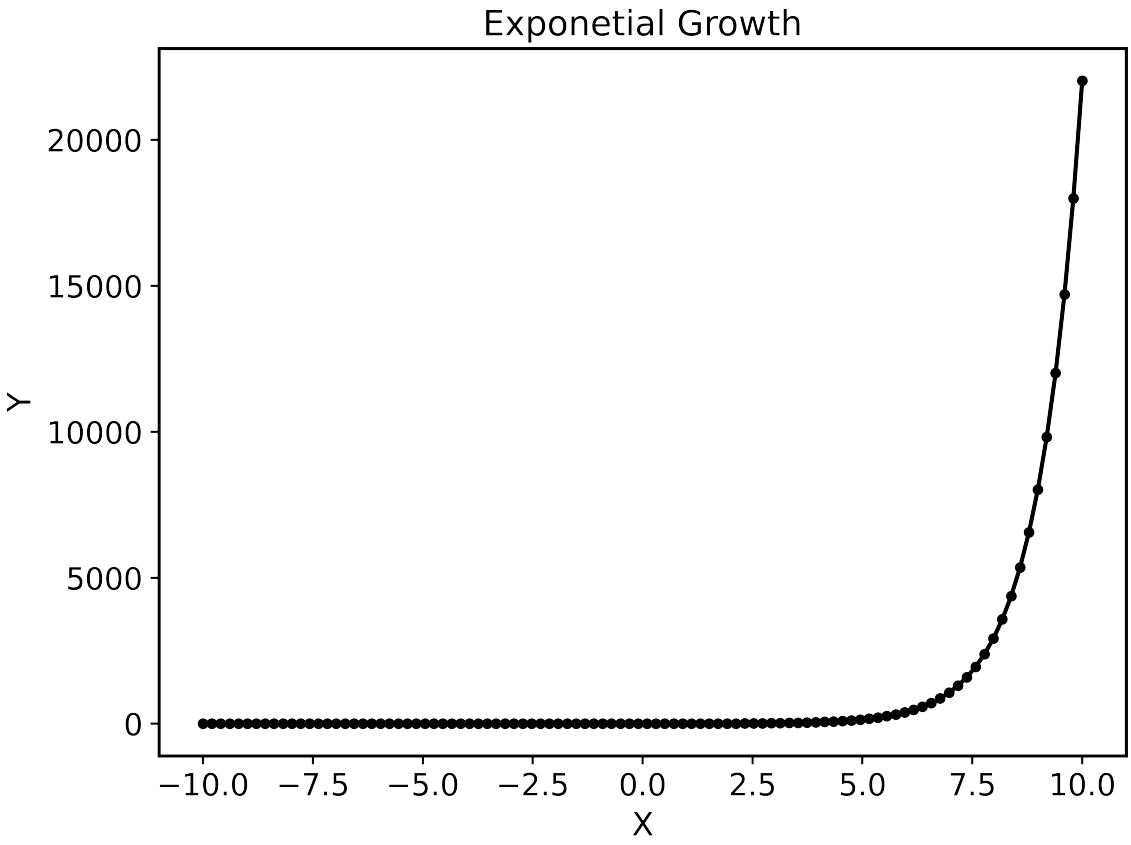
Modifying the scale of the axis

```
from masci_tools.vis.plot_methods import single_scatterplot
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

ax = single_scatterplot(x,y, scale={'y': 'log'})
```



Setting labels on the axis and a title

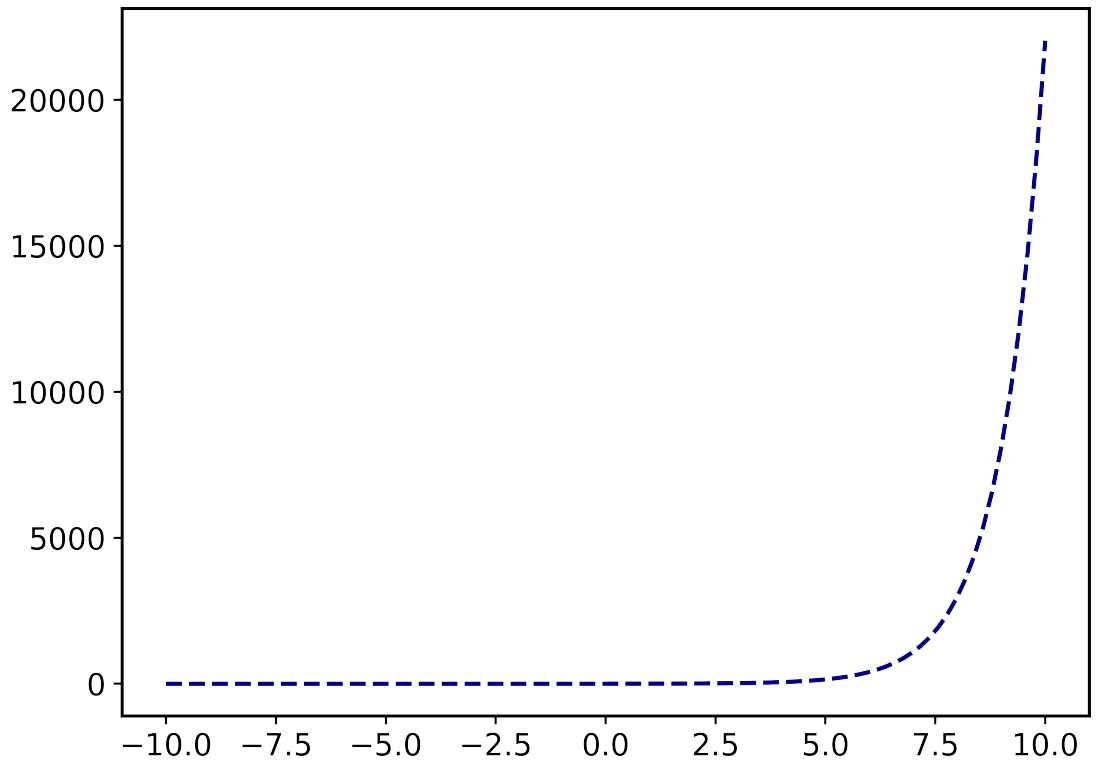
```
from masci_tools.vis.plot_methods import single_scatterplot
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

ax = single_scatterplot(x,y, xlabel='X', ylabel='Y', title='Exponential Growth')
```



Modifying plot parameters

See the matplotlib documentation for complete references of possible options

```
from masci_tools.vis.plot_methods import single_scatterplot
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

ax = single_scatterplot(x,y, color='darkblue', linestyle='--', marker=None)
```



Setting user defaults

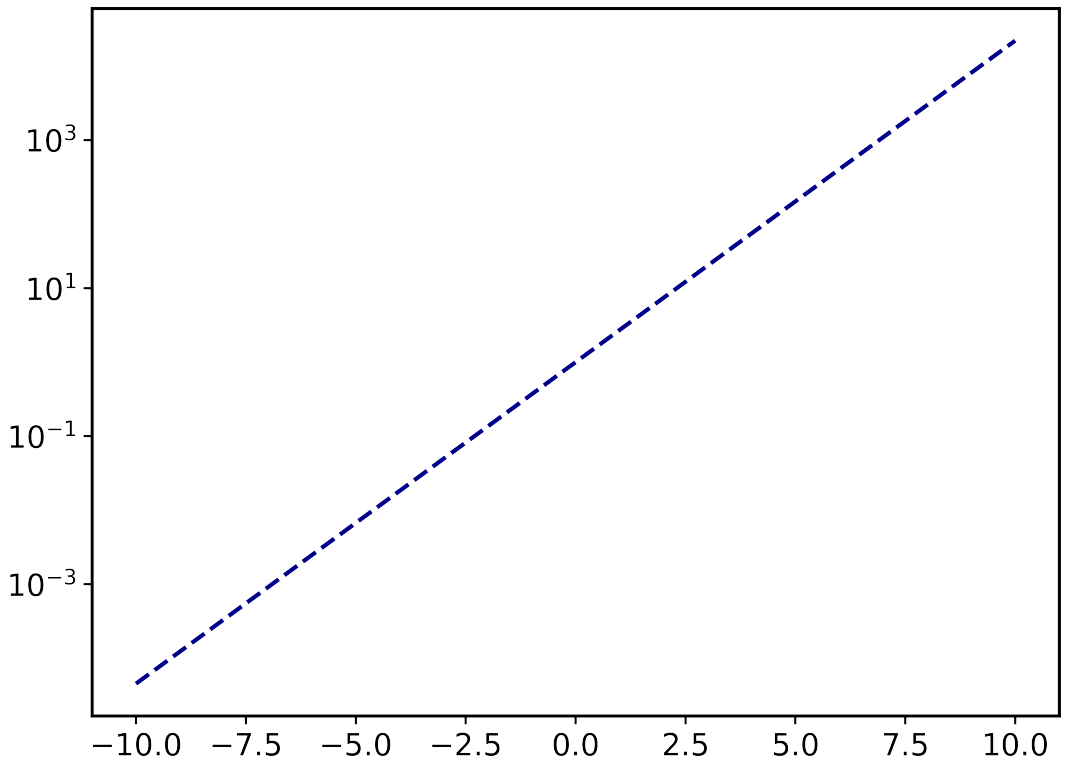
If you wish to change some parameters for all the plots you want to do, you can use the functions *set_mpl_plot_defaults()* or *set_bokeh_plot_defaults()* for the matplotlib and bokeh plotting library respectively. These functions accept the same keyword arguments as above and they will be applied to all the next plots that you do.

You can reset the changes to the defaults with *reset_mpl_plot_defaults()* or *reset_bokeh_plot_defaults()*

Note: You can still override these defaults by simply passing in another value for the parameter you wish to overwrite in the call to a plotting function

---

```
from masci_tools.vis.plot_methods import single_scatterplot, set_mpl_plot_defaults
import numpy as np

x = np.linspace(-10, 10, 100)
y = np.exp(x)

set_mpl_plot_defaults(color='darkblue', linestyle='--', marker=None)

ax = single_scatterplot(x,y, scale={'y': 'log'})
```



Multiple plots

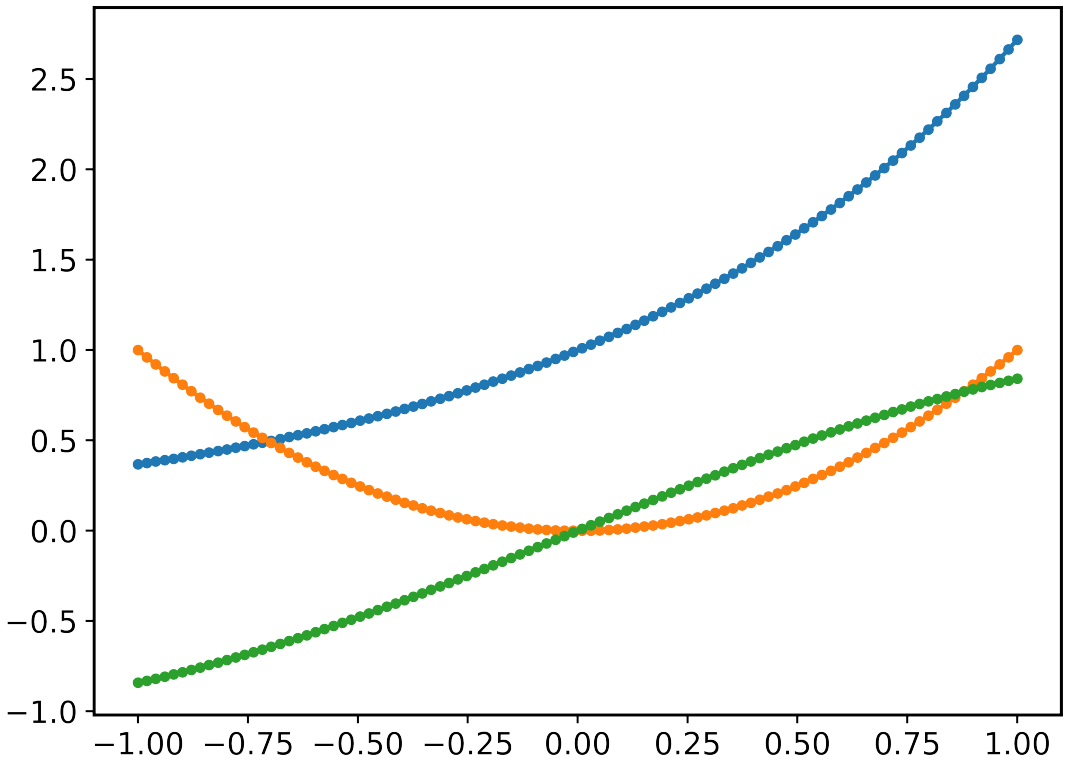
Many plotting routines accept multiple sets of data to plot. An example of this is the *multiple_scatterplots()* function. The usage of these is essentially the same. However, some parameters can be changed for each data set to plot. These include but are not limited to `linestyle`, `linewidth`, `marker`, `markersize` and `color`. These parameters can either be set to a single value applying it to all data sets, or can be specified for some/all data sets with unspecified values being replaced with the current defaults. This second way can be done in two ways (Both of the below examples have the same effect):

1. List of values (`None` for unspecified values) Example: `linestyle=['-', None, '--']`
2. Dictionary with integer indices Example: `linestyle={0:'-', 2:'--'}`

Warning: Specifying parameters for multiple data sets is only valid for the parameters passed into the function. Setting defaults with values for multiple data sets is not supported

Default plot

```
from masci_tools.vis.plot_methods import multiple_scatterplots
import numpy as np

x = np.linspace(-1,1,100)
y = np.exp(x)
y2 = x**2
y3 = np.sin(x)

ax = multiple_scatterplots([x, x, x], [y, y2, y3])
```



Changing parameters on all plots

```
from masci_tools.vis.plot_methods import multiple_scatterplots
import numpy as np

x = np.linspace(-1,1,100)
y = np.exp(x)
y2 = x**2
y3 = np.sin(x)
```

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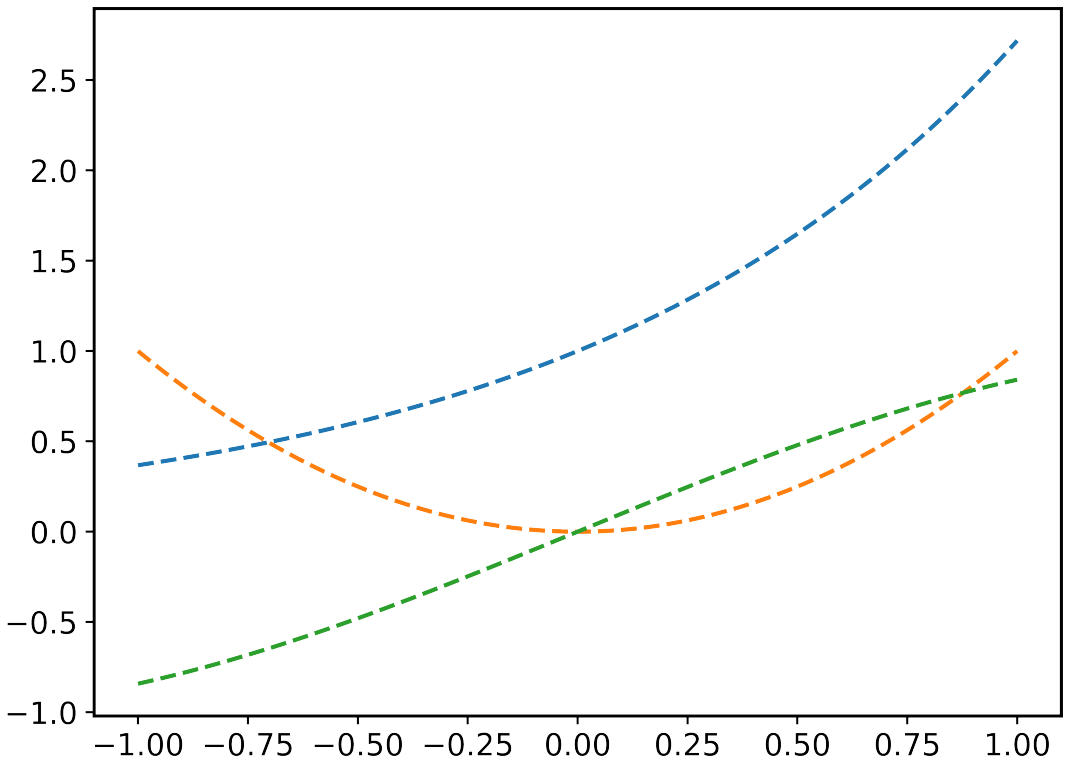
```
ax = multiple_scatterplots([x, x, x], [y, y2, y3], linestyle='--', marker=None)
```

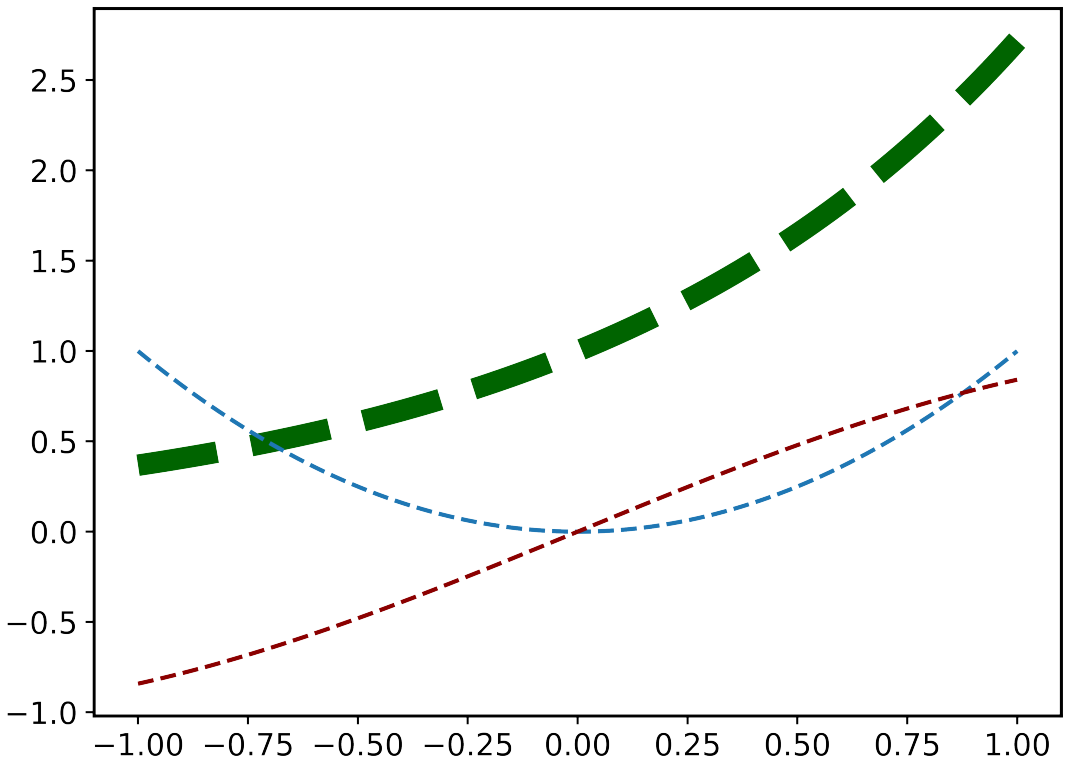


Changing parameters on specific plots

```
from masci_tools.vis.plot_methods import multiple_scatterplots
import numpy as np

x = np.linspace(-1,1,100)
y = np.exp(x)
y2 = x**2
y3 = np.sin(x)

ax = multiple_scatterplots([x, x, x], [y, y2, y3],
                           linestyle='--',
                           marker=None,
                           color=['darkgreen', None, 'darkred'],
                           linewidth={0: 10})
```


2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

CHAPTER

FIVE

DEVELOPER'S GUIDE

5.1 Developers Guide

This is the developers guide for masci-tools

5.1.1 Updating or adapting the Fleur Parsers

Each input and output file for Fleur has a correspong XML-Schema, where the structure of these files are defined.

To be able to parse such files efficiently and without hardcoding their structure we extract all necessary information about the schemas in the modules under *fleur_schema*. The resulting python dictionaries can be accessed via the classes *InputSchemaDict* and *OutputSchemaDict*. The easiest way to instantiate one of these objects is to use the *fromVersion()* or *fromVersion()* methods by providing the desired version string.

5.1.1.1 Adding/modifying a Fleur Schema:

The command `masci-tools fleur-schema add <path-to-schema-file>` can be used to add the schema to the repository. If the schema for the specified version already exists an error is raised. To ignore this error the option `--overwrite` can be used.

5.1.1.2 Adapting the outxml_parser:

In contrast to the input file parser *inpxml_parser()*, which parses all information available, the *outxml_parser()* has to be more flexible. The out file has much more information which might not be always useful for users. Therefore the selection of what is parsed has to be much more specific.

This selection is expressed in the context of tasks. In general this corresponds to things like:

- Total energy
- Charge density distances
- Magnetic moments
- and so on ...

These are expressed in a definition in form of a dictionary. Below a simple example (Total energy) is shown, which parses the `` `value` `` and `` `units` `` attribute of the `` `totalEnergy` `` tag. The hardcoded known parsing tasks can be found in *default_parse_tasks*

```
total_energy_definition = {
    'energy_hartree': {
        'parse_type': 'singleValue',
        'path_spec': {
            'name': 'totalEnergy'
        }
    },
}
```

The definition of a task can consist of multiple keys (in this case only `energy_hartree`), which by default correspond to the keys in the resulting output dictionary. Each key has to contain the `parse_type` and `path_spec` key. The `parse_type` defines the method used to extract the information.

The following are possible:

attrib Will parse the value of the given attribute

text Will parse the text of the given tag

numberNodes Will return the number of nodes for the given tag

exists Will return, whether the given tag exists

attrib_exists Will return, whether the given attribute exists

allAttribs Will parse all known attributes at the given tag into a dictionary

parentAttribs Will parse all known attributes at the given tag into a dictionary, but for the parent of the tag

singleValue Special case of allAttribs to parse value and units attribute for the given tag

The `path_spec` key specifies how the key can be uniquely identified.

It can contain the following specifications:

name Name of the wanted tag/attribute

contains A phrase, which has to occur in the path

not_contains A phrase, which has to not occur in the path

exclude list of str. Only valid for attributes (these are sorted into different categories `unique`, `unique_path` and `other`). This attribute can exclude one or more of these categories

All except the `name` key are optional and should be constructed so that there is only one possible choice. Otherwise an exception is raised. There are other keywords, which can be entered here. These control how the parsed data is entered into the output dictionary. For a definition of these keywords, please refer to *default_parse_tasks*.

Each task can also contain a number of control keys, determining when to peform the tasks. Each of these keys begins with an underscore. All of these are optional. The following are valid:

_general bool, if True (default False) the task is not performed for each iteration but once on the root of the file

_minimal bool, if True the task is peformed even when `minimal_mode = True` is given

_modes list of tuples specifying requirements on the `fleur_modes` for the task. For example `[('jspins', 2), ('soc', True)]` will only perform the task for a magnetic SOC calculation

_conversions list of str, giving the names of functions to call after this task. Functions given here have to be decorated with the *conversion_function()* decorator

_special bool, if True (default False) this task is NEVER added automatically and has to be added by hand

5.1.1.3 Migrating the parsing tasks

These task definitions might have to be adapted for new fleur versions. Some changes might be possible to make in *default_parse_tasks* directly without breaking backwards compatibility. If this is not possible there is a decorator *register_migration()* to define a function that is recognized by the class *ParseTasks* to convert between versions. A usage example is shown below.

```
from masci_tools.util.parse_tasks_decorators import register_migration
import copy

@register_migration(base_version='0.33', target_version='0.34')
def migrate_033_to034(definition_dict):
  """
  Ficticious migration from 0.33 to 0.34
  Moves the `number_of_atom_types` attribute from reading a simple
  attribute to counting the number of atomGroups in the input section
  And removes orbital_magnetic_moments task
  """

  #IMPORTANT: First copy the original dict
  new_dict = copy.deepcopy(definition_dict)

  #If a task is incompatible remove it from the defintion_dict
  new_dict.pop('orbital_magnetic_moments')

  new_dict['general_out_info'].pop('number_of_atom_types')
  new_dict['general_inp_info']['number_of_atom_types'] = {
      'parse_type': 'numberNodes',
      'path_spec': {
          'name': 'atomGroup'
      }
  }

  return new_dict
```

5.1.2 Using the `Plotter` class

5.1.2.1 Description

The *Plotter* class aims to provide a framework, which can be used to handle default values and collect common codeblocks needed for different plotting frameworks.

The *Plotter* class is a base class that should be subclassed for different Plotting backends. See *MatplotlibPlotter* or *BokehPlotter* for examples. The Subclass provides a dictionary of all the keys that should be handled by the plotter class. The Plotter class provides a hierachy of overwriting these parameters (Higher numbers take precedence).

1. Function defaults set with *set_defaults()* with `default_type='function'`
2. Global defaults set with *set_defaults()*
3. Parameters set with *set_parameters()*

The subclasses should then also provide the plotting backend specific useful code snippets. For example showing colorbars, legends, and so on ...

For a list of these functions you can look at the respective documentation (*MatplotlibPlotter* or *BokehPlotter*)

5.1.2.2 Writing a plotting function

In the following we will go through a few examples of how to write a simple plotting function using the *Plotter* class. We will be focusing on the *MatplotlibPlotter*, but all of this is very similar for other plotting backends.

Local instance

Even though the *Plotter* class is meant to be used globally or on the module level, it can also be useful locally for simplifying simple plotting scripts. Here we have a example of a function producing a single plot with the given data for the x and y coordinates.

```
def plot_with_defaults(x,y,**kwargs):
   from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter

   #First we instantiate the MatplotlibPlotter class
   plot_params = MatplotlibPlotter()

   #Now we process the given arguments
   plot_params.set_parameters(**kwargs)

   #Set up the axis, on which to plot the data
   ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

   #The plot_kwargs provides a way to get the keyword arguments for the
   #actual plotting call to `plot` in this case.
   plot_kwargs = plot_params.plot_kwargs()

   ax.plot(x, y, **plot_kwargs)

   #The MatplotlibPlotter has a lot of small helper functions
   #In this case we just want to set the limits and scale of the
   #axis if they were given
   plot_params.set_scale(ax)
   plot_params.set_limits(ax)

   return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

#Some examples
plot_with_defaults(x, y)
plot_with_defaults(x, y, limits={'x': (0,1)})
plot_with_defaults(x, y, marker='s', markersize=20)
```

Global/Module level instance

The local instance already gives us reusable code snippets to avoid common pitfalls when doing matplotlib/bokeh plots. But when instantiating the *Plotter* class locally we have no way of letting the user modify the global defaults.

However, when handling global state we need to be careful to not leave the instance of the *Plotter* class in an inconsistent state. If an error is thrown inside the plotting routine the parameters would stay set and may lead to very unexpected results. For this reason every plotting function using a global or module level instance of these plotters should be decorated with the *ensure_plotter_consistency()* decorator. This does two things:

1. If an error occurs in the decorated function the parameters will be reset before the error is raised
2. It makes sure that nothing inside the plotting routine changed the user defined defaults

Let us take the previous example and convert it to use a global instance

```
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency

#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

#The decorator needs to get the plotter object
#that is used inside the function
@ensure_plotter_consistency(plot_params)
def plot_with_defaults(x,y,**kwargs):

   #Now we process the given arguments
   plot_params.set_parameters(**kwargs)

   #Set up the axis, on which to plot the data
   ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

   #The plot_kwargs provides a way to get the keyword arguments for the
   #actual plotting call to `plot` in this case.
   plot_kwargs = plot_params.plot_kwargs()

   ax.plot(x, y, **plot_kwargs)

   #The MatplotlibPlotter has a lot of small helper functions
   #In this case we just want to set the limits and scale of the
   #axis if they were given
   plot_params.set_scale(ax)
   plot_params.set_limits(ax)

   return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

#Some examples
plot_with_defaults(x, y)
plot_params.set_defaults(marker='s', markersize=20)
```

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```
plot_with_defaults(x, y, limits={'x': (0,1)})
plot_with_defaults(x, y)
```

The *masci_tools.vis.parameters.Plotter.set_defaults()* method is exposed in the two main modules for plotting *masci_tools.vis.plot_methods* *masci_tools.vis.bokeh_plots* as the functions *masci_tools.vis.plot_methods.set_mpl_plot_defaults()* and *masci_tools.vis.bokeh_plots.set_bokeh_plot_defaults()* specific to the plotter instance that is used in these modules.

Function defaults

Some functions may want to set function specific defaults, that make sense inside the function, but may not be useful globally. The following example sets the default `linewidth` for our function to 6.

Note: Function defaults are also reset by the *ensure_plotter_consistency()* decorator, when the plotting function terminates successfully or in an error

---

```python
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency

#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

#The decorator needs to get the plotter object
#that is used inside the function
@ensure_plotter_consistency(plot_params)
def plot_with_defaults(x,y,**kwargs):

    #Set the function defaults
    plot_params.set_defaults(default_type='function', linewidth=6)

    #Now we process the given arguments
    plot_params.set_parameters(**kwargs)

    #Set up the axis, on which to plot the data
    ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

    #The plot_kwargs provides a way to get the keyword arguments for the
    #actual plotting call to `plot` in this case.
    plot_kwargs = plot_params.plot_kwargs()

    ax.plot(x, y, **plot_kwargs)

    #The MatplotlibPlotter has a lot of small helper functions
    #In this case we just want to set the limits and scale of the
    #axis if they were given
    plot_params.set_scale(ax)
    plot_params.set_limits(ax)

    return ax
```

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```
import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

#Some examples
plot_with_defaults(x, y)
plot_params.set_defaults(marker='s', markersize=20)
plot_with_defaults(x, y, limits={'x': (0,1)})
plot_with_defaults(x, y)
```

Passing keyword arguments directly to plot calls

The plotter classes have a restricted set of keys that they recognize as valid parameters. This set is of course not complete, since there is a vast number of parameters you can set for all plotting backends. In our previous examples unknown keys will immediately lead to an error in the call to *set_parameters()*. To enable this functionality we can provide the `continue_on_error=True` as an argument to this method.

Then the unknown keys are ignored and are returned in a dictionary. Additionally you can explicitly bypass the plotter object if you provide arguments in a dictionary with the name `extra_kwargs` it will be ignored, unpacked and returned along with the unknown keys

Warning: Be careful with the this feature and especially the `extra_kwargs`, since there is no check for name clashes with this argument. You might also run into situations, where arguments of different names collide with arguments provided by the *Plotter*

```
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency

#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

#The decorator needs to get the plotter object
#that is used inside the function
@ensure_plotter_consistency(plot_params)
def plot_with_defaults(x,y,**kwargs):

    #Set the function defaults
    plot_params.set_defaults(default_type='function', linewidth=6)

    #Now we process the given arguments (unknown ones are returned)
    kwargs = plot_params.set_parameters(continue_on_error=True, **kwargs)

    #Set up the axis, on which to plot the data
    ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

    #The plot_kwargs provides a way to get the keyword arguments for the
    #actual plotting call to `plot` in this case.
    plot_kwargs = plot_params.plot_kwargs()
```

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```
    ax.plot(x, y, **plot_kwargs, **kwargs)

    #The MatplotlibPlotter has a lot of small helper functions
    #In this case we just want to set the limits and scale of the
    #axis if they were given
    plot_params.set_scale(ax)
    plot_params.set_limits(ax)

    return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

#The key markerfacecolor is not known to the MatplotlibPlotter
plot_with_defaults(x, y, markerfacecolor='red', markersize=20)
```

Multiple plotting calls

The plotter classes also provide support for multiple plotting calls with different data sets in a single plotting function. To enable this feature we need to set two properties on the *masci_tools.vis.parameters.Plotter*; `single_plot` to *False* ` and `num_plots` to the number of plot calls made in this function. The plot specific parameters can then be specified in two ways. Shown behind the two ways is the way to set the color of the second data set to `red`.

1. List of values (`None` for unspecified values) `[None,'red']`
2. Dict with integer indices for the specified values `{1:  'red'}`

Unspecified values are replaced with the previously set defaults.

Note: The `num_plots` and `single_plot` properties are also reset by the *ensure_plotter_consistency()*

```
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency

#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

#The decorator needs to get the plotter object
#that is used inside the function
@ensure_plotter_consistency(plot_params)
def plot_2lines_with_defaults(x,y,**kwargs):

    plot_params.single_plot = False
    plot_params.num_plots = 2

    #Set the function defaults
    plot_params.set_defaults(default_type='function', linewidth=6)
```

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```
    #Now we process the given arguments (unknown ones are returned)
    kwargs = plot_params.set_parameters(continue_on_error=True, **kwargs)

    #Set up the axis, on which to plot the data
    ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

    #The plot_kwargs provides a way to get the keyword arguments for the
    #actual plotting call to `plot` in this case.
    #For multiple plots this will be a list of dicts
    #of length `num_plots`
    plot_kwargs = plot_params.plot_kwargs()

    ax.plot(x[0], y[0], **plot_kwargs[0], **kwargs)
    ax.plot(x[1], y[1], **plot_kwargs[1], **kwargs)

    #The MatplotlibPlotter has a lot of small helper functions
    #In this case we just want to set the limits and scale of the
    #axis if they were given
    plot_params.set_scale(ax)
    plot_params.set_limits(ax)

    return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2
y2 = x**3

#The key markerfacecolor is not known to the MatplotlibPlotter
plot_2lines_with_defaults([x,x], [y,y2])
plot_2lines_with_defaults([x,x], [y,y2],
                          color={1:'red'}, linestyle=['--',None])
```

Custom function specific parameters

You might have situations, where you want to have some function specific parameters, that should pull from the previously set defaults or even a custom default value.

The *add_parameter()* method is implemented exactly for this purpose. It creates a new key to be handled by the plotter class and with the arguments `default_from` or `default_value` we can specify what the defaults should be. `default_value` sets a specific value, `default_from` specifies a key from the plotter class from which to take the default value.

The *plot_kwargs()* method then can take keyword arguments to replace the arguments to take with your custom parameters

---

Note: These added parameters live on the function defaults and parameters level, meaning they will be removed by the *ensure_plotter_consistency()* decorator after the function finishes

---

```python
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency

#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

#The decorator needs to get the plotter object
#that is used inside the function
@ensure_plotter_consistency(plot_params)
def plot_shifted_with_defaults(x,y,**kwargs):

   #Set the function defaults
   plot_params.set_defaults(default_type='function', linewidth=6)

   plot_params.add_parameter('linestyle_shifted',
                             default_from='linestyle')

   #Now we process the given arguments (unknown ones are returned)
   kwargs = plot_params.set_parameters(continue_on_error=True, **kwargs)

   #Set up the axis, on which to plot the data
   ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

   #The plot_kwargs provides a way to get the keyword arguments for the
   #actual plotting call to `plot` in this case.
   plot_kwargs = plot_params.plot_kwargs()
   ax.plot(x, y, **plot_kwargs, **kwargs)

   #This call replaces the parameter linestyle with our custom
   #parameter linestyle_shifted
   plot_kwargs = plot_params.plot_kwargs(linestyle='linestyle_shifted')
   ax.plot(x, y+2, **plot_kwargs, **kwargs)

   #The MatplotlibPlotter has a lot of small helper functions
   #In this case we just want to set the limits and scale of the
   #axis if they were given
   plot_params.set_scale(ax)
   plot_params.set_limits(ax)

   return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

plot_shifted_with_defaults(x, y)
plot_shifted_with_defaults(x, y, linestyle_shifted='--')
```

Nested plotting functions

More complex plotting routines might want to call other plotting routines to simplify their structure. However, this has a side-effect when working with the *Plotter* class and the *ensure_plotter_consistency()* decorator. Since the decorator resets the parameters and function defaults after a plotting function has been called you lose everything that you might have modified in the enclosing plotting function.

If you do need access to these parameters after calling a nested plotting function the *NestedPlotParameters()* contextmanager is implemented. It defines a local scope, in which a plotting function can change the parameters and function defaults. After exiting the local scope the parameters and function defaults are always in the same state as when the `with` block was entered (Even if an error is raised). The nested plotting function will also start with the state that was set before.

Usage is shown here:

```
from masci_tools.vis.matplotlib_plotter import MatplotlibPlotter
from masci_tools.vis import ensure_plotter_consistency
from masci_tools.vis import NestedPlotParameters


#First we instantiate the MatplotlibPlotter class
plot_params = MatplotlibPlotter()

@ensure_plotter_consistency(plot_params)
def nested_plot_function(x, y, **kwargs):

   plot_params.set_defaults(default_type='function',
                            linewidth=10, linestyle='--')

   #The contextmanager also needs a reference to the plotter object
   #to manage
   with NestedPlotParameters(plot_params):
      ax = plot_with_defaults(x,y,**kwargs)

   #Will plot with the above set defaults
   plot_kwargs = plot_params.plot_kwargs()
   ax.plot(x, y+2, **plot_kwargs)

@ensure_plotter_consistency(plot_params)
def plot_with_defaults(x,y,**kwargs):

   #Set the function defaults
   plot_params.set_defaults(default_type='function', linewidth=6)

   #Now we process the given arguments
   plot_params.set_parameters(**kwargs)

   #Set up the axis, on which to plot the data
   ax = plot_params.prepare_plot(xlabel='X', ylabel='Y', title='Single Scatterplot')

   #The plot_kwargs provides a way to get the keyword arguments for the
   #actual plotting call to `plot` in this case.
   plot_kwargs = plot_params.plot_kwargs()
```

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```
    ax.plot(x, y, **plot_kwargs)

    #The MatplotlibPlotter has a lot of small helper functions
    #In this case we just want to set the limits and scale of the
    #axis if they were given
    plot_params.set_scale(ax)
    plot_params.set_limits(ax)

    return ax

import numpy as np

x = np.linspace(-1, 1, 10)
y = x**2

nested_plot_function(x, y)
nested_plot_function(x, y, linewidth=1)
```

5.1.3 Using the `PlotData` class

5.1.3.1 Description

The *PlotData* class simplifies supporting data to plotting functions in multiple ways, while keeping the plotting functions themselves simple and easy to understand.

The basic idea of *PlotData* is to mimic the behaviour of the `data` argument in matplotlib or the `source` argument in bokeh. Suppose we have our data for a plot in a dictionary `d`, which has the keys `x`, `y1` and `y2`. If we now want to plot both `y` keys against `x` we can do this in the following way.

```
from masci_tools.vis.data import PlotData

plot_data = PlotData(d, x='x', y=['y1', 'y2'])

for entry, source in plot_data.items():
    #entry has the keys needed to get the data from the source
    #and source is the mapping to use

    print(entry.x, entry.y) #Yields x, y1 in the first loop and x, y2 in the second

    #Now we can plot the data
    #for example plt.plot(entry.x, entry.y, data=source)
```

The keys are automatically expanded to be of the same length, if this is possible. There are three iteration modes, with the same names as for dicts:

- `keys`: Yields `namedtuple` with the keys for each plot
- `values`: Yields `namedtuple` with the values corresponding to the keys for each plot
- `items`: Yields the `keys` and their corresponding mapping for each plot

All of these functions have an argument `first`, which will only return the first element if it is given as `True`.

Note: The names `x` and `y` in the example above are completely arbitrary. The names for the columns and the fields on the `namedtuple` are determined by the keyword arguments given to *PlotData* at initialization

Note: At the moment the types of mappings accepted in the *PlotData* class are limited to `dict`, `pd.DataFrame` and `ColumnDataSource` (bokeh) objects

5.1.3.2 Initializing `PlotData` without a mapping

Users might want to provide data directly as arrays. If this should be allowed, there is a function *process_data_arguments()* to allow for this option. This function can either take a `data` argument with a mapping and the same keyword arguments as the *PlotData*.

```
from masci_tools.vis.data import process_data_arguments

plot_data = process_data_arguments(data=d, x='x', y=['y1','y2'])
```

Or you can provide the arrays directly without a `data` argument

```
from masci_tools.vis.data import process_data_arguments

#x,y1,y2 are the actual arrays
plot_data = process_data_arguments(x=x, y=[y1,y2])
```

If no `data` argument is given the keyword arguments are assumed to contain the data and they will be processed according to th

1. If the data is a multidimensional array (list of lists, etc.) and it is not forbidden by the given argument the first dimension of the array is iterated over and interpreted as separate entries (if the data was previously split up into multiple sets a length check is performed)
2. If the data is a one-dimensional array and of a different length than the number of defined data sets it is added to all previously existing entries
3. If the data is a one-dimensional array and of the same length as the number of defined data sets each entry is added to the corresponding data set

Note: List or array in this context refers to `list`, `np.array` and `pd.Series`

5.1.3.3 Available routines on `PlotData`

There are a couple of routines for mutating/copyying or getting information about the data in a *PlotData* instance. These are not meant to be used heavily and should be used for typical simple work done for plot data processing, i.e. scaling, shifting, getting limits, ...

Note: The term data key in the following section refers to the keys of the keyword arguments given to *PlotData* at initialization or the fields on the namedtuples returned by iterating over an instance

- *get_keys()*: Get all the keys for a given data key in a list

- *get_values()*: Get all the values for a given data key in a list
- *min()*: Get the minimum value for a given data key. A mask can be passed to further select the data. If `separate=True` is passed a list of minimum values for each plot is returned
- *max()*: Get the maximum value for a given data key. A mask can be passed to further select the data. If `separate=True` is passed a list of maximum values for each plot is returned
- *apply()*: Apply a lambda function to transform the data of a given data key (in-place!!)
- *get_function_result()*: Apply a function to a given data key and return the results (Does not change the data)
- *sort_data()*: Sort the data by the given data keys
- *group_data()*: Group the data by the given data keys
- *shift_data()*: Shift the data of a given data key either globally or with different shifts for each plot
- *copy_data()*: Copy data to a of one data key to a new data key
- *distinct_datasets()*: Return how many different datasets exist for a given data key

Warning: The methods *sort_data()* and *group_data()* will always convert the data sources to `pd.DataFrame` objects if they are not already.

CHAPTER

SIX

MODULE REFERENCE (API)

6.1 Source code Documentation (API reference)

6.1.1 Visualisation and Plotting

6.1.1.1 Fleur specific Plotting

Plotting routine for fleur density of states and bandstructures

masci_tools.vis.fleur.**plot_fleur_bands**(*bandsdata*, *bandsattributes*, *spinpol=True*, *only_spin=None*, *backend=None*, *weight=None*, ***kwargs*)

Plot the bandstructure previously extracted from a *banddos.hdf* via the *HDF5Reader*

This routine expects datasets and attributes read in with a *FleurBands* recipe from *recipes* or something producing equivalent data

Parameters

- **bandsdata** – dataset dict produced by the *FleurBands* recipe
- **attributes** – attributes dict produced by the *FleurBands* recipe
- **spinpol** – bool, if True (default) use the plot for spin-polarized bands if the data is spin-polarized
- **only_spin** – optional str, if given only the speicified spin components are plotted
- **backend** – specify which plotting library to use ('matplotlib' or 'bokeh')
- **weight** – str, name of the weight (without spin suffix *_up* or *_dn*) you want to emphasize

All other Kwargs are passed on to the underlying plot routines

- Matplotlib: *plot_bands()*, *plot_spinpol_bands()*
- Bokeh: *bokeh_bands()*, *bokeh_spinpol_bands()*

masci_tools.vis.fleur.**plot_fleur_bands_characterize**(*bandsdata*, *bandsattributes*, *weight_names*, *weight_colors*, *spinpol=True*, *only_spin=None*, *backend=None*, ***kwargs*)

Plot the bandstructure previously extracted from a *banddos.hdf* via the *HDF5Reader* with points colored according to the maximum weight from a selection of weights. Can be used to show what character dominates each band

This routine expects datasets and attributes read in with a *FleurBands* recipe from *recipes* or something producing equivalent data

Parameters

- **bandsdata** – dataset dict produced by the *FleurBands* recipe
- **attributes** – attributes dict produced by the *FleurBands* recipe
- **weight_names** – list of str with the names of the weights that should be considered in the characterization
- **weight_color** – list of colors associated with each weight. If spin-polarized bandstructures should be shown with different colors the list should be twice as long as the weights
- **spinpol** – bool, if True (default) use the plot for spin-polarized bands if the data is spin-polarized
- **only_spin** – optional str, if given only the speicified spin components are plotted
- **backend** – specify which plotting library to use ('matplotlib' or 'bokeh')

All other Kwargs are passed on to *plot_fleur_bands()*

masci_tools.vis.fleur.**plot_fleur_dos**(*dosdata*, *attributes*, *spinpol=True*, *multiply_by_equiv_atoms=True*, *plot_keys=None*, *show_total=True*, *show_interstitial=True*, *show_sym=False*, *show_atoms='all'*, *show_lresolved=None*, *key_mask=None*, *backend=None*, ***kwargs*)

Plot the density of states previously extracted from a *banddos.hdf* via the *HDF5Reader*

This routine expects datasets and attributes read in with the *FleurDOS* (Or related DOS modes) recipe from *recipes* or something producing equivalent data

The limits for the axes can be specified either with `x` and `y` or `energy` and `dos`. Mixing the two options is not possible

Parameters

- **dosdata** – dataset dict produced by the *FleurDOS* recipe
- **attributes** – attributes dict produced by the *FleurDOS* recipe
- **spinpol** – bool, if True (default) use the plot for spin-polarized dos if the data is spin-polarized
- **backend** – specify which plotting library to use ('matplotlib' or 'bokeh')

Arguments for selecting the DOS components to plot:

param plot_keys optional str list of str, defines the labels you want to plot

param show_total bool, if True (default) the total DOS is shown

param show_interstitial bool, if True (default) the interstitial DOS is shown

param show_atoms either 'all', None, or int or list of ints, defines, which total atom projections to show

param show_atoms either 'all', None, or int or list of ints, defines, which total atom projections to show

param key_mask list of bools of the same length as the number of datasets, alternative way to specify, which entries to plot

All other Kwargs are passed on to the underlying plot routines

- Matplotlib: *plot_dos()*, *plot_spinpol_dos()*
- Bokeh: *bokeh_dos()*, *bokeh_spinpol_dos()*

masci_tools.vis.fleur.**sum_weights_over_atoms**(*data*, *attributes*, *atoms_to_sum*, *entry_name*)
Create sums of atom components over specified atoms. They are entered with the same suffixes as in the original data, but with the given entry_name as prefix

Parameters

- **data** – datasets dict produced by the HDF5Reader with a recipe for DOS or bandstructure
- **attributes** – attributes dict produced by the HDF5Reader with a recipe for DOS or bandstructure
- **atoms_to_sum** – list of ints for the atoms, which should be summed
- **entry_name** – str prefix to be entered for the summed entries

Returns dict with the summed entries

6.1.1.2 KKR specific Plotting

masci_tools.vis.kkr_plot_FS_qdos.**FSqdos2D**(*p0='./'*, *totonly=True*, *s=20*, *ls_ef=':'*, *lw_ef=1*, *color=''*, *reload_data=False*, *clrbar=True*, *atoms=[]*, *ax=None*, *nosave=False*, *noalat=False*, *cmap=<matplotlib.colors.LinearSegmentedColormap object>*, *noplot=False*, *return_data=False*, *pclrmesh=False*, *logscale=True*, *ef=None*)
plotting routine for dos files

dispersionplot function for plotting KKR bandstructures (i.e. qdos) files

masci_tools.vis.kkr_plot_bandstruc_qdos.**dispersionplot**(*p0='./'*, *totonly=True*, *s=20*, *ls_ef=':'*, *lw_ef=1*, *units='eV_rel'*, *noefline=False*, *color=''*, *reload_data=False*, *clrbar=True*, *logscale=True*, *nosave=False*, *atoms=None*, *ratios=False*, *atoms2=None*, *noscale=False*, *newfig=False*, *cmap=None*, *alpha=1.0*, *qcomponent=- 2*, *clims=None*, *xscale=1.0*, *raster=True*, *atoms3=None*, *alpha_reverse=False*, *return_data=False*, *xshift=0.0*, *yshift=0.0*, *plotmode='pcolor'*, *ptitle=None*, *ef=None*, *as_e_dimension=None*, *scale_alpha_data=False*, *shading='gouraud'*)
plotting routine for qdos files - dispersion (E vs. q)

masci_tools.vis.kkr_plot_dos.**dosplot**(*p0='./'*, *totonly=True*, *color=''*, *label=''*, *marker=''*, *lw=2*, *ms=5*, *ls='-'*, *ls_ef=':'*, *lw_ef=1*, *units='Ry'*, *noefline=False*, *interpol=False*, *allatoms=False*, *onespin=False*, *atoms=[]*, *lmdos=False*, *lm=[]*, *nofig=False*, *scale=1.0*, *shift=0*, *normalized=False*, *xyswitch=False*, *efcolor=''*, *return_data=False*, *xscale=1.0*, *xshift=0.0*, *yshift=0.0*, *filled=False*, *spins=2*)
plotting routine for dos files

masci_tools.vis.kkr_plot_shapefun.**change_zoom**(*ax*, *zoom_range*, *center=[0, 0, 0]*)
Change the zoom of a 3d plot

Author Philipp Ruessmann

Parameters

- **ax** – axis which is zoomed
- **zoom_range** – range to which the image is zoomed, total range from center-zoom_range to center+zoom_range
- **center** – center of the zoomed region (optional, defaults to origin)

masci_tools.vis.kkr_plot_shapefun.**plot_shapefun**(*pos*, *out*, *mode*)
Creates a simple matplotlib image to show the shapefunctions given it's positions in the unit cell, the atoms's vertices in *ut* and the plotting mode

Author Philipp Ruessmann

Parameters

- **pos** – positions of the centers of the cells
- **verts** – array of vertices of the shapefunction (outlines of shapes)
- **mode** – 'all' or 'single' determines whether or not all shapes are combined in a single figure or plotted as individual figures

Returns ax return the axis in which the plot was done (useful to pass to 'change_zoom' and 'zoom_in' functions of this module

masci_tools.vis.kkr_plot_shapefun.**zoom_in**(*ax*, *atm*, *pos*, *zoom_range=10*)
Zoom into shapefun of a single atom

Author Philipp Ruessmann

Parameters

- **ax** – axis in which shapefun plot is found
- **atm** – atom index whose shapefunction is zoomed
- **pos** – array of positions of centers of the shapes (needed to shift center of zommed region to correct atom
- **zoom_range** – range of the zoomed region (optional, defaults to 10)

6.1.1.3 General Plotting

Here basic functionality is provided for setting default parameters for plotting and ensuring consistent values for these

masci_tools.vis.parameters.**NestedPlotParameters**(*plotter_object*)
Contextmanager for nested plot function calls Will reset function defaults and parameters to previous values after exiting

Parameters **plotter_object** – Plotter instance

class masci_tools.vis.parameters.**Plotter**(*default_parameters*, *general_keys=None*, *key_descriptions=None*, ***kwargs*)
Base class for handling parameters for plotting methods. For different plotting backends a subclass can be created to represent the specific parameters of the backend.

Parameters

- **default_parameters** – dict with hardcoded default parameters
- **general_keys** – set of str optional, defines parameters which are not allowed to change for each entry in the plot data

Kwargs in the __init__ method are forwarded to *Plotter.set_defaults()* to change the current defaults away from the hardcoded parameters.

The Plotter class creates a hierachy of dictionaries for lookups on this object utilizing the *ChainMap* from the *collections* module.

The hierachy is as follows (First entries take precedence over later entries):

- *parameters*: set by *set_parameters()* (usually arguments passed into function)
- *user defaults*: set by *set_defaults()*
- *function defaults*: set by *set_defaults()* with *default_type='function'*
- *global defaults*: Hardcoded as fallback

Only the *parameters* can represent parameters for multiple sets of plot calls. All others are used as fallback for specifying non-specified values for single plots

The current parameters can be accessed by bracket indexing the class. A example of this is shown below.

```
parameter_dict = {'fontsize': 16, 'linestyle': '-'}

params = Plotter(parameter_dict)

#Accessing a parameter
print(params['fontsize']) # 16

#Modifying a parameter
params['fontsize'] = 20
print(params['fontsize']) # 20

#Creating a parameter set for multiple plots

#1. Set the properties to the correct values
params.single_plot = False
params.num_plots = 3

#2. Now we can set a property either by providing a list or a integer indexed dict
#   Both of the following examples set the linestyle of the second and third plot␣
↪to '--'
params['linestyle'] = [None, '--', '--']
params['linestyle'] = {1: '--', 2: '--'}

# Not specified values are replaced with the default value for a single plot
print(params['linestyle']) # ['-', '--', '--']

#In lists properties can also be indexed via tuples
print(params[('linestyle', 0)]) # '-'
print(params[('linestyle', 1)]) # '--'

#Changes to the parameters and properties are reset
params.reset_parameters()

print(params['linestyle']) # '-'
```

add_parameter(*name*, *default_from=None*, *default_val=None*)
Add a new parameter to the parameters dictionary.

Parameters

- **name** – str name of the parameter
- **default_from** – str (optional), if given a entry is created in the curent defaults with the name and the default value of the key *default_from*

static convert_to_complete_list(*given_value*, *single_plot*, *num_plots*, *default=None*, *key=''*)
Converts given value to list with length num_plots with None for the non-specified values

Parameters

- **given_value** – value passed in, for multiple plots either list or dict with integer keys
- **single_plot** – bool, if True only a single parameter is allowed
- **num_plots** – int, if single_plot is False this defines the number of plots
- **default** – default value for unspecified entries
- **key** – str of the key to process

static dict_of_lists_to_list_of_dicts(*dict_of_lists*, *single_plot*, *num_plots*, *repeat_after=None*, *ignore_repeat=None*)
Converts dict of lists and single values to list of length num_plots or single dict for single_plot=True

Parameters

- **dict_of_lists** – dict to be converted
- **single_plot** – boolean, if True only a single parameter set is allowed
- **num_plots** – int of the number of allowed plots

Returns list of dicts

expand_parameters(*original_length*, ***kwargs*)
Expand parameters to a bigger number of plots. New length has to be a multiple of original length. Only lists of length <= orginal_length are expanded. Also expands function defaults

Parameters

- **orginal_length** – int of the old length
- **kwargs** – arguments to expand

Returns expanded kwargs

get_description(*key*)
Get the description of the given key

Parameters **key** – str of the key, for which the description should be printed

get_dict()
Return the dictionary of the current defaults. For use of printing

get_multiple_kwargs(*keys*, *ignore=None*)
Get multiple parameters and return them in a dictionary

Parameters

- **keys** – set of keys to process
- **ignore** – str or list of str (optional), defines keys to ignore in the creation of the dict

is_general(*key*)
Return, whether the key is general (meaning only related to the whole plots)

Parameters **key** – str of the key to check

Returns bool, whether the key is general

load_defaults(*filename='plot_defaults.json'*)
Load defaults from a json file.

Parameters **filename** – filename,from where the defaults should be taken

property num_plots
Integer property for number of plots produced

remove_added_parameters()
Remove the parameters added via *Plotter.add_parameter()*

reset_defaults()
Resets the defaults to the hardcoded defaults in _PLOT_DEFAULTS.

reset_parameters()
Reset the parameters to the current defaults. The properties single_plot and num_plots are also set to default values

save_defaults(*filename='plot_defaults.json'*, *save_complete=False*)
Save the current defaults to a json file.

Parameters

- **filename** – filename, where the defaults should be stored
- **save_complete** – bool if True not only the overwritten user defaults but also the unmodified harcoded defaults are stored

set_defaults(*continue_on_error=False*, *default_type='global'*, ***kwargs*)
Set the current defaults. This method will only work if the parameters are not changed from the defaults. Otherwise a error is raised. This is because after changing the defaults the changes will be propagated to the parameters to ensure consistency.

Parameters **continue_on_error** – bool, if True unknown key are simply skipped

Default_type either 'global' or 'function'. Specifies, whether to set the global defaults (not reset after function) or the function defaults

Kwargs are used to set the defaults.

set_parameters(*continue_on_error=False*, ***kwargs*)
Set the current parameters.

Parameters **continue_on_error** – bool, if True unknown key are simply skipped and returned

Kwargs are used to set the defaults.

set_single_default(*key*, *value*, *default_type='global'*)
Set default value for a single key/value pair

Parameters

- **key** – str of the key to set
- **value** – value to set the key to

Default_type either 'global' or 'function'. Specifies, whether to set the global defaults (not reset after function) or the function defaults

property single_plot
Boolean property if True only a single Plot parameter set is allowed

masci_tools.vis.parameters.**ensure_plotter_consistency**(*plotter_object*)

Decorator for plot functions to ensure that the Parameters are reset even if an error occurs in the function Additionally checks are performed that the parameters are reset after execution and the defaults are never changed in a plot function

Parameters **plotter_object** – Plotter instance to be checked for consistency

This module contains classes and functions to make plotting functions more flexible with respect to the used data. This way plotting functions can both allow the flexible usage of lists, arrays directly or dataframes together with the keys that should be used

class masci_tools.vis.data.**ColumnDataSourceWrapper**(*wrapped*)

Wrapper around `bokeh.models.ColumnDataSource` to give it a `__getitem__` and `__setitem__` method

Used in the *PlotDataIterator* for easier handling of these types

class masci_tools.vis.data.**PlotData**(*data*, *use_column_source=False*, *same_length=False*, *strict_data_keys=False*, *copy_data=False*, ***kwargs*)

Class for iterating over the data in a dict or dataframe with automatic filling in of single defined keys to get a list of keys to extract.

The iteration allows for implicit definition of data for multiple plot sets, without excessive copying of the given data

Usage Example

```
from masci_tools.vis.data import PlotData
import numpy as np

#Let's say we have one energy grid and a couple of functions
#defined on this energy grid.
#We collect these in a dict

x = np.linspace(-10,10,100)
data = {'x': x, 'y1': np.sin(x), 'y2':np.cos(x), 'y3', x**2}

p = PlotData(data, x='x', y=['y1', 'y2', 'y3'])

#If we now iterate over this object it will result in the data
#for y being returned together with the x data (The same would work the other way␣
↪around)
for entry in p:
   print(entry.x) #'x' entry
   print(entry.y) #'y1' then 'y2' and finally 'y3'

#Additionally data for z, color and size can be defined
```

Parameters **data** – object or list of objects which can be bracket indexed with the given keys e.g. dicts, pandas dataframes, …

Same_length bool if True and any sources are dicts it will be checked for same dimensions in (ALL) entries (not only for keys plotted against each other)

Strict_data_keys bool if True no new data keys are allowed to be entered via *copy_data()*

Kwargs are used to specify the columns in a namedtuple If a list is given for any of the keys the data will be expanded to a list of namedtuple with the same length

add_data_key(*data_key*, *keys=None*)
Add a new column of data keys

Parameters

- **data_key** – string of the new data key to add
- **keys** – None, Index into data or list of index into the data to initialize the values to

apply(*data_key*, *lambda_func*, *apply_to_whole_array=True*, ***kwargs*)
Apply a function to a given data column for all entries

> **Warning:** This operation is done in-place. Meaning if there are multiple data entries pointing to the same data set and only one should be modified by this method, the data needs to be copied beforehand using *copy_data()*

Parameters

- **data_key** – name of the data key to apply the function
- **lambda_func** – function to apply to the data

copy_data(*data_key_from*, *data_key_to*, *prefix=None*, *rename_original=False*, *force=False*)
Copy the data for a given data key to another one

Parameters

- **data_key_from** – data key to copy from
- **data_key_to** – data key to copy to
- **prefix** – optional prefix to use for the renamed data entries. Can be used to avoid name clashes. If not given the data keys are used
- **rename_original** – optional bool (default False). If True the original entries are renamed instead of the ones under `data_key_to`

property data_keys
Return the registered data keys for this instance

distinct_datasets(*data_key*)
Return how many different data sets are present for the given data key

Parameters **data_key** – The data key to analyse

Returns int of the number of different datasets

get_function_result(*data_key*, *func*, *list_return=False*, *as_numpy_array=False*, ***kwargs*)
Apply a function to a given data column for all entries and return the results

Parameters

- **data_key** – name of the data key to apply the function to
- **func** – function to apply to the data to get the results if func is a string then it will be used to get the attribute with the corresponding name from the source and call it

get_keys(*data_key*)
Get the keys for a given data column for all entries

Parameters **data_key** – name of the data key to return the keys

Returns list of keys, corresponding to the entries for the given data in the sources

get_mask(*mask*, *data_key=None*)
Get mask list for use with the Data in this instance

Parameters

- **mask** – either list of callable, if it is callable it is used in *get_function_result()* together with the `data_key` argument
- **data_key** – str to be used for the data key if mask is a callable

:param

get_values(*data_key*)
Get the values for a given data column for all entries

Parameters **data_key** – name of the data key to return the values

Returns list of values, corresponding to the entries for the given data in the sources

group_data(*by*, ***kwargs*)
Group the data by the given data_key(s) or other arguments for groupby

Note: This function will convert the data arguments to `pd.Dataframe` objects

Parameters **by** – str or list of str of the data_keys to sort by or other valid arguments for by in `pd.Dataframe.groupby()`

Kwargs are passed on to `pd.Dataframe.groupby()`

items(*first=False*, *mappable=False*)
Iterate over PlotData items. Returns the key and corresponding source for the data

Parameters

- **first** – bool, if True only the first entry is returned
- **mappable** – bool, if True only the data ColumnDataSources are wrapped to be mappable

keys(*first=False*)
Iterate over PlotData keys. Returns the keys for the corresponding sources

Parameters **first** – bool, if True only the first entry is returned

mask_data(*mask*, *data_key=None*)
Apply a given mask to the data inplace.

Note: This function will convert the data arguments to `pd.Dataframe` objects

Parameters

- **mask** – mask rgument passed to *get_mask()*
- **data_key** – data_key argument used by *get_mask()*

max(*data_key*, *separate=False*, *mask=None*, *mask_data_key=None*)
Get the maximum value for a given data column for all entries

Parameters

- **data_key** – name of the data key to determine the maximum

- **separate** – bool if True the maximum will be determined and returned for all entries separately
- **mask** – optional mask to select specifc rows from the data entries
- **mask_data_key** – optional data key to be used when `mask` is a function

Returns maximum value for all entries either combined or as a list

min(*data_key*, *separate=False*, *mask=None*, *mask_data_key=None*)
Get the minimum value for a given data column for all entries

Parameters

- **data_key** – name of the data key to determine the minimum
- **separate** – bool if True the minimum will be determined and returned for all entries separately
- **mask** – optional mask to select specifc rows from the data entries
- **mask_data_key** – optional data key to be used when `mask` is a function

Returns minimum value for all entries either combined or as a list

shift_data(*data_key*, *shifts*, *shifted_data_key=None*, *separate_data=True*, *negative=False*)
Apply shifts to a given data column for all entries

Parameters

- **data_key** – name of the data key to shift
- **shifts** – float or array of floats with the shifts to apply
- **shifted_data_key** – optional string, if given the data will be copied to this data key
- **separate_data** – bool, if True and shifted_data_key is not given the data will be copied to itself (This separates the data for all columns)
- **negative** – bool if True the shifts are applied with a minus sign

sort_data(*by_data_keys*, ***kwargs*)
Sort the data by the given data_key(s)

Note: This function will convert the data arguments to `pd.Dataframe` objects

---

Note: If there are multiple plot sets and only one data source. This function will expand the data to be one data source sorted according to the data_keys for each plot

---

Parameters **by_data_keys** – str or list of str of the data_keys to sort by

Kwargs are passed on to `pd.Dataframe.sort_values()`

values(*first=False*)
Iterate over PlotData values. Returns the values for the data

Parameters **first** – bool, if True only the first entry is returned

class masci_tools.vis.data.**PlotDataIterator**(*plot_data*, *mode='values'*, *mappable=False*)
Class containing the iteration behaviour over the *PlotData* class. Can be used in three modes:

- *keys*: Returns the keys to be entered in the corresponding data sources for each entry

- *values*: Returns the data for each entry
- *items*: Returns the keys and the data sources in a tuple

The keys and values are always returned in a `namedtuple` with fields corresponding to the set data keys

masci_tools.vis.data.**normalize_list_or_array**(*data*, *key*, *out_data*, *flatten_np=False*, *forbid_split_up=False*)

Split up a given list/numpy array or pd.Series to be used in the plotting methods

Parameters

- **data** – The (array-like) data to be normalized
- **key** – key under which to enter the new data
- **out_data** – dict containining previously normalized data
- **flatten_np** – bool, if True multidimensional numpy arrays are flattened
- **forbid_split_up** – bool, if True multidimensional arrays are not split up

The rules are the following:

- if `data` is a multidimensional array (list of lists, etc.) and it is not forbidden by the given argument the first dimension of the array is iterated over and interpreted as separate entries (if the data was previously split up into multiple sets a length check is performed)
- if `data` is a one-dimensional array and of a different length than the number of defined data sets it is added to all previously existing entries
- if `data` is a one-dimensional array and of the same length as the number of defined data sets each entry is added to the corresponding data set

Returns list of dicts or dict containing the nomralized data

masci_tools.vis.data.**process_data_arguments**(*data=None*, *single_plot=False*, *use_column_source=False*, *flatten_np=False*, *forbid_split_up=None*, *same_length=False*, *copy_data=False*, ***kwargs*)

Initialize PlotData from np.arrays or lists of np.arrays or lists or a already given data argument, i.e. mapping

Parameters

- **data** – either None or Mapping to be used as the data in the PlotData class
- **single_plot** – bool, if True only a single dataset is allowed
- **use_column_source** – bool, if True all data arguments are converted to ColumnDataSource of bokeh
- **flatten_np** – bool, if True multidimensional numpy arrays are flattened (Only if data not given)
- **forbid_split_up** – set of keys for which not to split up multidimensional arrays
- **same_length** – bool if True and any sources are dicts it will be checked for same dimensions in (ALL) entries (not only for keys plotted against each other)
- **copy_data** – bool, if True the data argument will be copied

Kwargs define which keys belong to which data entries if data is given or they contain the data to be normalized

The following two example calls will both create a PlotData object with the same two plot data sets with the entries `x` and `y`:

```
import numpy as np

x = np.linspace(-10,10,100)
y1 = y**2
y2 = np.sin(x)

#Use a predefined data argument (a dict in this case) and the keys in the kwargs
p = process_data_arguments({'x': x, 'y1': y1, 'y2': y2}, x='x', y=['y1','y2'])

#Let the function normalize the given arrays
p = process_data_arguments=(x=x,y=[y1, y2])
```

Returns A *PlotData* object corresponding to the given data

This modules provides common plotting functions dispatching to different plotting backends. At the moment the following backends are used:

- `matplotlib` ('mpl', 'matplotlib')
- `bokeh` ('bokeh')

The underlying plotting routines collected here should have the same signature for the data arguments; keyword arguments can be different.

class masci_tools.vis.common.**PlotBackend**(*value*)

Enumeration containing the possible names for each plotting backend Initialize using the *from_str()* method

At the moment the following are supported (case-insensitive)

- `matplotlib`: either *'mpl'* or *'matplotlib'*
- `bokeh`: *'bokeh'*

static default()

Return a *PlotBackend* instance corresponding to the current default backend

static from_str(*label*)

Initialize the *PlotBackend* from a given string

Parameters **label** – str to use to initialize the backend if it is *None* the default is returned

Returns *PlotBackend* instance corresponding to the label

masci_tools.vis.common.**bands**(*kpath*, *eigenvalues*, *backend=None*, *data=None*, ***kwargs*)

Plot the provided data for a bandstructure (non spin-polarized) Non-weighted, weighted, as a line plot or scatter plot, color-mapped or fixed colors are all possible options

Parameters

- **kpath** – data for the kpoints path (flattened to 1D)
- **eigenvalues** – data for the eigenvalues
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- `matplotlib`: *plot_bands()*
- `bokeh`: *bokeh_bands()*

Returns Figure object for the used plotting backend

masci_tools.vis.common.**dos**(*energy_grid*, *dos_data*, *backend=None*, *data=None*, ***kwargs*)
Plot the provided data as a density of states (not spin-polarized). Can be done horizontally or vertical via the switch *xyswitch*

Parameters

- **energy_grid** – data for the energy grid of the DOS
- **dos_data** – data for all the DOS components to plot
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- matplotlib: *plot_dos()*
- bokeh: *bokeh_dos()*

Returns Figure object for the used plotting backend

masci_tools.vis.common.**get_help**(*key*, *backend=None*)
Get a help string for a given parameter.

Parameters

- **key** – name of the parameter to get the parameter for
- **backend** – For which backend to get the description of the parameter

masci_tools.vis.common.**get_plotter**(*backend=None*)
Get the instance of the *Plotter* subclass used for the given plotting backend

Parameters **backend** – For which backend to get the Plotter instace

masci_tools.vis.common.**line**(*xdata*, *ydata*, *backend=None*, *data=None*, ***kwargs*)
Plot the provided data as a line plot. Multiple data sets are possible

Parameters

- **xdata** – data for the x-axis
- **xdata** – data for the y-axis
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- matplotlib: *multiple_scatterplots()*
- bokeh: *bokeh_line()*

Returns Figure object for the used plotting backend

masci_tools.vis.common.**load_defaults**(*backend=None*, *filename='plot_defaults.json'*)
Load defaults for the plot parameters from a file and set the contained defaults.

Parameters

- **backend** – For which backend to save the parameters

- **filename** – str of the filename to load the defaults from

masci_tools.vis.common.**reset_defaults**(*backend=None*)
Reset the defaults for theplot parameters to the original state.

Parameters **backend** – For which backend to reset the parameters

masci_tools.vis.common.**save_defaults**(*backend=None*, *filename='plot_defaults.json'*, *save_complete=False*)
Save the defaults for the plot parameters.

Parameters

- **backend** – For which backend to save the parameters
- **filename** – str of the filename to save the defaults to
- **save_complete** – bool, if True also the hardcoded defaults are included

masci_tools.vis.common.**scatter**(*xdata*, *ydata*, *backend=None*, *data=None*, ***kwargs*)
Plot the provided data as a scatter plot. Varying size and color are possible. Multiple data sets are possible

Parameters

- **xdata** – data for the x-axis
- **xdata** – data for the y-axis
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- matplotlib: *multi_scatter_plot()*
- bokeh: *bokeh_multi_scatter()*

Returns Figure object for the used plotting backend

masci_tools.vis.common.**set_default_backend**(*backend*)
Sets the default backend used when no explicit backend is specified.

Parameters **backend** – Name of the backend to use

masci_tools.vis.common.**set_defaults**(*backend=None*, ***kwargs*)
Sets defaults for the plot parameters.

Parameters **backend** – For which backend to set the parameters

The Kwargs are used to set the parameters of the specified backend

masci_tools.vis.common.**show_defaults**(*backend=None*)
Show the current set defaults for the plot parameters.

Parameters **backend** – For which backend to show the parameters

masci_tools.vis.common.**spinpol_bands**(*kpath*, *eigenvalues_up*, *eigenvalues_dn*, *backend=None*, *data=None*, ***kwargs*)
Plot the provided data for a bandstructure (spin-polarized) Non-weighted, weighted, as a line plot or scatter plot, color-mapped or fixed colors are all possible options

Parameters

- **kpath** – data for the kpoints path (flattened to 1D)
- **eigenvalues_up** – data for the eigenvalues for spin-up

- **eigenvalues_dn** – data for the eigenvalues for spin-down
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- matplotlib: *plot_spinpol_bands()*
- bokeh: *bokeh_spinpol_bands()*

Returns Figure object for the used plotting backend

masci_tools.vis.common.**spinpol_dos**(*energy_grid*, *dos_data_up*, *dos_data_dn*, *backend=None*, *data=None*, ***kwargs*)

Plot the provided data as a density of states (spin-polarized). Can be done horizontally or vertical via the switch *xyswitch*

Parameters

- **energy_grid** – data for the energy grid of the DOS
- **dos_data_up** – data for all the DOS components to plot for spin-up
- **dos_data_dn** – data for all the DOS components to plot for spin-down
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **backend** – name of the backend to use (uses a default if None is given)

Kwargs are passed on to the backend plotting functions:

- matplotlib: *plot_spinpol_dos()*
- bokeh: *bokeh_spinpol_dos()*

Returns Figure object for the used plotting backend

Matplotlib

This module contains a subclass of *Plotter* for the matplotlib library

class masci_tools.vis.matplotlib_plotter.**MatplotlibPlotter**(***kwargs*)

Class for plotting parameters and standard code snippets for plotting with the matplotlib backend.

Kwargs in the __init__ method are forwarded to setting default values for the instance

For specific documentation about the parameter/defaults handling refer to *Plotter*.

Below the current defined default values are shown:

Table 1: Plot Parameters

Name	Description	Default value
title_fontsize	Fontsize for the title of the figure	16

continues on next page

Table 1 – continued from previous page

Name	Description	Default value
figure_kwargs	Arguments passed to *plt.figure* when creating the figure. Includes things like figsize, dpi, background color, ...	{'figsize': (8, 6), 'dpi': 100, 'facecolor': 'w', 'edgecolor': 'k', 'constrained_layout': False}
alpha	Float specifying the transparency of the title	1
axis_linewidth	Linewidth of the lines for the axis	1.5
use_axis_formatter	If True the labels will always not be formatted with an additive constant at the top	False
set_powerlimits	If True the threshold for switching to scientific notation is adjusted to 0,3	True
xticks	Positions of the ticks on the x axis	No Default
xticklabels	Labels for the ticks on the x-axis	No Default
yticks	Positions for the ticks on the y-axis	No Default
yticklabels	Labels for the ticks on the y-axis	No Default
invert_xaxis	If True the direction of the x-axis is inverted	False
invert_yaxis	If True the direction of the y-axis is inverted	False
color_cycle	If set this will override the default color cycle of matplotlib. Can be given as name of a colormap cycle or list of colors	No Default
sub_colormap	If a colormap is used this can be used to cut out a part of the colormap. For example (0.5,1.0) will only use the upper half of the colormap	No Default
linewidth	Linewidth for the plot(s)	2.0
linestyle	Linestyle for the plot(s)	-
marker	Shape of the marker to use for the plot(s)	o
markersize	Size of the markers to use in the plot(s)	4.0
color	Color to use in the plot(s)	No Default
zorder	z-position to use for the plot(s) (Is used to define fore- and background)	No Default
repeat_parameters	If set as integer the parameters for single plots (except labels) will be repeated after the given number of plots. Only implemented for multiple_scatterplots	No Default
edgecolor	Edgecolor to use in the plot(s)	No Default
facecolor	Facecolor to use in the plot(s)	No Default
plot_label	Label to use in the plot(s) for the legend	No Default
area_plot	If True fill_between(x) will be used to produce the plot(s)	False
area_vertical	Determines, whether to use fill_between or fill_betweenx for area plots	False
area_enclosing_line	If True a enclosing line will be drawn around the area	True
area_alpha	Transparency to use for the area in the area plot(s)	1.0
area_linecolor	Color for the enclosing line in the area plot(s)	No Default
plot_alpha	Transparency to use for the plot(s)	1.0
cmap	Colormap to use for scatter/pcolormesh or 3D plots	viridis
norm	If set this norm will be used to normalize data for the colormapping	No Default
shading	Shading to use for pcolormesh plots	gouraud

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Table 1 – continued from previous page

Name	Description	Default value
rasterized	Rasterize the pcolormesh when drawing vector graphics.	True
scale	Dict specifying the scales of the axis, e.g {'y': 'log'} will create a logarithmic scale on the y-axis	No Default
limits	Dict specifying the limits of the axis, e.g {'x': (-5,5)}	No Default
labelfontsize	Fontsize for the labels on the axis	15
lines	Dict specifying straight help-lines to draw. For example {'vertical': 0, 'horizontal': [-1,1]} will draw a vertical line at 0 and two horizontal at -1 and 1	No Default
line_options	Color, width, and more options for the help-lines	{'linestyle': '--', 'color': 'k', 'linewidth': 1.0}
font_options	Default font options that can be used for text annotations	{'family': 'serif', 'color': 'black', 'weight': 'normal', 'size': 16}
tick_paramsx	Parameters for major ticks on the x-axis (Size, fontsize, ...)	{'size': 4.0, 'width': 1.0, 'labelsize': 14, 'length': 5, 'labelrotation': 0}
tick_paramsy	Parameters for major ticks on the y-axis (Size, fontsize, ...)	{'size': 4.0, 'width': 1.0, 'labelsize': 14, 'length': 5, 'labelrotation': 0}
tick_paramsx_minor	Parameters for minor ticks on the x-axis (Size, fontsize, ...)	{'size': 2.0, 'width': 1.0, 'labelsize': 0, 'length': 2.5}
tick_paramsy_minor	Parameters for minor ticks on the y-axis (Size, fontsize, ...)	{'size': 2.0, 'width': 1.0, 'labelsize': 0, 'length': 2.5}

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Table 1 – continued from previous page

Name	Description	Default value
colorbar	If True and the function implements color mapping, a colorbar is shown	True
colorbar_padding	Specifies the space between plot and colorbar	0.1
legend	If True a legend for the plot is shown	False
legend_show_data_labels	If True the column names from the data argument are shown if not overwritten	False
legend_remove_duplicates	If True duplicate legend labels are removed	False
legend_options	Parameters for displaying the legend (Fontsize, location, ...)	{'fontsize': 'large', 'linewidth': 3.0, 'loc': 'best', 'fancybox': True}
save_plots	if True the plots will be saved to file	False
save_format	Formats to save the plots to, can be single or list of formats	png
save_options	Additional options for saving the plots to file	{'transparent': True}
tightlayout	If True the tight layout will be used (NOT IMPLEMENTED)	False
show	If True plt.show will be called at the end of the routine	True
save_raw_plot_data	If True the data for the plot is saved to file (NOT IMPLEMENTED)	False
raw_plot_data_format	Format in which to save the data for the plot (NOT IMPLEMENTED)	txt

draw_lines(*ax*)

Draw horizontal and vertical lines specified in the lines argument

Parameters **ax** – Axes object on which to perform the operation

plot_kwargs(*ignore=None*, *extra_keys=None*, *plot_type='default'*, *post_process=True*, *list_of_dicts=True*, ***kwargs*)

Creates a dict or list of dicts (for multiple plots) with the defined parameters for the plotting calls fo matplotlib

Parameters

- **ignore** – str or list of str (optional), defines keys to ignore in the creation of the dict
- **extra_keys** – optional set for addtional keys to retrieve
- **post_process** – bool, if True the parameters are cleaned up for inserting them directly into matplotlib plitting functions

Kwargs are used to replace values by custom parameters:

Example for using a custom markersize:

```
p = MatplotlibPlotter()
p.add_parameter('marker_custom', default_from='marker')
p.plot_kwargs(marker='marker_custom')
```

This code snippet will return the standard parameters for a plot, but the value for the marker will be taken from the key *marker_custom*

prepare_plot(*title=None*, *xlabel=None*, *ylabel=None*, *zlabel=None*, *axis=None*, *minor=False*, *projection=None*)

Prepares the figure of a matplotlib plot, setting the labels/titles, ticks, ...

Parameters

- **title** – str for the title of the figure
- **xlabel** – str for the label on the x-axis
- **ylabel** – str for the label on the y-axis
- **zlabel** – str for the label on the z-axis
- **axis** – matplotlib axes object, optional, if given the operations are performed on the object otherwise a new figure and subplot are created
- **minor** – bool, if True minor tick parameters are set
- **projection** – str, passed on to the add_subplot call

Returns the created or modified axis object

save_plot(*saveas*)

Save the current figure or show the current figure

Parameters **saveas** – str, filename for the resulting file

set_limits(*ax*)

Set limits of the axis

Parameters **ax** – Axes object on which to perform the operation

set_scale(*ax*)

Set scale of the axis (for example 'log')

Parameters **ax** – Axes object on which to perform the operation

show_colorbar(*ax*)

Print a colorbar for the plot

Parameters **ax** – Axes object on which to perform the operation

show_legend(*ax*, *leg_elems=None*)

Print a legend for the plot

Parameters **ax** – Axes object on which to perform the operation

static truncate_colormap(*cmap*, *minval=0.0*, *maxval=1.0*, *n=256*)

Cut off parts of colormap

Parameters

- **cmap** – cmap to truncate
- **minval** – minimum value of new colormap
- **maxval** – maximum value of new colormap
- **n** – number of colors in new colormap

Returns colormap truncated to only hold colors between minval and maxval from old colormap

In this module are plot routines collected to create default plots out of certain ouput nodes from certain workflows with matplot lib.

Comment: Do not use any aiida methods, otherwise the methods in here can become tricky to use inside a virtual environment. Make the user extract thing out of aiida objects before hand or write something on top. Since usually parameter nodes, or files are plotted, parse a dict or filepath.

Each of the plot_methods can take keyword arguments to modify parameters of the plots There are keywords that are handled by a special class for defaults. All other arguments will be passed on to the matplotlib plotting calls

For the definition of the defaults refer to *MatplotlibPlotter*

masci_tools.vis.plot_methods.**CDF_voigt_profile**(*x*, *fwhm_g*, *fwhm_l*, *mu*)
Cumulative distribution function of a voigt profile implementation of formula found here: https://en.wikipedia.org/wiki/Voigt_profile # TODO: is there an other way then to calc 2F2? # or is there an other way to calc the integral of wofz directly, or use different error functions.

class masci_tools.vis.plot_methods.**PDF**(*pdf*, *size=(200, 200)*)
Display a PDF file inside a Jupyter notebook.

masci_tools.vis.plot_methods.**asymmetric_lorentz**(*x*, *fwhm*, *mu*, *alpha=1.0*, *beta=1.5*)
asymetric lorentz function

L^alpha for x<=mu L^beta for x>mu See casexps LA

masci_tools.vis.plot_methods.**asymmetric_lorentz_gauss_conv**(*x*, *mu*, *fwhm_l*, *fwhm_g*, *alpha=1.0*, *beta=1.5*)
asymmetric Lorentzian with Gauss convoluted

masci_tools.vis.plot_methods.**asymmetric_lorentz_gauss_sum**(*x*, *mu*, *fwhm_l*, *fwhm_g*, *alpha=1.0*, *beta=1.5*)
asymmetric Lorentzian with Gauss convoluted

masci_tools.vis.plot_methods.**barchart**(*positions*, *heights*, ***, *width=0.35*, *xlabel='x'*, *ylabel='y'*, *title=''*, *bottom=None*, *alignment='vertical'*, *saveas='barchart'*, *bar_type='stacked'*, *axis=None*, *xerr=None*, *yerr=None*, *data=None*, *copy_data=False*, ***kwargs*)
Create a standard bar chart plot (this should be flexible enough) to do all the basic bar chart plots.

Parameters

- **positions** – arraylike data for the positions of the bars
- **heights** – arraylike data for the heights of the bars
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **width** – float determines the width of the bars
- **axis** – Axes object where to add the plot
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **xerr** – optional data for errorbar in x-direction
- **yerr** – optional data for errorbar in y-direction
- **bottom** – bottom values for the lowest end of the bars
- **bar_type** – type of the barchart plot. Either `stacked`, `grouped` or `independent`
- **alignment** – which direction the bars should be plotted (`horizontal` or `vertical`)

- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *bar*

TODO: grouped barchart (meaing not stacked)

masci_tools.vis.plot_methods.**colormesh_plot**(*xdata*, *ydata*, *cdata*, ***, *xlabel=''*, *ylabel=''*, *title=''*, *data=None*, *saveas='colormesh'*, *axis=None*, *copy_data=False*, ***kwargs*)

Create plot with pcolormesh

Parameters

- **xdata** – arraylike, data for the x coordinate
- **ydata** – arraylike, data for the y coordinate
- **cdata** – arraylike, data for the color values with a colormap
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **title** – str, title of the figure
- **saveas** – str specifying the filename (without file format)
- **axis** – Axes object, if given the plot will be applied to this object
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *pcolormesh*

masci_tools.vis.plot_methods.**construct_corelevel_spectrum**(*coreleveldict*, *natom_typesdict*, *exp_references=None*, *scale_to=- 1*, *fwhm_g=0.6*, *fwhm_l=0.1*, *energy_range=None*, *xspec=None*, *energy_grid=0.2*, *peakfunction='voigt'*, *alpha_l=1.0*, *beta_l=1.5*)

Constructrs a corelevel spectrum from a given corelevel dict

Params

Returns list: [xdata_spec, ydata_spec, ydata_single_all, xdata_all, ydata_all, xdatalabel]

masci_tools.vis.plot_methods.**default_histogram**(**args*, ***kwargs*)

Create a standard looking histogram (DEPRECATED)

masci_tools.vis.plot_methods.**doniach_sunjic**(*x*, *scale=1.0*, *E_0=0*, *gamma=1.0*, *alpha=0.0*)

Doniach Sunjic asymmetric peak function. tail to higher binding energies.

param x: list values to evaluate this function param scale: multiply the function with this factor param E_0: position of the peak param gamma, 'lifetime' broadening param alpha: 'asymmetry' parametera

See Doniach S. and Sunjic M., J. Phys. 4C31, 285 (1970) or http://www.casaxps.com/help_manual/line_shapes.htm

masci_tools.vis.plot_methods.**gauss_one**(*x*, *fwhm*, *mu*)

Returns a Lorentzian line shape at x with FWHM fwhm and mean mu

masci_tools.vis.plot_methods.**gaussian**(*x*, *fwhm*, *mu*)

Returns Gaussian line shape at x with FWHM fwhm and mean mu

masci_tools.vis.plot_methods.**get_mpl_help**(*key*)
Print the decription of the given key in the matplotlib backend

Available defaults can be seen in *MatplotlibPlotter*

masci_tools.vis.plot_methods.**histogram**(*xdata*, *density=False*, *histtype='bar'*, *align='mid'*, *orientation='vertical'*, *log=False*, *axis=None*, *title='hist'*, *xlabel='bins'*, *ylabel='counts'*, *saveas='histogram'*, *return_hist_output=False*, *data=None*, *copy_data=False*, ***kwargs*)
Create a standard looking histogram

Parameters

- **xdata** – arraylike, Data for the histogram
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **density** – bool, if True the histogram is normed and a normal distribution is plotted with the same mu and sigma as the data
- **histtype** – str, type of the histogram
- **align** – str, defines where the bars for the bins are aligned
- **orientation** – str, is the histogram vertical or horizontal
- **log** – bool, if True a logarithmic scale is used for the counts
- **axis** – Axes object where to add the plot
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **return_hist_output** – bool, if True the data output from hist will be returned
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *hist*

masci_tools.vis.plot_methods.**hyp2f2**(*a*, *b*, *z*)
Calculation of the 2F2() hypergeometric function, since it is not part of scipy with the identity 2. from here: https://en.wikipedia.org/wiki/Generalized_hypergeometric_function a, b,z array like inputs TODO: not clear to me how to do this… the identity is only useful if we mange the adjust the arguments in a way that we can use them… also maybe go for the special case we need first: 1,1,3/2;2;-z2

masci_tools.vis.plot_methods.**load_mpl_defaults**(*filename='plot_mpl_defaults.json'*)
Load defaults for the matplotlib backend from a json file.

Parameters **filename** – filename,from where the defaults should be taken

masci_tools.vis.plot_methods.**lorentzian**(*x*, *fwhm*, *mu*)
Returns a Lorentzian line shape at x with FWHM fwhm and mean mu

masci_tools.vis.plot_methods.**lorentzian_one**(*x*, *fwhm*, *mu*)
Returns a Lorentzian line shape at x with FWHM fwhm and mean mu

masci_tools.vis.plot_methods.**multi_scatter_plot**(*xdata*, *ydata*, ***, *size_data=None*, *color_data=None*, *xlabel=''*, *ylabel=''*, *title=''*, *data=None*, *saveas='mscatterplot'*, *axis=None*, *copy_data=False*, *exclude_points_outside_plot_area=False*, ***kwargs*)

Create a scatter plot with varying marker size Info: x, y, size and color data must have the same dimensions.

Parameters

- **xdata** – str or arraylike, data for the x coordinate
- **ydata** – str or arraylike, data for the y coordinate
- **size_data** – str or arraylike, data for the markersizes (optional)
- **color_data** – str or arraylike, data for the color values with a colormap (optional)
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **title** – str, title of the figure
- **data** – Mapping giving the data for the plots (required if data arguments are str)
- **saveas** – str specifying the filename (without file format)
- **axis** – Axes object, if given the plot will be applied to this object
- **xerr** – optional data for errorbar in x-direction
- **yerr** – optional data for errorbar in y-direction
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *scatter*

masci_tools.vis.plot_methods.**multiaxis_scatterplot**(*xdata*, *ydata*, ***, *axes_loc*, *xlabel=''*, *ylabel=''*, *title=''*, *num_cols=1*, *num_rows=1*, *saveas='mscatterplot'*, ***kwargs*)

Create a scatter plot with multiple axes.

Parameters

- **xdata** – list of arraylikes, passed on to the plotting functions for each axis (x-axis)
- **ydata** – list of arraylikes, passed on to the plotting functions for each axis (y-axis)
- **axes_loc** – list of tuples of two integers, location of each axis
- **xlabel** – str or list of str, labels for the x axis
- **ylabel** – str or list of str, labels for the y-axis
- **title** – str or list of str, titles for the subplots
- **num_rows** – int, how many rows of axis are created
- **num_cols** – int, how many columns of axis are created
- **saveas** – str filename of the saved file

Special Kwargs:

param subplot_params dict with integer keys, can contain all valid kwargs for *multiple_scatterplots()* with the integer key denoting to which subplot the changes are applied

param axes_kwargs dict with integer keys, additional arguments to pass on to *subplot2grid* for the creation of each axis (e.g colspan, rowspan)

Other Kwargs will be passed on to all *multiple_scatterplots()* calls (If they are not overwritten by parameters in *subplot_params*).

masci_tools.vis.plot_methods.**multiple_scatterplots**(*xdata*, *ydata*, ***, *xlabel=''*, *ylabel=''*, *title=''*, *data=None*, *saveas='mscatterplot'*, *axis=None*, *xerr=None*, *yerr=None*, *area_curve=0*, *copy_data=False*, *exclude_points_outside_plot_area=False*, ***kwargs*)

Create a standard scatter plot with multiple sets of data (this should be flexible enough) to do all the basic plots.

Parameters

- **xdata** – str or arraylike, data for the x coordinate
- **ydata** – str or arraylike, data for the y coordinate
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, title of the figure
- **data** – Mapping giving the data for the plots (required if xdata and ydata are str)
- **saveas** – str specifying the filename (without file format)
- **axis** – Axes object, if given the plot will be applied to this object
- **xerr** – optional data for errorbar in x-direction
- **yerr** – optional data for errorbar in y-direction
- **area_curve** – if an area plot is made this arguments defines the other enclosing line defaults to 0
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib functions (*errorbar* or *fill_between*)

masci_tools.vis.plot_methods.**multiplot_moved**(*xdata*, *ydata*, ***, *xlabel=''*, *ylabel=''*, *title=''*, *data=None*, *scale_move=1.0*, *min_add=0*, *saveas='mscatterplot'*, *copy_data=False*, ***kwargs*)

Plots all the scatter plots above each other. It adds an arbitrary offset to the ydata to do this and calls *multiple_scatterplots*. Therefore you might not want to show the yaxis ticks

Parameters

- **xdata** – arraylike, data for the x coordinate
- **ydata** – arraylike, data for the y coordinate
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis

- **ylabel** – str, label written on the y axis
- **title** – str, title of the figure
- **scale_move** – float, max*scale_move determines size of the shift
- **min_add** – float, minimum shift
- **saveas** – str specifying the filename (without file format)
- **copy_data** – bool, if True the data argument will be copied

Kwargs are passed on to the *multiple_scatterplots()* call

masci_tools.vis.plot_methods.**plot_bands**(*kpath*, *bands*, *, *data=None*, *size_data=None*, *color_data=None*, *special_kpoints=None*, *e_fermi=0*, *xlabel=''*, *ylabel='$E-E_F$ [eV]'*, *title=''*, *saveas='bandstructure'*, *markersize_min=0.5*, *markersize_scaling=5.0*, *scale_color=True*, *separate_bands=False*, *line_plot=False*, *band_index=None*, *copy_data=False*, ***kwargs*)

Plot the provided data for a bandstrucuture (non spin-polarized). Can be used to illustrate weights on bands via *size_data*

Parameters

- **kpath** – arraylike data for the kpoint data
- **bands** – arraylike data for the eigenvalues
- **size_data** – arraylike data the weights to emphasize (optional)
- **color_data** – str or arraylike, data for the color values with a colormap (optional)
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value
- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label
- **markersize_min** – minimum value used in scaling points for weight
- **markersize_scaling** – factor used in scaling points for weight
- **scale_color** – bool, if True (default) the weight will be additionally shown via a colormapping
- **line_plot** – bool, if True the bandstructure will be plotted with lines Here no weights are supported
- **separate_bands** – bool, if True the bandstructure will be separately plotted for each band allows more specific parametrization
- **band_index** – data for which eigenvalue belongs to which band (needed for line_plot and separate_bands)
- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the *multi_scatter_plot()* call

masci_tools.vis.plot_methods.**plot_bands_and_dos**()
PLot a Bandstructure with a density of states on the right side.

masci_tools.vis.plot_methods.**plot_certain_bands**()
Plot only certain bands from a bands.1 file from FLEUR

masci_tools.vis.plot_methods.**plot_colortable**(*colors*, *title*, *sort_colors=False*, *emptycols=0*)
Plot a legend of named colors.

Reference: https://matplotlib.org/3.1.0/gallery/color/named_colors.html

Parameters

- **colors** (Dict) – a dict color_name : color_value (hex str, rgb tuple, ...)
- **title** (str) – plot title
- **sort_colors** (bool) – True: sort legend entries not by dict position, but by color hue, staturation, value.
- **emptycols** (int) –

Returns figure

masci_tools.vis.plot_methods.**plot_convergence**(*iteration*, *distance*, *total_energy*, ***, *data=None*, *saveas_energy='energy_convergence'*, *saveas_distance='distance_convergence'*, *axis_energy=None*, *axis_distance=None*, *xlabel='Iteration'*, *ylabel_energy='Total energy difference [Htr]'*, *ylabel_distance='Distance [me/bohr^3]'*, *title_energy='Total energy difference over scf-Iterations'*, *title_distance='Convergence (log)'*, *copy_data=False*, *drop_last_iteration=False*, ***kwargs*)
Plot the total energy differences versus the scf iteration and plot the distance of the density versus iterations.

Parameters

- **iteration** – data for the number of iterations
- **distance** – data of distances
- **total_energy** – data of total energies
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label for the x-axis of both plots
- **saveas_energy** – str, filename for the energy convergence plot
- **axis_energy** – Axes object for the energy convergence plot
- **title_energy** – str, title for the energy convergence plot
- **ylabel_energy** – str, label for the y-axis for the energy convergence plot
- **saveas_distance** – str, filename for the distance plot
- **axis_distance** – Axes object for the distance plot
- **title_distance** – str, title for the distance plot
- **ylabel_distance** – str, label for the y-axis for the distance plot
- **copy_data** – bool if True the data argument is copied
- **drop_last_iteration** – bool if True the last iteration is dropped for the distance plot

Other Kwargs will be passed on to all *multiple_scatterplots()* calls

masci_tools.vis.plot_methods.**plot_convergence_results**(*iteration*, *distance*, *total_energy*, ***, *saveas1='t_energy_convergence'*, *axis1=None*, *saveas2='distance_convergence'*, *axis2=None*, ***kwargs*)

DEPRECATED Plot the total energy versus the scf iteration and plot the distance of the density versus iterations.

Parameters

- **iteration** – array for the number of iterations
- **distance** – array of distances
- **total_energy** – array of total energies
- **saveas1** – str, filename for the energy convergence plot
- **axis1** – Axes object for the energy convergence plot
- **saveas2** – str, filename for the distance plot
- **axis2** – Axes object for the distance plot

Other Kwargs will be passed on to all *single_scatterplot()* calls

masci_tools.vis.plot_methods.**plot_convergence_results_m**(*iterations*, *distances*, *total_energies*, ***, *modes*, *nodes=None*, *saveas1='t_energy_convergence'*, *saveas2='distance_convergence'*, *axis1=None*, *axis2=None*, ***kwargs*)

DEPRECATED Plot the total energy versus the scf iteration and plot the distance of the density versus iterations.

Parameters

- **iterations** – array for the number of iterations
- **distances** – array of distances
- **total_energies** – array of total energies
- **modes** – list of convergence modes (if ‘force’ is in the list the last distance is removed)
- **saveas1** – str, filename for the energy convergence plot
- **axis1** – Axes object for the energy convergence plot
- **saveas2** – str, filename for the distance plot
- **axis2** – Axes object for the distance plot

Other Kwargs will be passed on to all *multiple_scatterplots()* calls

masci_tools.vis.plot_methods.**plot_convex_hull2d**(*hull*, ***, *title='Convex Hull'*, *xlabel='Atomic Percentage'*, *ylabel='Formation energy / atom [eV]'*, *saveas='convex_hull'*, *axis=None*, ***kwargs*)

Plot method for a 2d convex hull diagramm

Parameters

- **hull** – pyhull.Convexhull #scipy.spatial.ConvexHull
- **axis** – Axes object where to add the plot
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis

- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot

Function specific parameters:

param marker_hull defaults to *marker*, marker type for the hull plot

param markersize_hull defaults to *markersize*, markersize for the hull plot

param color_hull defaults to *color*, color for the hull plot

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib functions *plot*

masci_tools.vis.plot_methods.**plot_corelevel_spectra**(*coreleveldict*, *natom_typesdict*, *exp_references=None*, *scale_to=- 1*, *show_single=True*, *show_ref=True*, *energy_range=None*, *title=''*, *fwhm_g=0.6*, *fwhm_l=0.1*, *energy_grid=0.2*, *peakfunction='voigt'*, *linestyle_spec='-'*, *marker_spec='o'*, *color_spec='k'*, *color_single='g'*, *xlabel='Binding energy [eV]'*, *ylabel='Intensity [arb] (natoms*nelectrons)'*, *saveas=None*, *xspec=None*, *alpha_l=1.0*, *beta_l=1.0*, ***kwargs*)

Plotting function of corelevel in the form of a spectrum.

Convention: Binding energies are positiv!

Args: coreleveldict: dict of corelevels with a list of corelevel energy of atomstypes # (The given corelevel accounts for a weight (number of electrons for full occupied corelevel) in the plot.) natom_typesdict: dict with number of atom types for each entry

Kwargs: exp_references: dict with experimental refereces, will be ploted as vertical lines show_single (bool): plot all single peaks. scale_to float: the maximum 'intensity' will be scaled to this value (useful for experimental comparisons) title (string): something for labeling fwhm (float): full width half maximum of peaks (gaus, lorentz or voigt_profile) energy_grid (float): energy resolution linetyp_spec : linetype for spectrum peakfunction (string): what the peakfunction should be {'voigt', 'pseudo-voigt', 'lorentz', 'gaus'}

example: coreleveldict = {u'Be': {'1s1/2' : [-1.0220669053033051, -0.3185614920138805,-0.7924091040092139]}} n_atom_types_Be12Ti = {'Be' : [4,4,4]}

masci_tools.vis.plot_methods.**plot_corelevels**(*coreleveldict*, *compound=''*, *axis=None*, *saveas='scatterplot'*, ***kwargs*)

Ploting function to visualize corelevels and corelevel shifts

masci_tools.vis.plot_methods.**plot_dos**(*energy_grid*, *dos_data*, ***, *data=None*, *saveas='dos_plot'*, *energy_label='$E-E_F$ [eV]'*, *dos_label='DOS [1/eV]'*, *title='Density of states'*, *xyswitch=False*, *e_fermi=0*, *copy_data=False*, ***kwargs*)

Plot the provided data for a density of states (not spin-polarized). Can be done horizontally or vertical via the switch *xyswitch*

Parameters

- **energy_grid** – arraylike data for the energy grid of the DOS
- **dos_data** – arraylike data for all the DOS components to plot
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)

- **title** – str, Title of the plot
- **energy_label** – str, label for the energy-axis
- **dos_label** – str, label for the DOS-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value
- **xyswitch** – bool if True, the enrgy axis will be plotted vertically
- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the *multiple_scatterplots()* call

masci_tools.vis.plot_methods.**plot_lattice_constant**(*scaling*, *total_energy*, *, *fit_data=None*, *data=None*, *relative=True*, *ref_const=None*, *title='Equation of states'*, *saveas='lattice_constant'*, *axis=None*, *copy_data=False*, ***kwargs*)

Plot a lattice constant versus Total energy Plot also the fit. On the x axis is the scaling, it

Parameters

- **scaling** – arraylike, data for the scaling factor
- **total_energy** – arraylike, data for the total energy
- **fit_data** – arraylike, optional data of fitted data
- **relative** – bool, scaling factor given (True), or lattice constants given?
- **ref_const** – float (optional), or list of floats, lattice constant for scaling 1.0
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **copy_data** – bool if True the data argument will be copied

Function specific parameters:

param marker_fit defaults to *marker*, marker type for the fit data

param markersize_fit defaults to *markersize*, markersize for the fit data

param linewidth_fit defaults to *linewidth*, linewidth for the fit data

param plotlabel_fit str label for the fit data

Other Kwargs will be passed on to *multiple_scatterplots()*

masci_tools.vis.plot_methods.**plot_one_element_corelv**(*corelevel_dict*, *element*, *compound=''*, *axis=None*, *saveas='scatterplot'*, ***kwargs*)

This routine creates a plot which visualizes all the binding energies of one element (and currenlty one corelevel) for different atomtypes.

example: corelevels = {'W' : {'4f7/2' : [123, 123.3, 123.4 ,123.1], '4f5/2' : [103, 103.3, 103.4, 103.1]}, 'Be' : {'1s': [118, 118.2, 118.4, 118.1, 118.3]}}

masci_tools.vis.plot_methods.**plot_relaxation_results**()

Plot from the result node of a relaxation workflow, All forces of every atom type versus relaxation cycle. Average force of all atom types versus relaxation cycle. Absolut relaxation in Angstroem of every atom type. Relative realxation of every atom type to a reference structure. (if none given use the structure from first relaxation cycle as reference)

masci_tools.vis.plot_methods.**plot_residuen**(*xdata*, *fitdata*, *realdata*, ***, *errors=None*, *xlabel='Energy [eV]'*, *ylabel='cts/s [arb]'*, *title='Residuen'*, *saveas='residuen'*, *hist=True*, *return_residuen_data=True*, ***kwargs*)

Calculates and plots the residuen for given xdata fit results and the real data.

If hist=True also the normed residual distribution is ploted with a normal distribution.

Parameters

- **xdata** – arraylike data for the x-coordinate
- **fitdata** – arraylike fitted data for the y-coordinate
- **realdata** – arraylike data to plot residuen against the fit
- **errors** – dict, can be used to provide errordata for the x and y direction
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **title** – str, title for the plot
- **saveas** – str, filename for the saved plot
- **hist** – bool, if True a normed residual distribution is ploted with a normal distribution.
- **return_residuen_data** – bool, if True in addition to the produced axis object also the residuen data is returned

Special Kwargs:

param hist_kwargs dict, these arguments will be passed on to the *histogram()* call (if hist=True)

Other Kwargs will be passed on to all *single_scatterplot()* call

masci_tools.vis.plot_methods.**plot_spectral_function**(*kpath*, *energy_grid*, *spectral_function*, ***, *data=None*, *special_kpoints=None*, *e_fermi=0*, *xlabel=''*, *ylabel='$E-E_F$ [eV]'*, *title=''*, *saveas='spectral_function'*, *copy_data=False*, ***kwargs*)

Create a colormesh plot of a spectral function

Parameters

- **kpath** – data for the kpoint coordinates
- **energy_grid** – data for the energy grid
- **spectral_function** – 2D data for the spectral function
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value

- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label
- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the *colormesh_plot()* call

masci_tools.vis.plot_methods.**plot_spinpol_bands**(*kpath*, *bands_up*, *bands_dn*, ***, *size_data=None*, *color_data=None*, *data=None*, *show_spin_pol=True*, *special_kpoints=None*, *e_fermi=0*, *xlabel=''*, *ylabel='$E-E_F$ [eV]'*, *title=''*, *saveas='bandstructure'*, *markersize_min=0.5*, *markersize_scaling=5.0*, *scale_color=True*, *line_plot=False*, *separate_bands=False*, *band_index=None*, *copy_data=False*, ***kwargs*)

Plot the provided data for a bandstrucuture (spin-polarized). Can be used to illustrate weights on bands via *size_data*

Parameters

- **kpath** – arraylike data for the kpoint data
- **bands_up** – arraylike data for the eigenvalues (spin-up)
- **bands_dn** – arraylike data for the eigenvalues (spin-dn)
- **size_data** – arraylike data the weights to emphasize BOTH SPINS (optional)
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value
- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label
- **markersize_min** – minimum value used in scaling points for weight
- **markersize_scaling** – factor used in scaling points for weight
- **show_spin_pol** – bool, if True (default) the two different spin channles will be shown in blue and red by default
- **scale_color** – bool, if True (default) the weight will be additionally shown via a colormapping
- **line_plot** – bool, if True the bandstructure will be plotted with lines Here no weights are supported
- **separate_bands** – bool, if True the bandstructure will be separately plotted for each band allows more specific parametrization
- **band_index** – data for which eigenvalue belongs to which band (needed for line_plot and separate_bands)
- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the *multi_scatter_plot()* call

masci_tools.vis.plot_methods.**plot_spinpol_dos**(*energy_grid*, *spin_up_data*, *spin_dn_data*, ***, *data=None*, *saveas='spinpol_dos_plot'*, *energy_label='$E-E_F$ [eV]'*, *dos_label='DOS [1/eV]'*, *title='Density of states'*, *xyswitch=False*, *e_fermi=0*, *spin_dn_negative=True*, *spin_arrows=True*, *copy_data=False*, ***kwargs*)

Plot the provided data for a density of states (spin-polarized). Can be done horizontally or vertical via the switch *xyswitch*

Parameters

- **energy_grid** – arraylike data for the energy grid of the DOS
- **spin_up_data** – arraylike data for all the DOS spin-up components to plot
- **spin_dn_data** – arraylike data for all the DOS spin-down components to plot
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, Title of the plot
- **energy_label** – str, label for the energy-axis
- **dos_label** – str, label for the DOS-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value
- **xyswitch** – bool if True, the enrgy axis will be plotted vertically
- **energy_grid_dn** – arraylike data for the energy grid of the DOS of the spin-down component (optional)
- **spin_dn_negative** – bool, if True (default) the spin-down components are plotted downwards
- **spin_arrows** – bool, if True (default) small arrows will be plotted on the left side of the plot indicating the spin directions (if spin_dn_negative is True)
- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the *multiple_scatterplots()* call

masci_tools.vis.plot_methods.**pseudo_voigt_profile**(*x*, *fwhm_g*, *fwhm_l*, *mu*, *mix=0.5*)

Linear combination of gaussian and loretzian instead of convolution

Args: x: array of floats fwhm_g: FWHM of gaussian fwhm_l: FWHM of Lorentzian mu: Mean mix: ratio of gaus to lorentz, mix* gaus, (1-mix)*Lorentz

masci_tools.vis.plot_methods.**reset_mpl_plot_defaults**()

Reset the defaults for matplotib backend to the hardcoded defaults

Available defaults can be seen in *MatplotlibPlotter*

masci_tools.vis.plot_methods.**save_mpl_defaults**(*filename='plot_mpl_defaults.json'*, *save_complete=False*)

Save the current defaults for the matplotlib backend to a json file.

Parameters

- **filename** – filename, where the defaults should be stored
- **save_complete** – bool if True not only the overwritten user defaults but also the unmodified harcoded defaults are stored

masci_tools.vis.plot_methods.**set_mpl_plot_defaults**(***kwargs*)
Set defaults for matplotib backend according to the given keyword arguments

Available defaults can be seen in *MatplotlibPlotter*

masci_tools.vis.plot_methods.**show_mpl_plot_defaults**()
Show the currently set defaults for matplotib backend to the hardcoded defaults

Available defaults can be seen in *MatplotlibPlotter*

masci_tools.vis.plot_methods.**single_scatterplot**(*xdata*, *ydata*, ***, *xlabel=''*, *ylabel=''*, *title=''*, *data=None*, *saveas='scatterplot'*, *axis=None*, *xerr=None*, *yerr=None*, *area_curve=0*, *copy_data=False*, ***kwargs*)
Create a standard scatter plot (this should be flexible enough) to do all the basic plots.

Parameters

- **xdata** – str or arraylike, data for the x coordinate
- **ydata** – str or arraylike, data for the y coordinate
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **title** – str, title of the figure
- **data** – Mapping giving the data for the plot (required if xdata and ydata are str)
- **saveas** – str specifying the filename (without file format)
- **axis** – Axes object, if given the plot will be applied to this object
- **xerr** – optional data for errorbar in x-direction
- **yerr** – optional data for errorbar in y-direction
- **area_curve** – if an area plot is made this arguments defines the other enclosing line defaults to 0
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib functions (*errorbar* or *fill_between*)

masci_tools.vis.plot_methods.**surface_plot**(*xdata*, *ydata*, *zdata*, ***, *xlabel=''*, *ylabel=''*, *zlabel=''*, *title=''*, *data=None*, *saveas='surface_plot'*, *axis=None*, *copy_data=False*, ***kwargs*)
Create a standard surface plot

Parameters

- **xdata** – arraylike, data for the x coordinate
- **ydata** – arraylike, data for the y coordinate
- **zdata** – arraylike, data for the z coordinate
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **zlabel** – str, label written on the z axis

- **title** – str, title of the figure
- **axis** – Axes object, if given the plot will be applied to this object
- **saveas** – str specifying the filename (without file format)
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *plot_surface*

masci_tools.vis.plot_methods.**voigt_profile**(*x*, *fwhm_g*, *fwhm_l*, *mu*)

Return the Voigt line shape at x with Lorentzian component FWHM fwhm_l and Gaussian component FWHM fwhm_g and mean mu. There is no closed form for the Voigt profile, but it is related to the real part of the Faddeeva function (wofz), which is used here.

masci_tools.vis.plot_methods.**waterfall_plot**(*xdata*, *ydata*, *zdata*, ***, *xlabel=''*, *ylabel=''*, *zlabel=''*, *title=''*, *data=None*, *saveas='waterfallplot'*, *axis=None*, *copy_data=False*, ***kwargs*)

Create a standard waterfall plot

Parameters

- **xdata** – arraylike, data for the x coordinate
- **ydata** – arraylike, data for the y coordinate
- **zdata** – arraylike, data for the z coordinate
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label written on the x axis
- **ylabel** – str, label written on the y axis
- **zlabel** – str, label written on the z axis
- **title** – str, title of the figure
- **axis** – Axes object, if given the plot will be applied to this object
- **saveas** – str specifying the filename (without file format)
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.matplotlib_plotter.MatplotlibPlotter*. If the arguments are not recognized they are passed on to the matplotlib function *scatter3D*

Bokeh

Here the *masci_tools.vis.parameters.Plotter* subclass for the bokeh plotting backend is defined with default values and many helper methods

class masci_tools.vis.bokeh_plotter.**BokehPlotter**(***kwargs*)

Class for plotting parameters and standard code snippets for plotting with the bokeh backend.

Kwargs in the __init__ method are forwarded to setting default values for the instance

For specific documentation about the parameter/defaults handling refer to *Plotter*.

Below the current defined default values are shown:

Table 2: Plot Parameters

Name	Description	Default value
`figure_kwargs`	Parameters for creating the bokeh figure. Includes things like axis type (x and y), tools plot width/height	`{'tools': 'pan,poly_select,tap,wheel_zoom,box_zoom,redo,undo,reset,save,crosshair,zoom_out,zoom_in', 'y_axis_type': 'linear', 'x_axis_type': 'linear', 'active_inspect': None, 'toolbar_location': 'right'}`
`additional_tools`	Tools to add to the tools already specified in `figure_kwargs` (Has to be in the same format)	No Default
`show_tooltips`	Switch whether to add hover tooltips	`True`
`global_tooltips`	Switch whether to add individual (for each renderer) or global hover tooltips.	`False`
`format_tooltips`	Switch whether to enable the processing of formatted strings in tooltips.	`True`
`tooltips`	List of tuples specifying the tooltips. For more information refer to the bokeh documentation. Strings can contain format specifiers with the data keys of the function e.g. `'@ ``{x}`. Here the `` ``{x}` `` will be replaced by the entry for x. If there are formatting specifications for bokeh they need to be escaped with double curly braces or `format_tooltips=False`.	`[('X', '@{x}'), ('Y', '@{y}')]`
`additional_tooltips`	Tooltips to add to the already defined `tooltips` (See above)	No Default
`axis_linewidth`	Linewidth for the lines of the axis	`2`
`label_fontsize`	Fontsize for the labels of the axis	`18pt`
`tick_label_fontsize`	Fontsize for the ticks on the axis	`16pt`
`background_fill_color`	Color for the background of the plot	`#ffffff`
`x_axis_formatter`	If set this formatter will be used for the ticks on the x-axis	No Default
`y_axis_formatter`	If set this formatter will be used for the ticks on the y-axis	No Default
`x_ticks`	Tick specification for the x-axis	No Default
`x_ticklabels_override`	Override the labels for the ticks on the x-axis	No Default
`y_ticks`	Tick specification for the y-axis	No Default
`y_ticklabels_override`	Override the labels for the ticks on the y-axis	No Default
`x_range_padding`	Specifies the amount of padding on the edges of the x-axis	No Default
`y_range_padding`	Specifies the amount of padding on the edges of the y-axis	No Default
`limits`	Dict specifying the limits of the axis, e.g `{'x': (-5,5)}`	No Default
`legend_location`	Location of the legend inside the plot area	`top_right`
`legend_click_policy`	Policy for what happens when labels are clicked in the legend	`hide`
`legend_orientation`	Orientation of the legend	`vertical`
`legend_font_size`	Fontsize for the labels inside the legend	`14pt`
`legend_outside`	If True the legend will be placed outside of the plot area	`False`
`color_palette`	Color palette to use for the plot(s)	No Default

continues on next page

Table 2 – continued from previous page

Name	Description	Default value
color	Specific colors to use for the plot(s)	No Default
legend_label	Labels to use for the legend of the plot(s)	No Default
alpha	Transparency to use for the plot(s)	1.0
name	Name used for identifying elements in the plot (not shown only internally)	No Default
line_color	Color to use for line plot(s)	No Default
line_alpha	Transparency to use for line plot(s)	1.0
line_dash	Dash styles to use for line plot(s)	No Default
line_width	Line width to use for line plot(s)	2.0
marker	Type of marker to use for scatter plot(s)	circle
marker_size	Marker size to use for scatter plot(s)	6
area_plot	If True h(v)area will be used to produce the plot(s)	False
area_vertical	Determines, whether to use harea (False) or varea (True) for area plots	False
fill_alpha	Transparency to use for the area in area plot(s)	1.0
fill_color	Color to use for the area in area plot(s)	No Default
level	Can be used to specified, which elements are fore- or background	No Default
straight_lines	Dict specifying straight help-lines to draw. For example {'vertical': 0, 'horizontal': [-1,1]} will draw a vertical line at 0 and two horizontal at -1 and 1	No Default
straight_line_options	Color, width, and more options for the help-lines	{'line_color': 'black', 'line_width': 1.0, 'line_dash': 'dashed'}
save_plots	If True plots will be saved to file (Configuration beforehand is needed)	False
save_format	Formats to save the plots to, can be single or list of formats (html, png or svg)	html
show	If True bokeh.io.show will be called after the plotting routine	True

add_tooltips(*fig*, *renderers*, *columns=None*, *toggleable=False*)

Add Hover tooltips to the given renderers and figure

Parameters

- **fig** – bokeh figure to apply changes to
- **renderers** – bokeh renderers to activate the tooltips for
- **columns** – namedtuple containing the data keys used for evtl. formatting
- **toggleable** – bool, if True these tooltips will be toggleable in the toolbar

draw_straight_lines(*fig*)

Draw horizontal and vertical lines specified in the lines argument

Parameters **fig** – bokeh figure on which to perform the operation

plot_kwargs(*ignore=None*, *extra_keys=None*, *plot_type='default'*, *post_process=True*, *list_of_dicts=True*, ***kwargs*)

Creates a dict or list of dicts (for multiple plots) with the defined parameters for the plotting calls fo matplotlib

Parameters

- **ignore** – str or list of str (optional), defines keys to ignore in the creation of the dict
- **extra_keys** – optional set for addtional keys to retrieve
- **post_process** – bool, if True the parameters are cleaned up for inserting them directly into bokeh plotting functions

Kwargs are used to replace values by custom parameters:

Example for using a custom markersize:

```
p = BokehPlotter()
p.add_parameter('marker_custom', default_from='marker')
p.plot_kwargs(marker='marker_custom')
```

This code snippet will return the standard parameters for a plot, but the value for the marker will be taken from the key *marker_custom*

prepare_figure(*title*, *xlabel*, *ylabel*, *figure=None*)
Create a bokeh figure according to the set parameters or modify an existing one

Parameters

- **title** – title of the figure
- **xlabel** – label on the x-axis
- **ylabel** – label on the y-axis
- **figure** – bokeh figure, optional, if given the operations are performed on the object otherwise a new figure is created

Returns the created or modified bokeh figure

save_plot(*figure*, *saveas*)
Show/save the bokeh figure

Parameters **figure** – bokeh figure on which to perform the operation

set_color_palette_by_num_plots()
Set the colormap for the configured number of plots according to the set colormap or color

copied from https://github.com/PatrikHlobil/Pandas-Bokeh/blob/master/pandas_bokeh/plot.py credits to PatrikHlobil modified for use in this Plotter class

set_legend(*fig*)
Set legend options for the figure

Parameters **fig** – bokeh figure on which to perform the operation

set_limits(*fig*)
Set limits of the figure

Parameters **fig** – bokeh figure on which to perform the operation

Here are general and special bokeh plots to use

masci_tools.vis.bokeh_plots.**bokeh_bands**(*kpath*, *bands=None*, ***, *data=None*, *size_data=None*, *color_data=None*, *xlabel=''*, *ylabel='E-E_F [eV]'*, *title=''*, *special_kpoints=None*, *markersize_min=3.0*, *markersize_scaling=10.0*, *saveas='bands_plot'*, *scale_color=True*, *separate_bands=False*, *line_plot=False*, *band_index=None*, *copy_data=False*, ***kwargs*)

Create an interactive bandstructure plot (non-spinpolarized) with bokeh Can make a simple plot or weight the size and color of the points against a given weight

Parameters

- **kpath** – arraylike or key data for the kpoint data
- **bands** – arraylike or key data for the eigenvalues
- **size_data** – arraylike or key data the weights to emphasize (optional)
- **color_data** – str or arraylike, data for the color values with a colormap (optional)
- **data** – source for the bands data (optional) of the plot (pandas Dataframe for example)
- **xlabel** – label for the x-axis (default no label)
- **ylabel** – label for the y-axis
- **title** – title of the figure
- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label
- **e_fermi** – float, determines, where to put the line for the fermi energy
- **markersize_min** – minimum value used in scaling points for weight
- **markersize_scaling** – factor used in scaling points for weight
- **outfilename** – filename of the output file
- **scale_color** – bool, if True (default) the weight will be additionally shown via a colormapping
- **line_plot** – bool, if True the bandstructure will be plotted with lines Here no weights are supported
- **separate_bands** – bool, if True the bandstructure will be separately plotted for each band allows more specific parametrization
- **band_index** – data for which eigenvalue belongs to which band (needed for line_plot and separate_bands)
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *bokeh_multi_scatter()* or *bokeh_line()*

masci_tools.vis.bokeh_plots.**bokeh_dos**(*energy_grid*, *dos_data=None*, ***, *data=None*, *energy_label='E-E_F [eV]'*, *dos_label='DOS [1/eV]'*, *title='Density of states'*, *xyswitch=False*, *e_fermi=0*, *saveas='dos_plot'*, *copy_data=False*, ***kwargs*)

Create an interactive dos plot (non-spinpolarized) with bokeh Both horizontal or vertical orientation are possible

Parameters

- **energy_grid** – arraylike or key data for the energy grid
- **spin_up_data** – arraylike or key data for the DOS

- **data** – source for the DOS data (optional) of the plot (pandas Dataframe for example)
- **energy_label** – label for the energy-axis
- **dos_label** – label for the dos-axis
- **title** – title of the figure
- **xyswitch** – bool if True, the energy will be plotted along the y-direction
- **e_fermi** – float, determines, where to put the line for the fermi energy
- **outfilename** – filename of the output file
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *bokeh_line()*

masci_tools.vis.bokeh_plots.**bokeh_line**(*x*, *y=None*, ***, *data=None*, *figure=None*, *xlabel='x'*, *ylabel='y'*, *title=''*, *saveas='line'*, *plot_points=False*, *area_curve=0*, *copy_data=False*, *set_default_legend=True*, ***kwargs*)

Create an interactive multi-line plot with bokeh

Parameters

- **x** – arraylike or key for data for the x-axis
- **y** – arraylike or key for data for the y-axis
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – label for the x-axis
- **ylabel** – label for the y-axis
- **title** – title of the figure
- **figure** – bokeh figure (optional), if provided the plot will be added to this figure
- **outfilename** – filename of the output file
- **plot_points** – bool, if True also plot the points with a scatterplot on top
- **copy_data** – bool, if True the data argument will be copied
- **set_default_legend** – bool if True the data names are used to generate default legend labels

Kwargs will be passed on to *masci_tools.vis.bokeh_plotter.BokehPlotter*. If the arguments are not recognized they are passed on to the bokeh function *line*

masci_tools.vis.bokeh_plots.**bokeh_multi_scatter**(*x*, *y=None*, ***, *data=None*, *figure=None*, *xlabel='x'*, *ylabel='y'*, *title=''*, *saveas='scatter'*, *copy_data=False*, *set_default_legend=True*, ***kwargs*)

Create an interactive scatter (muliple data sets possible) plot with bokeh

Parameters

- **x** – arraylike or key for data for the x-axis
- **y** – arraylike or key for data for the y-axis
- **data** – source for the data of the plot (pandas Dataframe for example)
- **xlabel** – label for the x-axis
- **ylabel** – label for the y-axis
- **title** – title of the figure

- **figure** – bokeh figure (optional), if provided the plot will be added to this figure
- **outfilename** – filename of the output file
- **copy_data** – bool, if True the data argument will be copied
- **set_default_legend** – bool if True the data names are used to generate default legend labels

Kwargs will be passed on to *masci_tools.vis.bokeh_plotter.BokehPlotter*. If the arguments are not recognized they are passed on to the bokeh function *scatter*

masci_tools.vis.bokeh_plots.**bokeh_scatter**(*x*, *y=None*, ***, *xlabel='x'*, *ylabel='y'*, *title=''*, *figure=None*, *data=None*, *saveas='scatter'*, *copy_data=False*, ***kwargs*)

Create an interactive scatter plot with bokeh

Parameters

- **x** – arraylike or key for data for the x-axis
- **y** – arraylike or key for data for the y-axis
- **data** – source for the data of the plot (pandas Dataframe for example)
- **xlabel** – label for the x-axis
- **ylabel** – label for the y-axis
- **title** – title of the figure
- **figure** – bokeh figure (optional), if provided the plot will be added to this figure
- **outfilename** – filename of the output file
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *masci_tools.vis.bokeh_plotter.BokehPlotter*. If the arguments are not recognized they are passed on to the bokeh function *scatter*

masci_tools.vis.bokeh_plots.**bokeh_spectral_function**(*kpath*, *energy_grid*, *spectral_function*, ***, *data=None*, *special_kpoints=None*, *e_fermi=0*, *xlabel=''*, *ylabel='$E-E_F$ [eV]'*, *title=''*, *saveas='spectral_function'*, *copy_data=False*, *figure=None*, ***kwargs*)

Create a colormesh plot of a spectral function

Parameters

- **kpath** – data for the kpoint coordinates
- **energy_grid** – data for the energy grid
- **spectral_function** – 2D data for the spectral function
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **title** – str, Title of the plot
- **xlabel** – str, label for the x-axis
- **ylabel** – str, label for the y-axis
- **saveas** – str, filename for the saved plot
- **e_fermi** – float (default 0), place the line for the fermi energy at this value
- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label

- **copy_data** – bool, if True the data argument will be copied

All other Kwargs are passed on to the image call of bokeh

masci_tools.vis.bokeh_plots.**bokeh_spinpol_bands**(*kpath*, *bands_up=None*, *bands_dn=None*, ***, *size_data=None*, *color_data=None*, *data=None*, *xlabel=''*, *ylabel='E-E_F [eV]'*, *title=''*, *special_kpoints=None*, *markersize_min=3.0*, *markersize_scaling=10.0*, *saveas='bands_plot'*, *scale_color=True*, *line_plot=False*, *separate_bands=False*, *band_index=None*, *copy_data=False*, ***kwargs*)

Create an interactive bandstructure plot (spinpolarized) with bokeh Can make a simple plot or weight the size and color of the points against a given weight

Parameters

- **kpath** – arraylike or key data for the kpoint data
- **bands_up** – arraylike or key data for the eigenvalues spin-up
- **bands_dn** – arraylike or key data for the eigenvalues spin-dn
- **size_data** – arraylike or key data the weights to emphasize (optional)
- **color_data** – str or arraylike, data for the color values with a colormap (optional)
- **data** – source for the bands data (optional) of the plot (pandas Dataframe for example)
- **xlabel** – label for the x-axis (default no label)
- **ylabel** – label for the y-axis
- **title** – title of the figure
- **special_kpoints** – list of tuples (str, float), place vertical lines at the given values and mark them on the x-axis with the given label
- **e_fermi** – float, determines, where to put the line for the fermi energy
- **markersize_min** – minimum value used in scaling points for weight
- **markersize_scaling** – factor used in scaling points for weight
- **outfilename** – filename of the output file
- **scale_color** – bool, if True (default) the weight will be additionally shown via a colormapping
- **line_plot** – bool, if True the bandstructure will be plotted with lines Here no weights are supported
- **separate_bands** – bool, if True the bandstructure will be separately plotted for each band allows more specific parametrization
- **band_index** – data for which eigenvalue belongs to which band (needed for line_plot and separate_bands)
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *bokeh_multi_scatter()* or *bokeh_line()*

masci_tools.vis.bokeh_plots.**bokeh_spinpol_dos**(*energy_grid*, *spin_up_data=None*, *spin_dn_data=None*, ***, *data=None*, *spin_dn_negative=True*, *energy_label='E-E_F [eV]'*, *dos_label='DOS [1/eV]'*, *title='Density of states'*, *xyswitch=False*, *e_fermi=0*, *spin_arrows=True*, *saveas='dos_plot'*, *copy_data=False*, ***kwargs*)

Create an interactive dos plot (spinpolarized) with bokeh Both horizontal or vertical orientation are possible

Parameters

- **energy_grid** – arraylike or key data for the energy grid
- **spin_up_data** – arraylike or key data for the DOS spin-up
- **spin_dn_data** – arraylike or key data for the DOS spin-dn
- **data** – source for the DOS data (optional) of the plot (pandas Dataframe for example)
- **spin_dn_negative** – bool, if True (default), the spin down components are plotted downwards
- **energy_label** – label for the energy-axis
- **dos_label** – label for the dos-axis
- **title** – title of the figure
- **xyswitch** – bool if True, the energy will be plotted along the y-direction
- **e_fermi** – float, determines, where to put the line for the fermi energy
- **spin_arrows** – bool, if True (default) small arrows will be plotted on the left side of the plot indicating the spin directions (if spin_dn_negative is True)
- **outfilename** – filename of the output file
- **copy_data** – bool, if True the data argument will be copied

Kwargs will be passed on to *bokeh_line()*

masci_tools.vis.bokeh_plots.**get_bokeh_help**(*key*)

Print the decription of the given key in the bokeh backend

Available defaults can be seen in *BokehPlotter*

masci_tools.vis.bokeh_plots.**load_bokeh_defaults**(*filename='plot_bokeh_defaults.json'*)

Load defaults for the bokeh backend from a json file.

Parameters **filename** – filename,from where the defaults should be taken

masci_tools.vis.bokeh_plots.**periodic_table_plot**(*source*, *display_values=[]*, *display_positions=[]*, *color_value=None*, *tooltips=[('Name', '@name'), ('Atomic number', '@{atomic number}'), ('Atomic mass', '@{atomic mass}'), ('CPK color', '$color[hex, swatch]:CPK'), ('Electronic configuration', '@{electronic configuration}')]*, *title=''*, *outfilename='periodictable.html'*, *value_color_range=[None, None]*, *log_scale=0*, *color_map=None*, *bokeh_palette='Plasma256'*, *toolbar_location=None*, *tools='hover'*, *blank_color='#c4c4c4'*, *blank_outsiders=[True, True]*, *include_legend=True*, *copy_source=True*, *legend_labels=None*, *color_bar_title=None*, *show=True*)

Plot function for an interactive periodic table plot. Heat map and hover tool. source must be a panda dataframe containing, period, group,

param source: pandas dataframe containing everything param tooltips: what is shown with hover tool. values have to be in source example:

```
Keys of panda DF. group, period symbol and atomic number or required...
Index([u'atomic number', u'symbol', u'name', u'atomic mass', u'CPK',
   u'electronic configuration', u'electronegativity', u'atomic radius',
   u'ion radius', u'van der Waals radius', u'IE-1', u'EA',
   u'standard state', u'bonding type', u'melting point', u'boiling point',
   u'density', u'metal', u'year discovered', u'group', u'period',
   u'rmt_mean', u'rmt_std', u'number_of_occ', u'type_color', u'c_value'],
  dtype='object')

tooltips_def = [("Name", "@name"),
            ("Atomic number", "@{atomic number}"),
            ("Atomic mass", "@{atomic mass}"),
            ("CPK color", "$color[hex, swatch]:CPK"),
            ("Electronic configuration", "@{electronic configuration}")]
```

param display_values: list of strings, have to match source. Values to be displayed on the element rectangles example:[“rmt_mean”, “rmt_std”, “number_of_occ”] param display_positions: list of floats, length has to match display_values, At which y offset the display values should be displayed.

masci_tools.vis.bokeh_plots.**plot_convergence**(*iteration*, *distance*, *total_energy*, ***, *data=None*, *saveas_energy='energy_convergence'*, *saveas_distance='distance_convergence'*, *figure_energy=None*, *figure_distance=None*, *xlabel='Iteration'*, *ylabel_energy='Total energy difference [Htr]'*, *ylabel_distance='Distance [me/bohr^3]'*, *title_energy='Total energy difference over scf-Iterations'*, *title_distance='Convergence (log)'*, *copy_data=False*, *drop_last_iteration=False*, ***kwargs*)

Plot the total energy differences versus the scf iteration and plot the distance of the density versus iterations.

Parameters

- **iteration** – data for the number of iterations
- **distance** – data of distances
- **total_energy** – data of total energies

- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **xlabel** – str, label for the x-axis of both plots
- **saveas_energy** – str, filename for the energy convergence plot
- **figure_energy** – Axes object for the energy convergence plot
- **title_energy** – str, title for the energy convergence plot
- **ylabel_energy** – str, label for the y-axis for the energy convergence plot
- **saveas_distance** – str, filename for the distance plot
- **figure_distance** – Axes object for the distance plot
- **title_distance** – str, title for the distance plot
- **ylabel_distance** – str, label for the y-axis for the distance plot
- **copy_data** – bool if True the data argument is copied
- **drop_last_iteration** – bool if True the last iteration is dropped for the distance plot

Other Kwargs will be passed on to all *bokeh_line()* calls

masci_tools.vis.bokeh_plots.**plot_convergence_results**(*iteration*, *distance*, *total_energy*, ***, *saveas='convergence'*, ***kwargs*)

Plot the total energy versus the scf iteration and plot the distance of the density versus iterations. Uses bokeh_line and bokeh_scatter

Parameters

- **iteration** – list of Int
- **distance** – list of floats
- **show** – bool, if True call show

Total_energy list of floats

Kwargs will be passed on to *bokeh_line()*

Returns grid bokeh grid with figures

masci_tools.vis.bokeh_plots.**plot_convergence_results_m**(*iterations*, *distances*, *total_energies*, ***, *link=False*, *nodes=None*, *modes=None*, *plot_label=None*, *saveas='convergence'*, ***kwargs*)

Plot the total energy versus the scf iteration and plot the distance of the density versus iterations in a bokeh grid for several SCF results.

Parameters

- **distances** – list of lists of floats
- **iterations** – list of lists of Int
- **link** – bool, optional default=False:
- **nodes** – list of node uuids or pks important for links
- **saveas1** – str, optional default='t_energy_convergence', save first figure as
- **saveas2** – str, optional default='distance_convergence', save second figure as
- **figure_kwargs** – dict, optional default={'plot_width': 600, 'plot_height': 450}, gets parsed to bokeh_line

- **kwargs** – further key-word arguments for bokeh_line

Total_energies list of lists of floats

Returns grid bokeh grid with figures

masci_tools.vis.bokeh_plots.**plot_convex_hull2d**(*hull*, *title='Convex Hull'*, *xlabel='Atomic Procentage'*, *ylabel='Formation energy / atom [eV]'*, *linestyle='-'*, *marker='o'*, *legend=True*, *legend_option={}*, *saveas='convex_hull'*, *limits=[None, None]*, *scale=[None, None]*, *axis=None*, *color='k'*, *color_line='k'*, *linewidth=2*, *markersize=8*, *marker_hull='o'*, *markersize_hull=8*, ***kwargs*)

Plot method for a 2d convex hull diagram

Parameters **hull** – scipy.spatial.ConvexHull

masci_tools.vis.bokeh_plots.**plot_lattice_constant**(*scaling*, *total_energy*, ***, *fit_data=None*, *data=None*, *figure=None*, *relative=True*, *ref_const=None*, *title='Equation of states'*, *saveas='lattice_constant'*, *copy_data=False*, ***kwargs*)

Plot a lattice constant versus Total energy Plot also the fit. On the x axis is the scaling, it

Parameters

- **scaling** – arraylike, data for the scaling factor
- **total_energy** – arraylike, data for the total energy
- **fit_data** – arraylike, optional data of fitted data
- **relative** – bool, scaling factor given (True), or lattice constants given?
- **ref_const** – float (optional), or list of floats, lattice constant for scaling 1.0
- **data** – source for the data of the plot (optional) (pandas Dataframe for example)
- **copy_data** – bool if True the data argument will be copied
- **figure** – bokeh figure (optional), if provided the plot will be added to this figure

Function specific parameters:

param marker_fit defaults to *marker*, marker type for the fit data

param marker_size_fit defaults to *marker_size*, markersize for the fit data

param line_width_fit defaults to *line_width*, linewidth for the fit data

param legend_label_fit str label for the fit data

Other Kwargs will be passed on to *bokeh_line()*

masci_tools.vis.bokeh_plots.**reset_bokeh_plot_defaults**()

Reset the defaults for bokeh backend to the hardcoded defaults

Available defaults can be seen in *BokehPlotter*

masci_tools.vis.bokeh_plots.**save_bokeh_defaults**(*filename='plot_bokeh_defaults.json'*, *save_complete=False*)

Save the current defaults for the matplotlib backend to a json file.

Parameters

- **filename** – filename, where the defaults should be stored
- **save_complete** – bool if True not only the overwritten user defaults but also the unmodified harcoded defaults are stored

masci_tools.vis.bokeh_plots.**set_bokeh_plot_defaults**(***kwargs*)
Set defaults for bokeh backend according to the given keyword arguments

Available defaults can be seen in *BokehPlotter*

masci_tools.vis.bokeh_plots.**show_bokeh_plot_defaults**()
Show the currently set defaults for bokeh backend

Available defaults can be seen in *BokehPlotter*

6.1.2 Calculation tools

This file contains a class to compute the crystalfield coefficients from convoluting the charge density with the potential which produces the crystalfield. This is both compatible with the Yttrium-Analogue approximation and self-consitent calculation of the potential

class masci_tools.tools.cf_calculation.**CFCalculation**(*radial_points=4000*, *reference_radius='pot'*, *pot_cutoff=0.001*, *only_m0=False*, *quiet=False*)
Class for calculating Crystal Field coefficients using the procedure described in C.E. Patrick, J.B. Staunton: J. Phys.: Condens. Matter 31, 305901 (2019)

Using the formula:

$$B_{lm} = \sqrt{\frac{2l+1}{4\pi}} \int^{R_{MT}} drr^2 V_{lm}(r) n_{4f}(r)$$

The read in quantities are interpolated from logarithmic meshes to equidistant meshes

The function constructs an equidistant mesh between 0 and the muffin tin radius defined in *self.reference_radius* and with *self.radial_points* points

Parameters

- **radial_points** – int, number of radial points in the interpolated mesh
- **reference_radius** – stror float; Either 'pot' or 'cdn' or explicit number. Defines which muffin-tin radius is used for the equidistant mesh. IMPORTANT! If txt files are used the muffin-tin radius has to be provided explicitly
- **pot_cutoff** – float Defines minimum value that has to appear in potentials to not be omitted (Only HDF)
- **only_m0** – bool, Ignores coefficients with m!=0 if True
- **quiet** – bool, supresses print statements if True

performIntegration(*convert=True*)
Performs the integration to obtain the crystal field coefficients If the data was not already interpolated, the interpolation will be performed beforehand

Parameters:

param convert bool, converts to Steven's coefficients (if True)

Returns list of CFCoefficient objects (namedtuple), with all the necessary information

prefactor(*l*, *m*)
Gives the lm dependent prefactor for conversion between Blm and Alm coefficients

Args:

param l int; orbital quantum number

param m int; magnetic quantum number

Returns float prefactor for conversion to Steven's Coefficients

readCDN(*file*, ***kwargs*)
Reads in the normed charge density for the CF coefficient calculation If hdf files are given also the muffin tin radius is read in

Parameters:

param file Expects string filename for the charge density to read in The function expects either HDF files or txt files with the format (rmesh,cdn). The charge density should be given as r^2n(r) and normed to 1

kwargs:

param atomType int, Defines the atomType to read in (only for HDF files)

param header int, Define how many lines to skip in the beginning of txt file

readPot(**args*, *lm=None*, ***kwargs*)
Reads in the potentials for the CF coefficient calculation If hdf files are given also the muffin tin radius is read in

Parameters

- **args** – Expects string filenames for the potentials to read in The function expects either HDF files or txt files with the format (rmesh,vlmup,vlmdn)
- **lm** – list of tuples, Defines the l and m indices for the given txt files
- **atomType** – int, Defines the atomType to read in (only for HDF files)
- **header** – int, Define how many lines to skip in the beginning of txt file
- **complexData** – bool, Define if the data in the text file is complex

Raises: ValueError: lm indices list length has to match number of files read in

class masci_tools.tools.cf_calculation.**CFCoefficient**(*l*, *m*, *spin_up*, *spin_down*, *unit*, *convention*)

convention
Alias for field number 5

l
Alias for field number 0

m
Alias for field number 1

spin_down
Alias for field number 3

spin_up
Alias for field number 2

unit
Alias for field number 4

masci_tools.tools.cf_calculation.**plot_crystal_field_calculation**(*cfcalc*, *filename='crystal_field_calc'*, *pot_title='Potential'*, *cdn_title='Density'*, *xlabel='R (Bohr)'*, *pot_ylabel='$Vpot$ (Hartree)'*, *cdn_ylabel='Density'*, *fontsize=12*, *labelsize=12*, *pot_colors=None*, *save=False*, *show=True*)

Plot the given potentials and charge densities

Parameters

- **cfcalc** – CFcalculation containing the data to plot
- **filename** – str, Define the filename to save the figure
- **pot_title** – Title for the potential subplot
- **cdn_title** – Title for the charge density subplot
- **xlabel** – label for the x axis of both subplots
- **pot_ylabel** – label for the y axis of the potential subplot
- **cdn_ylabel** – label for the y axis f the charge density subplot
- **fontsize** – fontsize for titles and labels on the axis
- **labelsize** – fontsize for the ticks on the axis,

masci_tools.tools.cf_calculation.**plot_crystal_field_potential**(*cfcoeffs*, *filename='crystal_field_potential_areaplot'*, *spin='avg'*, *phi=0.0*, *save=False*, *show=True*)

Plots the angular dependence of the calculated CF potential as well as a plane defined by phi.

Parameters

- **cfcoeffs** – list of CFCoefficients to construct the potential
- **filename** – str, defines the filename to save the figure
- **spin** – str; Either 'up', 'dn' or 'avg'. Which spin direction to plot ('avg'-> ('up'+'dn')/2.0)
- **phi** – float, defines the phi angle of the plane

Raises **AssertionError** – When coefficients are provided as wrong types or in the wrong convention

This module contains utility and functions to work with Green's functions calculated and written to `greensf.hdf` files by fleur

class masci_tools.tools.greensfunction.**GreensFunction**(*element*, *data*, *attributes*)

Class for working with Green's functions calculated by the fleur code

Parameters

- **element** (*GreensfElement*) – *GreensfElement* namedtuple containing the information about the element

- **data** (dict[str, Any]) – datasets dict produced by one of the hdf recipes for reading Green's functions
- **attributes** (dict[str, Any]) – attributes dict produced by one of the hdf recipes for reading Green's functions

energy_dependence(*, *m=None*, *mp=None*, *spin=None*, *imag=True*, *both_contours=False*)
Select data with energy dependence

Parameters

- **m** (Optional[int]) – optional integer magnetic quantum number between -l and l
- **mp** (Optional[int]) – optional integer magnetic quantum number between -lp and lp
- **spin** (Optional[int]) – optional integer spin between 1 and nspins
- **both_contours** (bool) – bool id True the data is not added for both energy contours
- **imag** (bool) – bool if True and both_contours is False the imaginary part 1/2i(G(z)-G(z^*)) is returned otherwise the real part 1/2(G(z)+G(z^*))

Return type ndarray

Returns numpy array with the selected data

classmethod fromFile(*file*, *index=None*, ***selection_params*)
Classmethod for creating a *GreensFunction* instance directly from a hdf file

Parameters

- **file** (Any) – path or opened file handle to a greensf.hdf file
- **index** (Optional[int]) – optional int index of the element to read in

If index is not given Keyword arguments with the keys being the names of the fields of *GreensfElement* can be given to select the right Green's function. The specification has to match only one element in the file

Return type *GreensFunction*

get_coefficient(*name*, *spin=None*, *radial=False*)
Get the coefficient with the given name from the data attribute

Parameters

- **name** (Literal['sphavg', 'uu', 'ud', 'du', 'dd', 'ulou', 'uulo', 'ulod', 'dulo', 'uloulo']) – name of the coefficient
- **radial** (bool) – if the Green's function is stored by coefficient and radial is True it is multiplied by the corresponding radial function otherwise the scalar product is multiplied
- **spin** (Optional[int]) – integer index of the spin to retrieve

Return type ndarray

Returns numpy.ndarray for the given coefficient and spin

property nspins: int
Return the number of spins of the current element. If mperp is True for the element it is 4 otherwise it is determined by the spins attribute

Return type int

static to_m_index(*m*)
Convert between magnetic quantum numbers between -l and l to 0 and 2l+1 for easier indexing

Parameters **m** (int) – int magnetic quantum number to convert

Return type int

Returns converted magnetic quantum number

static to_spin_indices(*spin*)
Convert between spin index (0 to 3) to the corresponding two spin indices (0 or 1)

Parameters **spin** (int) – int spin index to convert

Return type tuple[int, int]

Returns tuple of spin indices

trace_energy_dependence(*spin*, *imag=True*)
Select trace of data with energy dependence

Parameters

- **spin** (int) – integer spin between 1 and nspins
- **imag** (bool) – bool if True the imaginary part 1/2i(G(z)-G(z^*)) is returned otherwise the real part 1/2(G(z)+G(z^*))

Return type ndarray

Returns numpy array with the selected and traced over data

class masci_tools.tools.greensfunction.**GreensfElement**(*l*, *lp*, *atomType*, *atomTypep*, *sphavg*, *onsite*, *kresolved*, *contour*, *nLO*, *atomDiff*)

atomDiff
Alias for field number 9

atomType
Alias for field number 2

atomTypep
Alias for field number 3

contour
Alias for field number 7

kresolved
Alias for field number 6

l
Alias for field number 0

lp
Alias for field number 1

nLO
Alias for field number 8

onsite
Alias for field number 5

sphavg
Alias for field number 4

class masci_tools.tools.greensfunction.**colors**
Color strings for coloring terminal output

You may need to change color settings in iPython

masci_tools.tools.greensfunction.**intersite_shell_indices**(*elements*, *reference_atom*, *show=False*)
Construct the green's function pairs to calculate the Jij exchange constants for a given reference atom from a list of *GreensfElement*

Parameters

- **elements** (list[*GreensfElement*]) – list of GreenfElements to use
- **reference_atom** (int) – integer of the atom to calculate the Jij's for (correspinds to the i)
- **show** (bool) – if True the elements belonging to a shell are printed in a shell

Return type list[tuple[float, list[tuple[int, int]]]]

Returns list of tuples with distance and all indices of pairs in the shell

masci_tools.tools.greensfunction.**intersite_shells**(*greensfunctions*, *reference_atom*, *show=False*)
Construct the green's function pairs to calculate the Jij exchange constants for a given reference atom from a list of given *GreensFunction*

Parameters

- **greensfunctions** (list[*GreensFunction*]) – List of Greens Function to use
- **reference_atom** (int) – integer of the atom to calculate the Jij's for (correspinds to the i)
- **show** (bool) – if True the elements belonging to a shell are printed in a shell

Return type Iterator[tuple[float, *GreensFunction*, *GreensFunction*]]

Returns flat iterator with distance and the two corresponding *GreensFunction* instances for each Jij calculation

masci_tools.tools.greensfunction.**intersite_shells_from_file**(*hdffile*, *reference_atom*, *show=False*)
Construct the green's function pairs to calculate the Jij exchange constants for a given reference atom from a given `greensf.hdf` file

Parameters

- **hdffile** (Any) – filepath or file handle to a greensf.hdf file
- **reference_atom** (int) – integer of the atom to calculate the Jij's for (correspinds to the i)
- **show** (bool) – if True the elements belonging to a shell are printed in a shell

Return type Iterator[tuple[float, *GreensFunction*, *GreensFunction*]]

Returns flat iterator with distance and the two corresponding *GreensFunction* instances for each Jij calculation

masci_tools.tools.greensfunction.**listElements**(*hdffile*, *show=False*)
Find the green's function elements contained in the given `greens.hdf` file

Parameters

- **hdffile** (Any) – filepath or file handle to a greensf.hdf file
- **show** (bool) – bool if True the found elements are printed in a table

Return type list[*GreensfElement*]

Returns list of *GreensfElement*

masci_tools.tools.greensfunction.**printElements**(*elements*, *index=None*, *mark=None*)
Print the given list of *GreensfElement* in a nice table

Parameters

- **elements** (list[*GreensfElement*]) – list of *GreensfElement* to be printed
- **index** (Optional[list[int]]) – optional list of indices to show instead of the default index in the list
- **mark** (Optional[list[int]]) – optional list of int with elements to emphasize with an arrow and color

Return type None

masci_tools.tools.greensfunction.**select_element_indices**(*elements*, *show=False*, ***selection_params*)

Select *GreensfElement* objects from a list based on constraints on their values

Parameters

- **elements** (list[*GreensfElement*]) – list of *GreensfElement* to choose from
- **show** (bool) – bool if True the found elements will be printed

The Keyword arguments correspond to the names of the fields and their desired value

Return type list[int]

Returns list of the indices matching the criteria

masci_tools.tools.greensfunction.**select_elements**(*greensfunctions*, *show=False*, ***selection_params*)

Select *GreensFunction* objects from a list based on constraints on the values of their underlying *GreensfElement*

Parameters

- **greensfunctions** (list[*GreensFunction*]) – list of *GreensFunction* to choose from
- **show** (bool) – bool if True the found elements will be printed

The Keyword arguments correspond to the names of the fields and their desired value

Return type Iterator[*GreensFunction*]

Returns iterator over the matching *GreensFunction*

masci_tools.tools.greensfunction.**select_elements_from_file**(*hdffile*, *show=False*, ***selection_params*)

Construct the green's function mathcing specified criteria from a given `greensf.hdf` file

Parameters

- **hdffile** (Any) – file or file path to the `greensf.hdf` file
- **show** (bool) – bool if True the found elements will be printed

The Keyword arguments correspond to the names of the fields and their desired value

Return type Iterator[*GreensFunction*]

Returns iterator over the matching *GreensFunction*

This module collects functions for calculating properties with the greens functions calculated by Fleur. At the moment the following are implemented:

- Calculating Heisenberg J_0 (spin stiffness) from onsite Green's functions
- Calculating Heisenberg J_ij exchange constants from intersite Green's functions
- Calculating the hybridization function from onsite Greens functions

masci_tools.tools.greensf_calculations.**calculate_heisenberg_j0**(*greensfunction*, *onsite_delta*, *show=False*)

Calculate spin stiffness J_0 for the given green's function using the formula

$$J_0 = \frac{1}{4\pi}\mathrm{Im}\ \mathrm{Tr_L}\int_{-\infty}^{E_F} \mathrm{dz}\Delta\left(G^{\uparrow}(z) - G^{\downarrow}(z)\right) + \Delta^2 G^{\uparrow}(z)G^{\downarrow}(z)$$

Parameters

- **greensfunction** – *GreensFunction* to use for the calculation
- **onsite_delta** – onsite exchange splitting to use for the calculation
- **show** – bool if True additional information about the used Greens functions is printed out

Returns the value of the spin stiffness in meV

masci_tools.tools.greensf_calculations.**calculate_heisenberg_jij**(*hdffileORgreensfunctions*, *reference_atom*, *onsite_delta*, *show=False*)

Calculate the Heisenberg exchange constants form Green's functions using the formula

$$J_{ij} = \frac{1}{4\pi}\mathrm{Im}\ \mathrm{Tr_L}\int_{-\infty}^{E_F} \mathrm{dz}\Delta_i G_{ij}(z)\Delta_j G_{ji}(z)$$

Parameters

- **hdffileORgreensfunctions** – either pat/file-like object for the `greensf.hdf` file to use or list of *GreensFunction*
- **reference_atom** – integer index of the atom to calculate the Jijs from
- **onsite_delta** – List of floats containing the onsite exchange splitting for each atom type and l-channel
- **show** – bool if True additional information about the used Greens functions is printed out

Returns dict mapping the distances to all the calculated Jijs for that distance

masci_tools.tools.greensf_calculations.**calculate_hybridization**(*greensfunction*)

Calculate the hybridization function as

$$\Delta(z) = \frac{1}{2 * l + 1}\mathrm{Tr}G^{-1}(z)$$

Returns numpy array of the hybridization function

6.1.3 IO helper functions and file parsers

6.1.3.1 KKR related IO

In this module you find the kkrparams class that helps defining the KKR input parameters Also some defaults for the parameters are defined.

class masci_tools.io.kkr_params.**kkrparams**(***kwargs*)

Class for creating and handling the parameter input for a KKR calculation Optional keyword arguments are passed to init and stored in values dictionary.

Example usage: params = kkrparams(LMAX=3, BRAVAIS=array([[1,0,0], [0,1,0], [0,0,1]]))

Alternatively values can be set afterwards either individually with params.set_value('LMAX', 3)

or multiple keys at once with params.set_multiple_values(EMIN=-0.5, EMAX=1)

Other useful functions

- print the description of a keyword: params.get_description([key]) where [key] is a string for a keyword in params.values
- print a list of mandatory keywords: params.get_all_mandatory()
- print a list of keywords that are set including their value: params.get_set_values()

change_XC_val_kkrimp(*val*)
Convert integer value of KKRhost KEXCOR input to KKRimp XC string input.

fill_keywords_to_inputfile(*is_voro_calc=False*, *output='inputcard'*, *no_check=False*, *verbose=False*)
Fill new inputcard with keywords/values automatically check for input consistency (can be disabled by the no_check input) if is_voro_calc==True change mandatory list to match voronoi code, default is KKRcode

classmethod get_KKRcalc_parameter_defaults(*silent=False*)
set defaults (defined in header of this file) and returns dict, kkrparams_version

get_all_mandatory()
Return a list of mandatory keys

get_description(*key=None*, *search=None*)
Returns description of keyword 'key' If 'key' is None, print all descriptions of all available keywords If 'search' is not None, print all keys+descriptions where the search string is found

get_dict(*group=None*, *subgroup=None*)
Returns values dictionary.

Prints values belonging to a certain group only if the 'group' argument is one of the following: 'lattice', 'chemistry', 'accuracy', 'external fields', 'scf cycle', 'other'

Additionally the subgroups argument allows to print only a subset of all keys in a certain group. The following subgroups are available.

- in 'lattice' group '2D mode', 'shape functions'
- in 'chemistry' group 'Atom types', 'Exchange-correlation', 'CPA mode', '2D mode'
- in 'accuracy' group 'Valence energy contour', 'Semicore energy contour', 'CPA mode', 'Screening clusters', 'Radial solver', 'Ewald summation', 'LLoyd'

get_missing_keys(*use_aiida=False*)
Find list of mandatory keys that are not yet set

get_set_values()
Return a list of all keys/values that are set (i.e. not None)

get_type(*key*)
Extract expected type of 'key' from format info

get_value(*key*)
Gets value of keyword 'key'

is_mandatory(*key*)
Returns mandatory flag (True/False) for keyword 'key'

items()
make kkrparams.items() work

read_keywords_from_inputcard(*inputcard='inputcard'*, *verbose=False*)
Read list of keywords from inputcard and extract values to keywords dict

Example usage p = kkrparams(); p.read_keywords_from_inputcard('inputcard')

Note converts '<RBLEFT>', '<RBRIGHT>', 'ZPERIODL', and 'ZPERIODR' automatically to Ang. units!

remove_value(*key*)
Removes value of keyword 'key', i.e. resets to None

set_multiple_values(***kwargs*)
Set multiple values (in example value1 and value2 of keywords 'key1' and 'key2') given as key1=value1, key2=value2

set_value(*key*, *value*, *silent=False*)
Sets value of keyword 'key'

static split_kkr_options(*valtxt*)
Split keywords after fixed length of 8 :param valtxt: list of strings or single string :returns: List of keywords of maximal length 8

update_to_kkrimp()
Update parameter settings to match kkrimp specification. Sets self.__params_type and calls _update_mandatory_kkrimp()

update_to_voronoi()
Update parameter settings to match voronoi specification. Sets self.__params_type and calls _update_mandatory_voronoi()

masci_tools.io.kkr_read_shapefun_info.**read_shapefun**(*path='.'*)
Read vertices of shapefunctions with Zoom into shapefun of a single atom

Author Philipp Ruessmann

Parameters **path** – path where voronoi output is found (optional, defaults to './')

Returns pos positions of the centers of the shapefunctions

Returns out dictionary of the vertices of the shapefunctions

Here I collect all functions needed to parse the output of a KKR calculation. These functions do not need aiida and are therefore separated from the actual parser file where parse_kkr_outputfile is called

masci_tools.io.parsers.kkrparser_functions.**check_error_category**(*err_cat*, *err_msg*, *out_dict*)
Check if parser error of the non-critical category (err_cat != 1) are actually consistent and may be discarded.

Parameters

- **err_cat** – the error-category of the error message to be investigated
- **err_msg** – the error-message
- **out_dict** – the dict of results obtained from the parser function

Returns True/False if message is an error or warning

masci_tools.io.parsers.kkrparser_functions.**get_kmeshinfo**(*outfile_0init*, *outfile_000*)
Extract kmesh info from output.0.txt and output.000.txt

masci_tools.io.parsers.kkrparser_functions.**get_lattice_vectors**(*outfile_0init*)
read direct and reciprocal lattice vectors in internal units (useful for qdos generation)

masci_tools.io.parsers.kkrparser_functions.**get_natom**(*outfile_0init*)
extract NATYP value from output.0.txt

masci_tools.io.parsers.kkrparser_functions.**get_noco_rms**(*outfile*, *debug=False*)
Get average noco rms error

masci_tools.io.parsers.kkrparser_functions.**get_nspin**(*outfile_0init*)
extract NSPIN value from output.0.txt

masci_tools.io.parsers.kkrparser_functions.**get_orbmom**(*outfile*, *natom*)
read orbmom info from outfile and return array (iteration, atom)=orbmom

masci_tools.io.parsers.kkrparser_functions.**get_rms**(*outfile*, *outfile2*, *debug=False*)
Get rms error per atom (both values for charge and spin) and total (i.e. average) value

masci_tools.io.parsers.kkrparser_functions.**get_single_particle_energies**(*outfile_000*)
extracts single particle energies from outfile_000 (output.000.txt) returns the valence contribution of the single particle energies

masci_tools.io.parsers.kkrparser_functions.**get_spinmom_per_atom**(*outfile*, *natom*, *nonco_out_file=None*)
Extract spin moment information from outfile and nonco_angles_out (if given)

masci_tools.io.parsers.kkrparser_functions.**parse_array_float**(*outfile*, *searchstring*, *splitinfo*, *replacepair=None*, *debug=False*)
Search for keyword *searchstring* in *outfile* and extract array of results

Returns: array of results

masci_tools.io.parsers.kkrparser_functions.**parse_kkr_outputfile**(*out_dict*, *outfile*, *outfile_0init*, *outfile_000*, *timing_file*, *potfile_out*, *nonco_out_file*, *outfile_2='output.2.txt'*, *skip_readin=False*, *debug=False*)
Parser method for the kkr outfile. It returns a dictionary with results

masci_tools.io.parsers.kkrparser_functions.**use_BdG**(*outfile_0init*)
extract BdG run info from output.0.txt

masci_tools.io.parsers.kkrparser_functions.**use_newsosol**(*outfile_0init*)
extract NEWSOSOL info from output.0.txt

Everything that is needed to parse the output of a voronoi calculation.

masci_tools.io.parsers.voroparser_functions.**check_voronoi_output**(*potfile*, *outfile*, *delta_emin_safety=0.1*)
Read output from voronoi code and create guess of energy contour

masci_tools.io.parsers.voroparser_functions.**get_valence_min**(*outfile='out_voronoi'*)
Construct minimum of energy contour (between valence band bottom and core states)

masci_tools.io.parsers.voroparser_functions.**parse_voronoi_output**(*out_dict*, *outfile*, *potfile*, *atominfo*, *radii*, *inputfile*, *debug=False*)
Parse output of voronoi calculation and return (success, error_messages_list, out_dict)

Tools for the impurity caluclation plugin and its workflows

class masci_tools.io.parsers.kkrimp_parser_functions.**KkrimpParserFunctions**
Class of parser functions for KKRimp calculation

Usage success, msg_list, out_dict = parse_kkrimp_outputfile().parse_kkrimp_outputfile(out_dict, files)

parse_kkrimp_outputfile(*out_dict*, *file_dict*, *debug=False*)
Main parser function for kkrimp, read information from files in file_dict and fills out_dict :param out_dict: dictionary that is filled with parsed output of the KKRimp calculation :param file_dict: dictionary of files

that are parsed :returns: success (bool), msg_list(list of error/warning messages of parser), out_dict (filled dict of parsed output) :note: file_dict should contain the following keys

- 'outfile', the std_out of the KKRimp calculation
- 'out_log', the out_log.000.txt file
- 'out_pot', the output potential
- 'out_enersp_at', the out_energysp_per_atom_eV file
- 'out_enertot_at', the out_energytotal_per_atom_eV file
- 'out_timing', the timing file
- 'kkrflex_llyfac', the file for the Lloyd factor
- 'kkrflex_angles', the nonco_angles file for the KKRimp calculation
- 'out_spinmoms', the output spin moments file
- 'out_orbmoms', the output orbital moments file

6.1.3.2 Fleur related IO

Input/Output Parser

Load both the outxml_parser and inpxml_parser

masci_tools.io.parsers.fleur.**inpxml_parser**(*inpxmlfile*, *parser_info_out=None*, *strict=False*, *debug=False*, *base_url=None*)

Parses the given inp.xml file to a python dictionary utilizing the schema defined by the version number to validate and corretly convert to the dictionary

Parameters

- **inpxmlfile** – either path to the inp.xml file, opened file handle or a xml etree to be parsed
- **parser_info_out** – dict, with warnings, info, errors, ...
- **strict** – bool if True and no parser_info_out is provided any encountered error will immediately be raised

Returns python dictionary with the parsed inp.xml

Raises

- **ValueError** – If the validation against the schema failed, or an irrecoverable error occured during parsing
- **FileNotFoundError** – If no Schema file for the given version was found

masci_tools.io.parsers.fleur.**outxml_parser**(*outxmlfile*, *parser_info_out=None*, *iteration_to_parse='last'*, *minimal_mode=False*, *additional_tasks=None*, *optional_tasks=None*, *overwrite=False*, *append=False*, *list_return=False*, *strict=False*, *debug=False*, *ignore_validation=False*, *base_url=None*)

Parses the out.xml file to a dictionary based on the version and the given tasks

Parameters

- **outxmlfile** – either path to the out.xml file, opened file handle or a xml etree to be parsed
- **parser_info_out** – dict, with warnings, info, errors, ...

- **iteration_to_parse** – either str or int, (optional, default 'last') determines which iteration should be parsed. Accepted are 'all', 'first', 'last' or an index for the iteration
- **minimal_mode** – bool, if True only total Energy, iteration number and distances are parsed
- **additional_tasks** – dict to define custom parsing tasks. For detailed explanation See *default_parse_tasks*.
- **overwrite** – bool, if True and keys in additional_tasks collide with defaults The defaults will be overwritten
- **append** – bool, if True and keys in additional_tasks collide with defaults The inner tasks will be written into the dict. If inner keys collide they are overwritten
- **optional_tasks** – Iterable of strings, defines additional tasks to perform. See *default_parse_tasks* for examples.
- **list_return** – bool, if True one-item lists in the output dict are not converted to simple values
- **strict** – bool if True and no parser_info_out is provided any encountered error will immediately be raised
- **debug** – bool if True additional information is printed out in the logs
- **ignore_validation** – bool, if True schema validation errors are only logged

Returns python dictionary with the information parsed from the out.xml

Raises

- **ValueError** – If the validation against the schema failed, or an irrecoverable error occured during parsing
- **FileNotFoundError** – If no Schema file for the given version was found
- **KeyError** – If an unknown task is encountered

Inputgenerator related IO

This module contains functionality for writing input files for the input generator of fleur

class masci_tools.io.fleur_inpgen.**AtomDictProperties**
TypedDict for the atom properties

class masci_tools.io.fleur_inpgen.**Kinds**
TypedDict for the kinds

masci_tools.io.fleur_inpgen.**read_inpgen_file**(*file*, *convert_to_angstroem=True*)
Method which reads in an inpgen input file and parses the structure and name lists information.

Parameters

- **file** – path to the file to read or opened file handle
- **convert_to_angstroem** – bool if True the bravais matrix (and atom positions) are converted to angstroem

Returns tuple of bravais matrix, atom sites, periodic boundary conditions and parameters

masci_tools.io.fleur_inpgen.**write_inpgen_file**(*cell*, *atom_sites*, *kinds=None*, *return_contents=False*, *file='inpgen.in'*, *pbc=(True, True, True)*, *input_params=None*, *significant_figures_cell=9*, *significant_figures_positions=10*, *convert_from_angstroem=True*)

Write an input file for the fleur inputgenerator 'inpgen' from given inputs

Parameters

- **cell** – 3x3 arraylike. The bravais matrix of the structure, in Angstrom by default
- **atom_sites** – either list of a dict containing the keys absolute 'position' in Angstrom (default) and 'kind_name', i.e

```
[{'position': (0.0, 0.0, -1.0545708047819), 'kind_name': 'Fe123'},
 {'position': (1.4026317387183, 1.9836207751336, 0.0), 'kind_name':
↪'Pt'},
 {'position': (0.0, 0.0, 1.4026318234924), 'kind_name': 'Pt'}]
```

  In this case the argument `kinds` is required. The other possibility is a list of tuples of the form of *AtomSiteProperties*

- **kinds** – a list of kind information containing the keys symbols, weights, mass, name i.e.

```
[{'symbols': ('Fe',), 'weights': (1.0,), 'mass': 55.845, 'name':
↪'Fe123'},
 {'symbols': ('Pt',), 'weights': (1.0,), 'mass': 195.084, 'name
↪': 'Pt'}]
```

  Required when atom_sites is a list of dicts

- **file** – Path or filehandle where the file should be written to. Defaults to 'inpgen.in' in the current folder.
- **pbc** – tuple of boolean length 3, optional, Periodic boundary conditions of the structure. Defaults to (True, True, True).
- **input_params** – Optional dict containing further namelist which should be written to the file. Defaults to None.
- **significant_figures_cell** – int, how many decimal places should be written for the bravais matrix (default: 9)
- **significant_figures_positions** – int, how many decimal places should be written for the atom positions (default: 10)
- **convert_from_angstroem** – optional boolean, if True the positions and elements of the bravais matrix are converted to bohr from Angstroem

Raises `ValueError` – If some input is wrong or inconsistent.

Comments: This was extracted out of aiida-fleur for more general use, the datastructures stayed very close to what aiida provides (to_raw()), it may not yet be convenient for all usecases. I.e data so far has to be given in Angstrom and will be converted to fleur units. # This could be made optional

Functions for modifying the input file

This module contains a class for organizing and grouping changes to a input file of fleur in a robust way.

Essentially a low-level version of the FleurinpModifier in aiida_fleur.

class masci_tools.io.fleurxmlmodifier.**FleurXMLModifier**(*validate_signatures=True*)

Class for grouping and organizing changes to a inp.xml file of fleur via the xml setting methods in *xml_setters_names* and *xml_setters_basic*

The basic usage is shown below

```
from masci_tools.io.fleurxmlmodifier import FleurXMLModifier

fmode = FleurXMLModifier()

#Add changes by calling the methods on this class
#(names correspond to the setting methods in the xml_setters modules)
#They are not modifying a input file directly
#Instead all the tasks are collected and performed in one go

fmode.set_inpchanges({'Kmax': 4.0}) #Set Kmax to 4.0
fmode.shift_value({'Gmax': 5.0}) #Add 5 to the current value of Gmax

#Set the local orbital configuration on all iron atoms to '3s 3p'
fmode.set_species('all-Fe', {'lo': [{'n':3, 'l': 's', 'type': 'SCLO'},
                                    {'n':3, 'l': 'p', 'type': 'SCLO'}]})

#To undo the last change call undo
#fmode.undo()

#revert_all=True resets all added tasks
#fmode.undo(revert_all=True)

#To apply the changes to an input file use the modify_xmlfile method
new_xmltree = fmode.modify_xmlfile('/path/to/input/file/inp.xml')
```

add_number_to_attrib(**args*, ***kwargs*)

Appends a *add_number_to_attrib()* to the list of tasks that will be done on the xmltree.

Parameters

- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Return type None

add_number_to_first_attrib(**args*, ***kwargs*)

Appends a *add_number_to_first_attrib()* to the list of tasks that will be done on the xmltree.

Parameters

- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Return type None

add_task_list(*task_list*)

Add a list of tasks to be added

Parameters **task_list** (list[tuple[str, dict[str, Any]]]) – list of tuples first index is the name of the method second is defining the arguments by keyword in a dict

Return type None

classmethod apply_modifications(*xmltree*, *nmmp_lines*, *modification_tasks*, *validate_changes=True*)

Applies given modifications to the fleurinp lxml tree. It also checks if a new lxml tree is validated against schema. Does not rise an error if inp.xml is not validated, simple prints a message about it.

Parameters

- **xmltree** – a lxml tree to be modified (IS MODIFIED INPLACE)
- **nmmp_lines** – a n_mmp_mat file to be modified (IS MODIFIED INPLACE)
- **modification_tasks** – a list of modification tuples
- **validate_changes** – bool optional (default True), if True after all tasks are performed both the xmltree and nmmp_lines are checked for consistency

Returns a modified lxml tree and a modified n_mmp_mat file

changes()
Prints out all changes currently registered on this instance

Return type list[*ModifierTask*]

clone_species(**args*, ***kwargs*)
Appends a *clone_species()* to the list of tasks that will be done on the xmltree.

Parameters

- **species_name** – string, name of the specie you want to clone Has to correspond to one single species (no 'all'/'all-<search_string>')
- **new_name** – new name of the cloned species
- **changes** – a optional python dict specifying what you want to change.

Return type None

create_tag(**args*, ***kwargs*)
Appends a *create_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag** – str of the tag to create or etree Element with the same name
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **create_parents** – bool optional (default False), if True and the given xpath has no results the the parent tags are created recursively
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

delete_att(**args*, ***kwargs*)
Appends a *delete_att()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag** – str of the attribute to delete
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **occurrences** – int or list of int. Which occurence of the parent nodes to delete a attribute. By default all nodes are used.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Return type None

delete_tag(**args*, ***kwargs*)

Appends a *delete_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag** – str of the tag to delete
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **occurrences** – int or list of int. Which occurence of the parent nodes to delete a tag. By default all nodes are used.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

classmethod fromList(*task_list*, **args*, ***kwargs*)

Instantiate the FleurXMLModifier from a list of tasks to be added immediately

Parameters **task_list** (list[tuple[str, dict[str, Any]]]) – list of tuples first index is the name of the method second is defining the arguments by keyword in a dict

Other arguments are passed on to the __init__ method

Return type *FleurXMLModifier*

Returns class with the task list instantiated

get_avail_actions()

Returns the allowed functions from FleurXMLModifier

Return type dict[str, Callable]

modify_xmlfile(*original_inpxmlfile*, *original_nmmp_file=None*, *validate_changes=True*)

Applies the registered modifications to a given inputfile

Parameters

- **original_inpxmlfile** – either path to the inp.xml file, opened file handle or a xml etree to be parsed
- **original_nmmp_file** – path or list of str to a corresponding density matrix file

Raises **ValueError** – if the parsing of the input file

Returns a modified xmltree and if existent a modified density matrix file

replace_tag(**args*, ***kwargs*)

Appends a *replace_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag** – str of the tag to replace
- **newelement** – a new tag
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **occurrences** – int or list of int. Which occurence of the parent nodes to replace a tag. By default all nodes are used.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

rotate_nmmpmat(**args*, ***kwargs*)

Appends a *rotate_nmmpmat()* to the list of tasks that will be done on the xmltree.

Parameters

- **species_name** – string, name of the species you want to change
- **orbital** – integer, orbital quantum number of the LDA+U procedure to be modified
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Return type None

set_atomgroup(**args*, ***kwargs*)

Appends a *set_atomgroup()* to the list of tasks that will be done on the xmltree.

Parameters

- **attributedict** – a python dict specifying what you want to change.
- **position** – position of an atom group to be changed. If equals to 'all', all species will be changed
- **species** – atom groups, corresponding to the given species will be changed
- **create** – bool, if species does not exist create it and all subtags?
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a beta noco parameter it can be done via:

```
'attributedict': {'nocoParams': {'beta': val}}
```

Return type None

set_atomgroup_label(**args*, ***kwargs*)

Appends a *set_atomgroup_label()* to the list of tasks that will be done on the xmltree.

Parameters

- **atom_label** – string, a label of the atom which specie will be changed. 'all' to change all the species
- **attributedict** – a python dict specifying what you want to change.
- **create** – bool, if species does not exist create it and all subtags?

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a beta noco parameter it can be done via:

```
'attributedict': {'nocoParams': {'beta': val}}
```

Return type None

set_attrib_value(**args*, ***kwargs*)

Appends a *set_attrib_value()* to the list of tasks that will be done on the xmltree.

Parameters

- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Return type None

set_complex_tag(**args*, ***kwargs*)

Appends a *set_complex_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag_name** – name of the tag to set
- **attributedict** – Keys in the dictionary correspond to names of tags and the values are the modifications to do on this tag (attributename, subdict with changes to the subtag, ...)
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **create** – bool optional (default False), if True and the path, where the complex tag is set does not exist it is created

- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

set_first_attrib_value(**args*, ***kwargs*)

Appends a *set_first_attrib_value()* to the list of tasks that will be done on the xmltree.

Parameters

- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **create** – bool optional (default False), if True the tag is created if is missing
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Return type None

set_first_text(**args*, ***kwargs*)

Appends a *set_first_text()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag_name** – str name of the tag, where the text should be set
- **text** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **create** – bool optional (default False), if True the tag is created if is missing
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

set_inpchanges(**args*, ***kwargs*)
Appends a *set_inpchanges()* to the list of tasks that will be done on the xmltree.

Parameters

- **change_dict** – a dictionary with changes
- **path_spec** – dict, with ggf. necessary further specifications for the path of the attribute

An example of change_dict:

```
change_dict = {'itmax' : 1,
               'l_noco': True,
               'ctail': False,
               'l_ss': True}
```

Return type None

set_kpath(**args*, ***kwargs*)
Appends a *set_kpath()* to the list of tasks that will be done on the xmltree.

> **Warning:** This method is only supported for input versions before the Max5 release

Parameters

- **kpath** – a dictionary with kpoint name as key and k point coordinate as value
- **count** – number of k-points
- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Return type None

set_kpointlist(**args*, ***kwargs*)
Appends a *set_kpointlist()* to the list of tasks that will be done on the xmltree.

> **Warning:** For input versions Max4 and older **all** keyword arguments are not valid (*name*, *kpoint_type*, *special_labels*, *switch* and *overwrite*)

Parameters

- **kpoints** – list or array containing the **relative** coordinates of the kpoints
- **weights** – list or array containing the weights of the kpoints
- **name** – str for the name of the list, if not given a default name is generated
- **kpoint_type** – str specifying the type of the kPointList ('path', 'mesh', 'spex', 'tria', ...)
- **special_labels** – dict mapping indices to labels. The labels will be inserted for the kpoints corresponding to the given index
- **switch** – bool, if True the kPointlist will be used by Fleur when starting the next calculation
- **overwrite** – bool, if True and a kPointlist with the given name already exists it will be overwritten

Return type None

set_nkpts(**args*, ***kwargs*)
Appends a *set_nkpts()* to the list of tasks that will be done on the xmltree.

> **Warning:** This method is only supported for input versions before the Max5 release

Parameters

- **count** – number of k-points
- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Return type None

set_nmmpmat(**args*, ***kwargs*)
Appends a *set_nmmpmat()* to the list of tasks that will be done on the xmltree.

Parameters

- **species_name** – string, name of the species you want to change
- **orbital** – integer, orbital quantum number of the LDA+U procedure to be modified
- **spin** – integer, specifies which spin block should be modified
- **state_occupations** – list, sets the diagonal elements of the density matrix and everything else to zero
- **denmat** – matrix, specify the density matrix explicitely
- **phi** – float, optional angle (radian), by which to rotate the density matrix before writing it
- **theta** – float, optional angle (radian), by which to rotate the density matrix before writing it
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Return type None

set_simple_tag(**args*, ***kwargs*)
Appends a *set_simple_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag_name** – str name of the tag to modify/set
- **changes** – list of dicts or dict with the changes. Elements in list describe multiple tags. Keys in the dictionary correspond to {'attributename': attributevalue}
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **create_parents** – bool optional (default False), if True and the path, where the simple tags are set does not exist it is created
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

set_species(**args*, ***kwargs*)

Appends a *set_species()* to the list of tasks that will be done on the xmltree.

Parameters

- **species_name** – string, name of the specie you want to change Can be name of the species, 'all' or 'all-<string>' (sets species with the string in the species name)
- **attributedict** – a python dict specifying what you want to change.
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create** – bool, if species does not exist create it and all subtags?

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a MT radius it can be done via:

```
attributedict = {'mtSphere' : {'radius' : 2.2}}
```

Another example:

```
'attributedict': {'special': {'socscale': 0.0}}
```

that switches SOC terms on a sertain specie. `mtSphere`, `atomicCutoffs`, `energyParameters`, `lo`, `electronConfig`, `nocoParams`, `ldaU` and `special` keys are supported. To find possible keys of the inner dictionary please refer to the FLEUR documentation flapw.de

Return type None

set_species_label(**args*, ***kwargs*)

Appends a *set_species_label()* to the list of tasks that will be done on the xmltree.

Parameters

- **atom_label** – string, a label of the atom which specie will be changed. 'all' to change all the species
- **attributedict** – a python dict specifying what you want to change.

Return type None

set_text(**args*, ***kwargs*)

Appends a *set_text()* to the list of tasks that will be done on the xmltree.

Parameters

- **tag_name** – str name of the tag, where the text should be set
- **text** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

shift_value(**args*, ***kwargs*)

Appends a *shift_value()* to the list of tasks that will be done on the xmltree.

Parameters

- **change_dict** – a python dictionary with the keys to shift and the shift values.
- **mode** – 'abs' if change given is absolute, 'rel' if relative
- **path_spec** – dict, with ggf. necessary further specifications for the path of the attribute

An example of change_dict:

```
change_dict = {'itmax' : 1, 'dVac': -0.123}
```

Return type None

shift_value_species_label(**args*, ***kwargs*)

Appends a *shift_value_species_label()* to the list of tasks that will be done on the xmltree.

Parameters

- **atom_label** – string, a label of the atom which specie will be changed. 'all' if set up all species
- **attributename** – name of the attribute to change
- **value_given** – value to add or to multiply by
- **mode** – 'rel' for multiplication or 'abs' for addition

Kwargs if the attributename does not correspond to a unique path:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Return type None

switch_kpointset(**args*, ***kwargs*)

Appends a *switch_kpointset()* to the list of tasks that will be done on the xmltree.

Warning: This method is only supported for input versions after the Max5 release

Parameters **list_name** – name of the kPoint set to use

Return type None

switch_species(**args*, ***kwargs*)

Appends a *switch_species()* to the list of tasks that will be done on the xmltree.

Parameters

- **new_species_name** – name of the species to switch to

- **position** – position of an atom group to be changed. If equals to 'all', all species will be changed
- **species** – atom groups, corresponding to the given species will be changed
- **clone** – if True and the new species name does not exist and it corresponds to changing from one species the species will be cloned with *clone_species()*
- **changes** – changes to do if the species is cloned
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details`

Return type None

switch_species_label(**args*, ***kwargs*)

Appends a *switch_species_label()* to the list of tasks that will be done on the xmltree.

Parameters

- **atom_label** – string, a label of the atom which group will be changed. 'all' to change all the groups
- **new_species_name** – name of the species to switch to
- **clone** – if True and the new species name does not exist and it corresponds to changing from one species the species will be cloned with *clone_species()*
- **changes** – changes to do if the species is cloned

Return type None

undo(*revert_all=False*)

Cancels the last change or all of them

Parameters **revert_all** (bool) – set True if need to cancel all the changes, False if the last one.

Return type list[*ModifierTask*]

xml_create_tag(**args*, ***kwargs*)

Appends a *xml_create_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path where to place a new tag
- **element** – a tag name or etree Element to be created
- **place_index** – defines the place where to put a created tag
- **tag_order** – defines a tag order
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Return type None

xml_delete_att(**args*, ***kwargs*)

Appends a *xml_delete_att()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path to the attribute to be deleted
- **attrib** – the name of an attribute

- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Return type None

xml_delete_tag(**args*, ***kwargs*)
Appends a *xml_delete_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path to the tag to be deleted
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Return type None

xml_replace_tag(**args*, ***kwargs*)
Appends a *xml_replace_tag()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path to the tag to be replaced
- **newelement** – a new tag
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Return type None

xml_set_attrib_value_no_create(**args*, ***kwargs*)
Appends a *xml_set_attrib_value_no_create()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path where to set the attributes
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set (if not str they will be converted with *str(value)*)
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.

Return type None

xml_set_text_no_create(**args*, ***kwargs*)
Appends a *xml_set_text_no_create()* to the list of tasks that will be done on the xmltree.

Parameters

- **xpath** – a path where to set the attributes
- **text** – value or list of values to set (if not str they will be converted with *str(value)*)
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.

Return type None

class masci_tools.io.fleurxmlmodifier.**ModifierTask**(*name*, *args*, *kwargs*)

args: tuple[typing.Any, ...]
Alias for field number 1

kwargs: dict[str, typing.Any]
Alias for field number 2

name: str
Alias for field number 0

Functions/Classes for loading/validating fleur XML files

This module provides the classes for easy acces to information from the fleur input and output xsd schema files

masci_tools.io.parsers.fleur_schema.schema_dict.**F**
Generic Type variable for callable

alias of TypeVar('F', bound=Callable[[...], Any])

class masci_tools.io.parsers.fleur_schema.schema_dict.**InputSchemaDict**(**args*, *xmlschema=None*, ***kwargs*)
This class contains information parsed from the FleurInputSchema.xsd

The keys contain the following information:

inp_version Version string of the input schema represented in this object

tag_paths simple xpath expressions to all valid tag names Multiple paths or ambiguous tag names are parsed as a list

_basic_types Parsed definitions of all simple Types with their respective base type (int, float, ...) and evtl. length restrictions (Only used in the schema construction itself)

attrib_types All possible base types for all valid attributes. If multiple are possible a list, with 'string' always last (if possible)

simple_elements All elements with simple types and their type definition with the additional attributes

unique_attribs All attributes and their paths, which occur only once and have a unique path

unique_path_attribs All attributes and their paths, which have a unique path but occur in multiple places

other_attribs All attributes and their paths, which are not in 'unique_attribs' or 'unique_path_attribs'

omitt_contained_tags All tags, which only contain a list of one other tag

tag_info For each tag (path), the valid attributes and tags (optional, several, order, simple, text)

classmethod fromPath(*path*)
load the FleurInputSchema dict for the specified FleurInputSchema file

Parameters **path** (PathLike) – path to the input schema file

Return type *InputSchemaDict*

Returns InputSchemaDict object with the information for the provided file

classmethod fromVersion(*version*, *logger=None*, *no_cache=False*)
load the FleurInputSchema dict for the specified version

Parameters

- **version** – str with the desired version, e.g. '0.33'

- **logger** – logger object for warnings, errors and information, ...

Returns InputSchemaDict object with the information for the provided version

property inp_version: tuple[int, int]
Returns the input version as an integer for comparisons (> or <)

Return type tuple[int, int]

exception masci_tools.io.parsers.fleur_schema.schema_dict.**NoPathFound**
Exception raised when no path is found for a given tag/attribute

exception masci_tools.io.parsers.fleur_schema.schema_dict.**NoUniquePathFound**
Exception raised when no unique path is found for a given tag/attribute

class masci_tools.io.parsers.fleur_schema.schema_dict.**OutputSchemaDict**(**args*, *xmlschema=None*, ***kwargs*)
This object contains information parsed from the FleurOutputSchema.xsd

The keys contain the following information:

out_version Version string of the output schema represented in this class

input_tag Name of the element containing the fleur input

iteration_tags Names of the elements that can contain all iteration tags

tag_paths simple xpath expressions to all valid tag names not in an iteration Multiple paths or ambiguous tag names are parsed as a list

iteration_tag_paths simple relative xpath expressions to all valid tag names inside an iteration. Multiple paths or ambiguous tag names are parsed as a list

_basic_types Parsed definitions of all simple Types with their respective base type (int, float, ...) and evtl. length restrictions (Only used in the schema construction itself)

_input_basic_types Part of the parsed definitions of all simple Types with their respective base type (int, float, ...) and evtl. length restrictions from the input schema (Only used in the schema construction itself)

attrib_types All possible base types for all valid attributes. If multiple are possible a list, with 'string' always last (if possible)

simple_elements All elements with simple types and their type definition with the additional attributes

unique_attribs All attributes and their paths, which occur only once and have a unique path outside of an iteration

unique_path_attribs All attributes and their paths, which have a unique path but occur in multiple places outside of an iteration

other_attribs All attributes and their paths, which are not in 'unique_attribs' or 'unique_path_attribs' outside of an iteration

iteration_unique_attribs All attributes and their relative paths, which occur only once and have a unique path inside of an iteration

iteration_unique_path_attribs All attributes and their relative paths, which have a unique path but occur in multiple places inside of an iteration

iteration_other_attribs All attributes and their relative paths, which are not in 'unique_attribs' or 'unique_path_attribs' inside of an iteration

omitt_contained_tags All tags, which only contain a list of one other tag

tag_info For each tag outside of an iteration (path), the valid attributes and tags (optional, several, order, simple, text)

iteration_tag_info For each tag inside of an iteration (relative path), the valid attributes and tags (optional, several, order, simple, text)

classmethod fromPath(*path*, *inp_path=None*, *inpschema_dict=None*)
load the FleurOutputSchema dict for the specified paths

Parameters

- **path** – path to the FleurOutputSchema file
- **inp_path** – path to the FleurInputSchema file (defaults to same folder as path)

Returns OutputSchemaDict object with the information for the provided files

classmethod fromVersion(*version*, *inp_version=None*, *logger=None*, *no_cache=False*)
load the FleurOutputSchema dict for the specified version

Parameters

- **version** – str with the desired version, e.g. '0.33'
- **inp_version** – str with the desired input version, e.g. '0.33' (defaults to version)
- **logger** – logger object for warnings, errors and information, ...

Returns OutputSchemaDict object with the information for the provided versions

property inp_version: tuple[int, int]
Returns the input version as an integer for comparisons (> or <)

Return type tuple[int, int]

iteration_attrib_xpath(*name*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*, *iteration_tag='iteration'*)
Tries to find a unique path from the schema_dict based on the given name of the attribute and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the attribute
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *iteration_tag_xpath()*
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath to the tag with the given attribute

Raises

- ***NoPathFound*** – If no path matching the criteria could be found
- ***NoUniquePathFound*** – If multiple paths matching the criteria are found

iteration_tag_xpath(*name*, *contains=None*, *not_contains=None*, *iteration_tag='iteration'*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

property out_version: tuple[int, int]

Returns the output version as an integer for comparisons (> or <)

Return type tuple[int, int]

relative_iteration_attrib_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*, *iteration_tag='iteration'*)

Tries to find a unique relative path from the schema_dict based on the given name of the attribute name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *relative_iteration_tag_xpath()*
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

relative_iteration_tag_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *iteration_tag='iteration'*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the tag

- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

class masci_tools.io.parsers.fleur_schema.schema_dict.**SchemaDict**(**args*, *xmlschema=None*, ***kwargs*)

Base class for schema dictionaries. Is locked on initialization with *freeze()*. Holds a reference to the xmlSchema for validating files.

Also provides interfaces for utility functions

Parameters **xmlschema** – etree.XMLSchema object for validating files

All other arguments are passed on to *LockableDict*

attrib_xpath(*name*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

Tries to find a unique path from the schema_dict based on the given name of the attribute and additional further specifications

Parameters

- **name** – str, name of the attribute
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *tag_xpath()*

Returns str, xpath to the tag with the given attribute

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

classmethod clear_cache()

Remove all stored entries in the schema dictionary cache

Return type None

relative_attrib_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

Tries to find a unique relative path from the schema_dict based on the given name of the attribute name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **root_tag** – str, name of the tag from which the path should be relative

- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *relative_tag_xpath()*

Returns str, xpath for the given tag

Raises

- ***NoPathFound*** – If no path matching the criteria could be found
- ***NoUniquePathFound*** – If multiple paths matching the criteria are found

relative_tag_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*)

Tries to find a unique relative path from the schema_dict based on the given name of the tag name of the root, from which the path should be relative and additional further specifications

Parameters

- **name** – str, name of the tag
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises **ValueError** – If no unique path could be found

tag_info(*name*, *contains=None*, *not_contains=None*, *parent=False*, ***kwargs*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications and returns the tag_info entry for this tag

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **parent** – bool, if True the tag_info for the parent of the tag is returned

Returns dict, tag_info for the found xpath

tag_xpath(*name*, *contains=None*, *not_contains=None*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications

Parameters

- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

class masci_tools.io.parsers.fleur_schema.schema_dict.**SchemaDictDispatch**(**args*, ***kwargs*)
Protocol representing function decorated by the schema_dict_version_dispatch decorator

register(*min_version=...*, *max_version=...*)
Register a virtual subclass of an ABC.

Returns the subclass, to allow usage as a class decorator.

masci_tools.io.parsers.fleur_schema.schema_dict.**list_available_versions**(*output_schema*)
List the available versions for the schema

Parameters **output_schema** (bool) – bool, if True search for FleurOutputSchema.xsd otherwise FleurInputSchema.xsd

Return type list[str]

Returns list version string of the available versions

masci_tools.io.parsers.fleur_schema.schema_dict.**schema_dict_version_dispatch**(*output_schema=False*)
Decorator for creating variations of functions based on the inp/out version of the schema_dict. All functions here need to have the signature:

```
def f(node, schema_dict, *args, **kwargs):
    pass
```

So schema_dict is the second positional argument

Inspired by singledispatch in the functools module

Return type Callable[[~F], *SchemaDictDispatch*]

This module provides easy functions for loading a input/output xml file of fleur and providing a parsed xml etree together with its corresponding schema dict

masci_tools.io.io_fleurxml.**load_inpxml**(*inpxmlfile*, *logger=None*, *base_url=None*, ***kwargs*)
Loads a inp.xml file for fleur together with its corresponding schema dictionary

Parameters **inpxmlfile** – either path to the inp.xml file, opened file handle or a xml etree to be parsed

Returns parsed xmltree of the inpxmlfile and the schema dictionary for the corresponding input version

masci_tools.io.io_fleurxml.**load_outxml**(*outxmlfile*, *logger=None*, *base_url=None*, ***kwargs*)
Loads a out.xml file for fleur together with its corresponding schema dictionary

Parameters **outxmlfile** – either path to the out.xml file, opened file handle or a xml etree to be parsed

Returns parsed xmltree of the outxmlfile and the schema dictionary for the corresponding output version

Helper functions for the n_mmp_mat file

Simple IO routines for creating text for nmmp_mat files

masci_tools.io.io_nmmpmat.**format_nmmpmat**(*denmat*)
Format a given 7x7 complex numpy array into the format for the n_mmp_mat file

Results in list of 14 strings. Every 2 lines correspond to one row in array Real and imaginary parts are formatted with 20.13f in alternating order

Parameters **denmat** (ndarray) – numpy array (7x7) and complex for formatting

Raises **ValueError** – If denmat has wrong shape or datatype

Return type list[str]

Returns list of str formatted in lines for the n_mmp_mat file

masci_tools.io.io_nmmpmat.**read_nmmpmat_block**(*nmmp_lines*, *block_index*)
Convert 14 line block of given nmmp_lines into 7x7 complex numpy array

Parameters

- **nmmplines** – list of lines in the n_mmp_mat file
- **block_index** (int) – int specifying which 14 line block to convert

Return type ndarray

Returns 7x7 complex numpy array of the numbers in the given block

masci_tools.io.io_nmmpmat.**rotate_nmmpmat_block**(*denmat*, *orbital*, *phi=None*, *theta=None*)
Rotate the given 7x7 complex numpy array with the d-wigner matrix corresponding to the given orbital and angles

Parameters

- **denmat** – complex numpy array of shape 7x7
- **orbital** – int of the orbital for the current block
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix

Returns denmat rotated by the d-wigner matrix

masci_tools.io.io_nmmpmat.**write_nmmpmat**(*orbital*, *denmat*, *phi=None*, *theta=None*)
Generate list of str for n_mmp_mat file from given numpy array

Parameters

- **orbital** – int of the orbital for the current block
- **denmat** – complex numpy array of shape (2*orbital+1 x 2*orbital+1) with the wanted occupations
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix

Returns list of str formatted in lines for the n_mmp_mat file

masci_tools.io.io_nmmpmat.**write_nmmpmat_from_orbitals**(*orbital*, *orbital_occupations*, *phi=None*, *theta=None*)
Generate list of str for n_mmp_mat file from orbital occupations

orbital occupations are provided in the following order (expressed as the spherical harmonics since it can be used for all orbitals):

- Y_l^0
- 1/sqrt(2) (Y_l^-1 + Y_l^1)
- i/sqrt(2) (Y_l^-1 - Y_l^1)
- 1/sqrt(2) (Y_l^-2 + Y_l^2)
- i/sqrt(2) (Y_l^-2 - Y_l^2)
- and so on …

Parameters

- **orbital** – int of the orbital for the current block
- **orbital_occupations** – list like with length 2*orbital+1 with the occupations of the orbitals
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix

Returns list of str formatted in lines for the n_mmp_mat file

masci_tools.io.io_nmmpmat.**write_nmmpmat_from_states**(*orbital*, *state_occupations*, *phi=None*, *theta=None*)

Generate list of str for n_mmp_mat file from diagonal occupations

Parameters

- **orbital** – int of the orbital for the current block
- **state_occupations** – list like with length 2*orbital+1 with the occupations of the diagonals
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix

Returns list of str formatted in lines for the n_mmp_mat file

6.1.3.3 General HDF5 parser

This module contains a generic HDF5 reader

class masci_tools.io.parsers.hdf5.reader.**AttribTransformation**(*name*, *attrib_name*, *args=()*, *kwargs={}*)

args: tuple[typing.Any, ...]
Alias for field number 2

attrib_name: str
Alias for field number 1

kwargs: dict[str, typing.Any]
Alias for field number 3

name: str
Alias for field number 0

class masci_tools.io.parsers.hdf5.reader.**HDF5LimitedTransformation**

class masci_tools.io.parsers.hdf5.reader.**HDF5Reader**(*file*, *move_to_memory=True*)

Class for reading in data from hdf5 files using a specified recipe

Parameters

- **file** – filepath to hdf file or opened file handle (mode 'rb')
- **move_to_memory** – bool if True after reading and transforming the data all leftover h5py.Datasets are moved into np.arrays

The recipe is passed to the *HDF5Reader.read()* method and consists of a dict specifiying which attributes and datasets to read in and how to transform them

Each attribute/dataset entry corresponds to one entry point in the given *.hdf* file Available transformations can either be found in *transforms* or can be defined by the user with the *hdf5_transformation()* decorator

Basic Usage:

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
import masci_tools.io.parsers.hdf5.recipes as recipes

#This example shows the usage for producing data from a bandstructure calculation
#in Fleur
with HDF5Reader('/path/to/hdf/banddos.hdf') as h5reader:
    data, attributes = h5reader.read(recipe=recipes.FleurBands)
print(data, attributes)
```

read(*recipe=None*)

Extracts datasets from HDF5 file, transforms them and puts all into a namedtuple.

Parameters **recipe** – dict with the format given in *recipes*

Returns two dicts with the datasets/attributes read in and transformed according to the recipe

class masci_tools.io.parsers.hdf5.reader.**HDF5Recipe**

class masci_tools.io.parsers.hdf5.reader.**HDF5Transformation**

class masci_tools.io.parsers.hdf5.reader.**Transformation**(*name*, *args=()*, *kwargs={}*)

args: tuple[typing.Any, ...]

Alias for field number 1

kwargs: dict[str, typing.Any]

Alias for field number 2

name: str

Alias for field number 0

This module defines commonly used recipes for the *HDF5Reader*

Available are:

- Recipe for bandstructure calculations with Fleur
- Recipes for almost all DOS calculation modes of Fleur

A Recipe is a python dictionary in a specific format.

A Template Example:

```
from masci_tools.io.parser.hdf5.readers import Transformation, AttribTransformation

RecipeExample = {
    'datasets': {
        'example_dataset': {
            'h5path': '/path/in/hdf/file',
            'transforms': [Transformation(name='get_first_element')]
        },
        'example_attrib_transform': {
            'h5path': '/other/path/in/hdf/file',
            'transforms': [AttribTransformation(name='multiply_by_attribute', attrib_
↪name='example_attribute')]
        }
    },
    'attributes': {
        'example_attribute': {
            'h5path':
            '/path/in/hdf/file',
            'transforms':
            [Transformation(name='get_attribute', args=('attribName',)),
             Transformation(name='get_first_element')]
        }
    }
}
```

The Recipe consists of two sections 'datasets' and 'attributes'. All data from these two sections will be returned in separate python dictionaries by the *HDF5Reader* class

Each entry in those sections has to have a *h5path* entry, which will specify the dataset to initially read from the hdf file. Then each entry can define a entry *transforms* with a list of the namedtuples imported at the top of the code example. These correponds to function calls to functions in *transforms* to transform the read in data

Entries in the *attributes* section are read and transformed first and can subsequently be used in transformations for the *datasets*. These correpsond to the transforms created with the *AttribTransformation* namedtuple instead of *Transformation*.

masci_tools.io.parsers.hdf5.recipes.**bands_recipe_format**(*group*, *simple=False*)

Format for bandstructure calculations retrieving weights from the given group

Parameters

- **group** (Literal['Local', 'jDOS', 'Orbcomp', 'MCD']) – str of the group the weights should be taken from
- **simple** (bool) – bool, if True no additional weights are retrieved with the produced recipe

Return type *HDF5Recipe*

Returns dict of the recipe to retrieve a bandstructure calculation

masci_tools.io.parsers.hdf5.recipes.**dos_recipe_format**(*group*)

Format for denisty of states calculations retrieving the DOS from the given group

Parameters **group** (Literal['Local', 'jDOS', 'Orbcomp', 'MCD']) – str of the group the DOS should be taken from

Return type *HDF5Recipe*

Returns dict of the recipe to retrieve a DOS calculation

masci_tools.io.parsers.hdf5.recipes.**get_fleur_bands_specific_weights**(*weight_name*, *group='Local'*)

Recipe for bandstructure calculations only retrieving one additional weight besides the eigenvalues and kpath

Parameters

- **weight_name** – key or list of keys of the weight(s) to retrieve
- **group** – optional str (default Local) name of the group from where to take the weights

Returns dict of the recipe to retrieve a simple bandstructure plus the one specified weight

Collection of predefined transformations for the *HDF5Reader* class

All Transformation have to be able to handle (or fail gracefully with a clear error) for the following 3 cases:

1. The dataset is still a h5py.Dataset and might need to be transformed to a numpy array
2. The dataset is a numpy array
3. The dataset is a dict. This is needed to read arbitrary child dataset, where not all labels are known. Two options can be chosen apply the transformation to all keys in the dict or throw an error

exception masci_tools.io.parsers.hdf5.transforms.**HDF5TransformationError**

masci_tools.io.parsers.hdf5.transforms.**add_partial_sums**(*dataset*, *attribute_value*, *pattern_format*, *make_set=False*, *replace_entries=None*)

Add entries to the dataset dict (Only avalaible for dict datasets) with sums over entries containing a given pattern formatted with a attribute_value

Used for example in the FleurBands recipe to calculate total atom weights with the pattern_format *'MT:{}'.format* and the atomtype as the attribute_value

Parameters

- **dataset** – dataset to transform
- **attribute_value** – value to multiply by (attribute value passed in from *_transform_dataset*)
- **pattern_format** – callable returning a formatted string This will be called with every entry in the attribute_value list
- **replace_entries** – list of str under which to enter the entries back

Returns dataset with new entries containing the sums over entries matching the given pattern

masci_tools.io.parsers.hdf5.transforms.**add_partial_sums_fixed**(*dataset*, *patterns*, *replace_entries=None*)

Add entries to the dataset dict (Only avalaible for dict datasets) with sums over entries containing a given pattern

Used for example in the FleurBands recipe to calculate total atom weights with the patterns *['MT:1', 'MT:2', ...]*

Parameters

- **dataset** – dataset to transform
- **patterns** – list of str to sum entries over
- **replace_entries** – list of str under which to enter the entries back

Returns dataset with new entries containing the sums over entries matching the given pattern

masci_tools.io.parsers.hdf5.transforms.**apply_lambda**(*dataset*, *lambda_func*)

Applies a given lambda function to the dataset This should be used with care. One possible example is converting to a boolean with lambda x: x==1

Parameters

- **dataset** – dataset to transform
- **lambda_func** – lambda function to apply to the dataset

Returns return value of the lambda function

masci_tools.io.parsers.hdf5.transforms.**attributes**(*dataset*)
Extracts all attributes of the dataset

Parameters **dataset** – dataset to transform

Returns dict with all the set attributes on the dataset

masci_tools.io.parsers.hdf5.transforms.**calculate_norm**(*dataset*, *between_neighbours=False*)
Calculate norms on the given dataset. Calculates the norm of each row in the dataset

Parameters

- **dataset** – dataset to transform
- **between_neighbours** – bool, if True the distance between subsequent entries in the dataset is calculated

Returns norms of the given dataset

masci_tools.io.parsers.hdf5.transforms.**convert_to_complex_array**(*dataset*)
Converts the given dataset of real numbers into dataset of complex numbers. This follows the convention of how complex numbers are normally written out by Fleur (last index 0 real part, last index 1 imag part)

Parameters **dataset** – dataset to transform

Returns dataset with complex values

masci_tools.io.parsers.hdf5.transforms.**convert_to_str**(*dataset*, *join=False*)
Converts the given dataset to a numpy array of type string

Parameters

- **dataset** – dataset to transform
- **join** – bool if True the result will be joined together

Returns numpy array of dtype str

masci_tools.io.parsers.hdf5.transforms.**cumulative_sum**(*dataset*, *beginning_zero=True*)
Calculate the cumulative sum of the dataset

Parameters **dataset** – dataset to transform

Returns cumulative sum of the dataset

masci_tools.io.parsers.hdf5.transforms.**flatten_array**(*dataset*, *order='C'*)
Flattens the given dataset to one dimensional array. Copies the array !!

Parameters

- **dataset** – dataset to transform
- **order** – str $\{C, F, A, K\}$ flatten in column major or row-major order (see numpy.flatten documentation)

Returns flattened dataset

masci_tools.io.parsers.hdf5.transforms.**get_all_child_datasets**(*group*, *ignore=None*, *contains=None*)

Get all datasets contained in the given group

Parameters

- **group** – h5py object to extract from
- **ignore** – str or iterable of str (optional). These keys will be ignored
- **contains** – str or iterable of str (optional). This phrase has to be in the key

Returns a dict with the contained dataset entered with their names as keys

masci_tools.io.parsers.hdf5.transforms.**get_attribute**(*dataset*, *attribute_name*)

Extracts a specified attribute's value.

Parameters

- **dataset** – dataset to transform
- **attribute_name** – str of the attribute to extract from the dataset

Returns value of the attribute on the dataset

masci_tools.io.parsers.hdf5.transforms.**get_first_element**(*dataset*)

Get the first element of the dataset.

Parameters **dataset** – dataset to transform

Returns first element of the dataset

masci_tools.io.parsers.hdf5.transforms.**get_name**(*dataset*, *full_path=False*)

Get the name of the dataset.

Parameters

- **dataset** – dataset to get the shape
- **full_path** – bool, if True the full path to the dataset is returned

Returns name of the dataset

masci_tools.io.parsers.hdf5.transforms.**get_shape**(*dataset*)

Get the shape of the dataset.

Parameters **dataset** – dataset to get the shape

Returns shape of the dataset

masci_tools.io.parsers.hdf5.transforms.**hdf5_transformation**(*, *attribute_needed*)

Decorator for registering a function as a transformation functions on the *HDF5Reader* class

Parameters **attribute_needed** (bool) – bool if True this function takes a previously processed attribute value and is therefore only available for the entries in datasets

Return type Callable

masci_tools.io.parsers.hdf5.transforms.**index_dataset**(*dataset*, *index*)

Get the n-th element of the dataset.

Parameters **dataset** – dataset to transform

Returns first element of the dataset

masci_tools.io.parsers.hdf5.transforms.**merge_subgroup_datasets**(*group*, *ignore=None*, *contains=None*, *ignore_group=None*, *contains_group=None*, *stack_results=True*, *sort_key=None*)

Get all datasets contained in the given group

Parameters

- **group** – h5py object to extract from
- **ignore_group** – str or iterable of str (optional). These keys will be ignored
- **contains_group** – str or iterable of str (optional). This phrase has to be in the key
- **ignore** – str or iterable of str (optional). These keys of the datasets in the subgroup will be ignored
- **contains** – str or iterable of str (optional). This phrase has to be in the key of the datasets in the subgroup
- **stack_results** – bool if True the resulting list of datasets will be used to construct one numpy array

Returns a dict with the contained dataset of the subgroups of the given group entered with their names as keys

masci_tools.io.parsers.hdf5.transforms.**move_to_memory**(*dataset*)

Moves the given dataset to memory, if it's not already there Creates numpy arrays for each dataset it finds

Parameters **dataset** – dataset to transform

Returns dataset with h5py.Datasets converted to numpy arrays

masci_tools.io.parsers.hdf5.transforms.**multiply_array**(*dataset*, *matrix*, *transpose=False*)

Multiply the given dataset with a matrix

Parameters

- **dataset** – dataset to multiply
- **matrix** – matrix to multiply by
- **transpose** – bool, if True the given matrix is transposed

Returns dataset multiplied with the given matrix

masci_tools.io.parsers.hdf5.transforms.**multiply_by_attribute**(*dataset*, *attribute_value*, *transpose=False*)

Multiply the given dataset with a previously parsed attribute, either scalar or matrix like

Parameters

- **dataset** – dataset to transform
- **attribute_value** – value to multiply by (attribute value passed in from *_transform_dataset*)

Only relevant for matrix multiplication:

param transpose bool if True the Matrix order is transposed before multiplying

Returns dataset multiplied with the given attribute_value

masci_tools.io.parsers.hdf5.transforms.**multiply_scalar**(*dataset*, *scalar_value*)
Multiply the given dataset with a scalar_value

Parameters

- **dataset** – dataset to transform
- **scalar_value** – value to mutiply the dataset by

Returns the dataset multiplied by the scalar if it is a dict all entries are multiplied

masci_tools.io.parsers.hdf5.transforms.**periodic_elements**(*dataset*)

Converts the given dataset (int or list of ints) To the atomic symbols corresponding to the atomic number

Parameters **dataset** – dataset to transform

Returns str or array of str with the atomic elements

masci_tools.io.parsers.hdf5.transforms.**repeat_array**(*dataset*, *n_repeats*)
Use numpy.repeat to repeat each element in array n-times

Parameters

- **dataset** – dataset to transform
- **n_repeats** – int, time to repeat each element

Returns dataset with elements repeated n-times

masci_tools.io.parsers.hdf5.transforms.**repeat_array_by_attribute**(*dataset*, *attribute_value*)
Use numpy.repeat to repeat each element in array n-times (given by attribute_value)

Parameters

- **dataset** – dataset to transform
- **attribute_shape** – int, time to repeat the elements in the given array

Returns dataset with elements repeated n-times

masci_tools.io.parsers.hdf5.transforms.**shift_by_attribute**(*dataset*, *attribute_value*, *negative=False*)
Shift the dataset by the given value of the attribute

Parameters

- **dataset** – dataset to transform
- **attribute_value** – value to shift the dataset by
- **negative** – bool, if True the scalar_value will be substracted

Returns the dataset shifted by the scalar if it is a dict all entries are shifted

masci_tools.io.parsers.hdf5.transforms.**shift_dataset**(*dataset*, *scalar_value*, *negative=False*)
Shift the dataset by the given scalar_value

Parameters

- **dataset** – dataset to transform
- **scalar_value** – value to shift the dataset by
- **negative** – bool, if True the scalar_value will be substracted

Returns the dataset shifted by the scalar if it is a dict all entries are shifted

masci_tools.io.parsers.hdf5.transforms.**slice_dataset**(*dataset*, *slice_arg*)
Slice the dataset with the given slice argument.

Parameters

- **dataset** – dataset to transform
- **slice_arg** – slice to apply to the dataset

Returns first element of the dataset

masci_tools.io.parsers.hdf5.transforms.**split_array**(*dataset*, *suffixes=None*, *name=None*)
Split the arrays in a dataset into multiple entries by their first index

If the dataset is a dict the entries will be split up. If the dataset is not a dict a dict is created with the dataset entered under *name* and this will be split up

Parameters

- **dataset** – dataset to transform
- **suffix** – Optional list of str to use for suffixes for the split up entries. by default it is the value of the first index of the original array
- **name** – str for the case of the dataset not being a dict. Key for the entry in the new dict for the original dataset. The returned dataset will only contain the split up entries
- **dataset** – dict with the entries split up

masci_tools.io.parsers.hdf5.transforms.**stack_datasets**(*dataset*, *axis=0*, *sort_key=None*)
Stack the entries in the given dict dataset along the given axis

Parameters

- **dataset** – dict dataset to transform
- **axis** – int along which axis should be stacked

Returns the array resulting from stacking all entries in the dictionary

masci_tools.io.parsers.hdf5.transforms.**sum_over_dict_entries**(*dataset*, *overwrite_dict=False*, *entries=None*, *dict_entry='sum'*, *entry_format=None*)
Sum the datasets contained in the given dict dataset

Parameters

- **dataset** – dataset to transform
- **overwrite_dict** – bool if True, the result will overwrite the dictionary if False it is entered under *sum* in the dict

Returns dataset with summed entries

masci_tools.io.parsers.hdf5.transforms.**tile_array**(*dataset*, *n_repeats*)
Use numpy.tile to repeat array n-times

Parameters

- **dataset** – dataset to transform
- **attribute_shape** – int, time sto repeat the given array

Returns dataset repeated n-times

masci_tools.io.parsers.hdf5.transforms.**tile_array_by_attribute**(*dataset*, *attribute_value*)
Use numpy.tile to repeat array n-times (given by attribute_value)

Parameters

- **dataset** – dataset to transform
- **attribute_shape** – int, time sto repeat the given array

Returns dataset repeated n-times

6.1.3.4 Definition of default parsing tasks for fleur out.xml

This module contains the dictionary with all defined tasks for the outxml_parser. The entries in the TASK_DEFINITION dict specify how to parse specific attributes tags.

This needs to be maintained if the specifications do not work for a new schema version because of changed attribute names for example.

Each entry in the TASK_DEFINITION dict can contain a series of keys, which by default correspond to the keys in the output dictionary

The following keys are expected in each entry:

param parse_type str, defines which methods to use when extracting the information

param path_spec dict with all the arguments that should be passed to tag_xpath or attrib_xpath to get the correct path

param subdict str, if present the parsed values are put into this key in the output dictionary

param overwrite_last bool, if True no list is inserted and each entry overwrites the last

For the allAttribs parse_type there are more keys that can appear:

param base_value str, optional. If given the attribute with this name will be inserted into the key from the task_definition all other keys are formatted as {task_key}_{attribute_name}

param ignore list of str, these attributes will be ignored

param overwrite list of str, these attributes will not create a list and overwrite any value that might be there

param flat bool, if False the dict parsed from the tag is inserted as a dict into the correspondin key if True the values will be extracted and put into the output dictionary with the format {task_key}_{attribute_name}

Each task entry can have additional keys to specify, when to perform the task. These are denoted with underscores in their names and are all optional:

param _general bool, default False. If True the parsing is not performed for each iteration on the iteration node but beforehand and on the root node

param _modes list of tuples, sets conditions for the keys in fleur_modes to perform the task .e.g. [('jspins', 2), ('soc', True)] means only perform this task for a magnetic soc calculation

param _minimal bool, default False, denotes task to perform when minimal_mode=True is passed to the parser

param _special bool, default False, If true these tasks are not added by default and need to be added manually

param _conversions list of str, gives the names of functions in fleur_outxml_conversions to perform after parsing

The following keys are special at the moment:

- `fleur_modes` specifies how to identify the type of the calculation (e.g. SOC, magnetic, lda+u) this is used to determine, whether additional things should be parsed

Following is the current specification of tasks

```
__base_version__ = '0.34'

TASKS_DEFINITION = {
    #--------Definitions for general info from outfile (start, endtime, number_
↪iterations)--------
    'general_out_info': {
        '_general': True,
        '_minimal': True,
        '_conversions': ['calculate_walltime'],
        'creator_name': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'version',
                'not_contains': 'git'
            }
        },
        'creator_target_architecture': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'targetComputerArchitectures'
            }
        },
        'output_file_version': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'fleurOutputVersion'
            }
        },
        'number_of_iterations': {
            'parse_type': 'numberNodes',
            'path_spec': {
                'name': 'iteration'
            }
        },
        'number_of_atoms': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'nat'
            }
        },
        'number_of_atom_types': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'ntype'
            }
        },
        'number_of_kpoints': {
            'parse_type': 'attrib',
            'path_spec': {
```

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```
                'name': 'count',
                'contains': 'numericalParameters'
            }
        },
        'start_date': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'startDateAndTime'
            },
            'ignore': ['zone'],
            'flat': False,
        },
        'end_date': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'endDateAndTime'
            },
            'ignore': ['zone'],
            'flat': False,
        }
    },
    #--------Defintions for general info from input section of outfile (kmax, symmetries,
↪ ..)--------
    'general_inp_info': {
        '_general': True,
        '_minimal': True,
        'title': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'comment'
            }
        },
        'kmax': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'Kmax'
            }
        },
        'gmax': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'Gmax'
            }
        },
        'number_of_spin_components': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'jspins'
            }
        },
        'number_of_symmetries': {
            'parse_type': 'numberNodes',
```

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```
            'path_spec': {
                'name': 'symOp'
            }
        },
        'number_of_species': {
            'parse_type': 'numberNodes',
            'path_spec': {
                'name': 'species'
            }
        },
        'film': {
            'parse_type': 'exists',
            'path_spec': {
                'name': 'filmPos'
            }
        },
    },
    #--------Defintions for lda+u info from input section (species, ldau tags)--------
    'ldau_info': {
        '_general': True,
        '_modes': [('ldau', True)],
        '_conversions': ['convert_ldau_definitions'],
        'parsed_ldau': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'ldaU',
                'contains': 'species'
            },
            'subdict': 'ldau_info',
            'flat': False,
            'only_required': True
        },
        'ldau_species': {
            'parse_type': 'parentAttribs',
            'path_spec': {
                'name': 'ldaU',
                'contains': 'species'
            },
            'subdict': 'ldau_info',
            'flat': False,
            'only_required': True
        }
    },
    #--------Defintions for relaxation info from input section (bravais matrix, atompos)
    #--------for Bulk and film
    'bulk_relax_info': {
        '_general': True,
        '_modes': [('relax', True), ('film', False)],
        '_conversions': ['convert_relax_info'],
        'lat_row1': {
            'parse_type': 'text',
            'path_spec': {
```

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```
                'name': 'row-1',
                'contains': 'bulkLattice/bravais'
            }
        },
        'lat_row2': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'row-2',
                'contains': 'bulkLattice/bravais'
            }
        },
        'lat_row3': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'row-3',
                'contains': 'bulkLattice/bravais'
            }
        },
        'atom_positions': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'relPos'
            }
        },
        'position_species': {
            'parse_type': 'parentAttribs',
            'path_spec': {
                'name': 'relPos'
            },
            'flat': False,
            'only_required': True
        },
        'element_species': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'species'
            },
            'flat': False,
            'ignore': ['vcaAddCharge', 'magField']
        },
    },
    'film_relax_info': {
        '_general': True,
        '_modes': [('relax', True), ('film', True)],
        '_conversions': ['convert_relax_info'],
        'lat_row1': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'row-1',
                'contains': 'filmLattice/bravais'
            }
        },
```

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```
        'lat_row2': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'row-2',
                'contains': 'filmLattice/bravais'
            }
        },
        'lat_row3': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'row-3',
                'contains': 'filmLattice/bravais'
            }
        },
        'atom_positions': {
            'parse_type': 'text',
            'path_spec': {
                'name': 'filmPos'
            }
        },
        'position_species': {
            'parse_type': 'parentAttribs',
            'path_spec': {
                'name': 'filmPos'
            },
            'flat': False,
            'only_required': True
        },
        'element_species': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'species'
            },
            'flat': False,
            'ignore': ['vcaAddCharge', 'magField']
        },
    },
    #----General iteration tasks
    # iteration number
    # total energy (only total or also contributions, also lda+u correction)
    # distances (nonmagnetic and magnetic, lda+u density matrix)
    # charges (total, interstitial, mt sphere)
    # fermi energy and bandgap
    # magnetic moments
    # orbital magnetic moments
    # forces
    'iteration_number': {
        '_minimal': True,
        'number_of_iterations_total': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'overallNumber'
```

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```
            },
            'overwrite_last': True,
        }
    },
    'total_energy': {
        '_minimal': True,
        '_conversions': ['convert_total_energy'],
        'energy_hartree': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'value',
                'tag_name': 'freeEnergy'
            }
        },
        'energy_hartree_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'tag_name': 'totalEnergy'
            },
            'overwrite_last': True,
        },
    },
    'distances': {
        '_minimal': True,
        'density_convergence': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'distance',
                'tag_name': 'chargeDensity'
            }
        },
        'density_convergence_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'tag_name': 'densityConvergence',
            },
            'overwrite_last': True,
        }
    },
    'magnetic_distances': {
        '_minimal': True,
        '_modes': [('jspin', 2)],
        'overall_density_convergence': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'distance',
                'tag_name': 'overallChargeDensity'
            }
        },
        'spin_density_convergence': {
```

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```
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'distance',
                'tag_name': 'spinDensity'
            }
        }
    },
    'total_energy_contributions': {
        'sum_of_eigenvalues': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'sumOfEigenvalues'
            },
            'only_required': True
        },
        'energy_core_electrons': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'coreElectrons',
                'contains': 'sumOfEigenvalues'
            },
            'only_required': True
        },
        'energy_valence_electrons': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'valenceElectrons'
            },
            'only_required': True
        },
        'charge_den_xc_den_integral': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'chargeDenXCDenIntegral'
            },
            'only_required': True
        },
    },
    'ldau_energy_correction': {
        '_modes': [('ldau', True)],
        'ldau_energy_correction': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'dftUCorrection'
            },
            'subdict': 'ldau_info',
            'only_required': True
        },
    },
    'nmmp_distances': {
        '_minimal': True,
        '_modes': [('ldau', True)],
```

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```
        'density_matrix_distance': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'distance',
                'contains': 'ldaUDensityMatrixConvergence'
            },
            'subdict': 'ldau_info'
        },
    },
    'fermi_energy': {
        'fermi_energy': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'FermiEnergy'
            },
        }
    },
    'bandgap': {
        '_modes': [('bz_integration', 'hist')],
        'bandgap': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'bandgap'
            },
        }
    },
    'magnetic_moments': {
        '_modes': [('jspin', 2)],
        'magnetic_moments': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'magneticMoment'
            },
            'base_value': 'moment',
            'ignore': ['atomType']
        }
    },
    'orbital_magnetic_moments': {
        '_modes': [('jspin', 2), ('soc', True)],
        'orbital_magnetic_moments': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'orbMagMoment'
            },
            'base_value': 'moment',
            'ignore': ['atomType']
        }
    },
    'forces': {
        '_minimal': True,
        '_modes': [('relax', True)],
        '_conversions': ['convert_forces'],
```

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```
        'force_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'tag_name': 'totalForcesOnRepresentativeAtoms'
            },
            'overwrite_last': True
        },
        'parsed_forces': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'forceTotal'
            },
            'flat': False,
            'only_required': True
        }
    },
    'charges': {
        '_conversions': ['calculate_total_magnetic_moment'],
        'spin_dependent_charge': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'spinDependentCharge',
                'contains': 'allElectronCharges',
                'not_contains': 'fixed'
            },
            'only_required': True
        },
        'total_charge': {
            'parse_type': 'singleValue',
            'path_spec': {
                'name': 'totalCharge',
                'contains': 'allElectronCharges',
                'not_contains': 'fixed'
            },
            'only_required': True
        }
    },
    #-------Tasks for forcetheorem Calculations
    # DMI, JIJ, MAE, SSDISP
    'forcetheorem_dmi': {
        '_special': True,
        'dmi_force': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'Entry',
                'contains': 'DMI'
            }
        },
        'dmi_force_qs': {
            'parse_type': 'attrib',
            'path_spec': {
```

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```
                'name': 'qpoints',
                'contains': 'Forcetheorem_DMI'
            }
        },
        'dmi_force_angles': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'Angles',
                'contains': 'Forcetheorem_DMI'
            }
        },
        'dmi_force_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'contains': 'Forcetheorem_DMI'
            }
        }
    },
    'forcetheorem_ssdisp': {
        '_special': True,
        'spst_force': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'Entry',
                'contains': 'SSDISP'
            }
        },
        'spst_force_qs': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'qvectors',
                'contains': 'Forcetheorem_SSDISP'
            }
        },
        'spst_force_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'contains': 'Forcetheorem_SSDISP'
            }
        }
    },
    'forcetheorem_mae': {
        '_special': True,
        'mae_force': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'Angle',
                'contains': 'MAE'
            }
        },
```

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```
        'mae_force_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'contains': 'Forcetheorem_MAE'
            }
        }
    },
    'forcetheorem_jij': {
        '_special': True,
        'jij_force': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'Config',
                'contains': 'JIJ'
            }
        },
        'jij_force_units': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'units',
                'contains': 'Forcetheorem_JIJ'
            }
        }
    },
    'torques': {
        '_minimum_version': '0.35',  #Typo torgue/torque before
        '_optional': True,
        'torque_x': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'sigma_x',
                'contains': 'noncollinearTorque'
            }
        },
        'torque_y': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'sigma_y',
                'contains': 'noncollinearTorque'
            }
        }
    },
    'noco_angles': {
        '_general': True,
        '_optional': True,
        'noco_alpha': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'alpha',
                'tag_name': 'nocoParams',
                'contains': 'Group'
```

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```
            }
        },
        'noco_beta': {
            'parse_type': 'attrib',
            'path_spec': {
                'name': 'beta',
                'tag_name': 'nocoParams',
                'contains': 'Group'
            }
        }
    },
    'corelevels': {
        '_optional': True,
        'corestates': {
            'parse_type': 'allAttribs',
            'path_spec': {
                'name': 'coreStates'
            },
            'subtags': True,
            'flat': False
        }
    }
}
```

In this module migration functions for the task definitions are collected

masci_tools.io.parsers.fleur.task_migrations.**migrate_033_to_031**(*definition_dict*)
Migrate definitions for MaX5 release to MaX4 release

Changes:

- LDA+U density matrix distance output did not exist

Return type dict[str, dict[str, Any]]

masci_tools.io.parsers.fleur.task_migrations.**migrate_034_to_033**(*definition_dict*)
Migrate definitions for MaX5 bugfix release to MaX5 release

Changes:

- forcetheorem units attribute did not exist (get from 'sumValenceSingleParticleEnergies')

Return type dict[str, dict[str, Any]]

6.1.4 Commandline interface (CLI)

6.1.4.1 masci_tools

CLI for the *masci-tools* library.

```
masci_tools [OPTIONS] COMMAND [ARGS]...
```

Options

-v, --version
Show the version and exit.

fleur-schema

Commands related to the Fleur XML Schemas

```
masci_tools fleur-schema [OPTIONS] COMMAND [ARGS]...
```

add

Adds a new xml schema file to the folder in *masci_tools/io/parsers/fleur_schema* corresponding to its version number

```
masci_tools fleur-schema add [OPTIONS] SCHEMA_FILE
```

Options

--overwrite
Overwrite any exisiting schema-file

--branch <branch>
If the file does not exist the branch can be specified in the fleur git

--api-key <api_key>
API key for access to the Iff Gitlab instance

--test-xml-file <test_xml_file>
Example xmlfile for this schema version to test the file parser against

Arguments

SCHEMA_FILE
Required argument

list

Show the available fleur schemas

```
masci_tools fleur-schema list [OPTIONS]
```

validate-input

Validate the given inp.xml file against the Fleur schema stored for the version of the input

```
masci_tools fleur-schema validate-input [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

validate-output

Validate the given out.xml file against the Fleur schema stored for the version of the output

```
masci_tools fleur-schema validate-output [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

inpxml

Tool for converting inp.xml files to different versions

```
masci_tools inpxml [OPTIONS] COMMAND [ARGS]...
```

convert

Convert the given XML_FILE file to version TO_VERSION

XML_FILE is the file to convert TO_VERSION is the file version of the finale input file

```
masci_tools inpxml convert [OPTIONS] XML_FILE TO_VERSION
```

Options

-o, --output-file <output_file>
Name of the output file

--overwrite
If the flag is given and the file already exists it is overwritten

Arguments

XML_FILE
Required argument

TO_VERSION
Required argument

generate-conversion

Generate the conversions from FROM_VERSION to TO_VERSION

FROM_VERSION is the file version of the initial input file TO_VERSION is the file version of the finale input file

```
masci_tools inpxml generate-conversion [OPTIONS] FROM_VERSION TO_VERSION
```

Options

--show, --no-show
Show a summary of the conversion at the end

Arguments

FROM_VERSION
Required argument

TO_VERSION
Required argument

show-conversion

Show the actions for an already created conversion from FROM_VERSION to TO_VERSION

FROM_VERSION is the file version of the initial input file TO_VERSION is the file version of the finale input file

```
masci_tools inpxml show-conversion [OPTIONS] FROM_VERSION TO_VERSION
```

Arguments

FROM_VERSION
Required argument

TO_VERSION
Required argument

parse

Commands for parsing information from KKR/Fleur files

```
masci_tools parse [OPTIONS] COMMAND [ARGS]...
```

all-attribs

Parse all attributes of the specified tag from the given xml file

```
masci_tools parse all-attribs [OPTIONS] XML_FILE
```

Options

-n, **--name** <name>

-c, **--contains** <contains>

-nc, **--not-contains** <not_contains>

--subtags

--text

Arguments

XML_FILE
Required argument

attrib

Parse the specified attribute from the given xml file

```
masci_tools parse attrib [OPTIONS] XML_FILE
```

Options

-n, **--name** <name>

-c, **--contains** <contains>

-nc, **--not-contains** <not_contains>

-t, **--tag** <tag>

Arguments

XML_FILE
Required argument

cell

Parse the unit cell definition fo the given xml file

```
masci_tools parse cell [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

constants

Parse the mathematical constants used in the given xml-file

```
masci_tools parse constants [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

fleur-modes

Parse the Fleur modes of the given xml file

```
masci_tools parse fleur-modes [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

inp-file

Parse the Fleur inp.xml into a python dictionary

```
masci_tools parse inp-file [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

kpoints

Parse the used kpoints from the given xml-file

```
masci_tools parse kpoints [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

nkpts

Extract the number of kpoints used in the given xml file

```
masci_tools parse nkpts [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

number-nodes

Return how often the specified tag occurs in the given xml file

```
masci_tools parse number-nodes [OPTIONS] XML_FILE
```

Options

-n, --name <name>

-c, --contains <contains>

-nc, --not-contains <not_contains>

Arguments

XML_FILE
Required argument

out-file

Parse the Fleur out.xml into a python dictionary

```
masci_tools parse out-file [OPTIONS] XML_FILE
```

Options

--ignore-validation

Arguments

XML_FILE
Required argument

parameters

Parse the calculation parameters of the given xml file

```
masci_tools parse parameters [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

parent-attribs

Parse all attributes of the parent of the specified tag from the given xml file

```
masci_tools parse parent-attribs [OPTIONS] XML_FILE
```

Options

-n, --name <name>

-c, --contains <contains>

-nc, --not-contains <not_contains>

Arguments

XML_FILE
Required argument

relaxation

Parse the relaxation information for the given xml file

```
masci_tools parse relaxation [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

structure

Parse the structure information in the given Fleur xml file

```
masci_tools parse structure [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

symmetry

Parse the symmetry information for the given xml file

```
masci_tools parse symmetry [OPTIONS] XML_FILE
```

Arguments

XML_FILE
Required argument

tag-exists

Return whether the specified tag exists in the given xml file

```
masci_tools parse tag-exists [OPTIONS] XML_FILE
```

Options

-n, --name <name>

-c, --contains <contains>

-nc, --not-contains <not_contains>

Arguments

XML_FILE
Required argument

text

Parse the text of the specified tag from the given xml file

```
masci_tools parse text [OPTIONS] XML_FILE
```

Options

-n, --name <name>

-c, --contains <contains>

-nc, --not-contains <not_contains>

Arguments

XML_FILE
Required argument

plot

Commands for visualizing data

```
masci_tools plot [OPTIONS] COMMAND [ARGS]...
```

fleur-bands

Plot bandstructures from the banddos.hdf file from Fleur

```
masci_tools plot fleur-bands [OPTIONS] BANDDOS_FILE
```

Options

-w, --weight <weight>

--backend <backend>

Options matplotlib | mpl | bokeh

--save

--show

-r, --recipe <recipe>

Options FleurBands | FleurOrbcompBands | FleurjDOSBands | FleurSimpleBands | FleurMCD-Bands

Arguments

BANDDOS_FILE
Required argument

fleur-dos

Plot density of states from the banddos.hdf file from Fleur

```
masci_tools plot fleur-dos [OPTIONS] BANDDOS_FILE
```

Options

--total <total>

--interstitial <interstitial>

--atoms <atoms>

--l_resolved <l_resolved>

--backend <backend>

Options matplotlib | mpl | bokeh

--save

--show

-r, --recipe <recipe>

Options FleurDOS | FleurORBCOMP | FleurJDOS | FleurMCD

Arguments

BANDDOS_FILE
Required argument

6.1.5 Utility Functions/Classes

6.1.5.1 Custom Datatypes

This module defines subclasses of UserDict and UserList to be able to prevent unintended modifications

masci_tools.util.lockable_containers.**LockContainer**(*lock_object*)
Contextmanager for temporarily locking a lockable object. Object is unfrozen when exiting with block

Parameters **lock_object** – lockable container (not yet frozen)

class masci_tools.util.lockable_containers.**LockableDict**(**args*, *recursive=True*, ***kwargs*)
Subclass of UserDict, which can prevent modifications to itself. Raises *RuntimeError* if modification is attempted.

Use *LockableDict.freeze()* to enforce. *LockableDict.get_unlocked()* returns a copy of the locked object with builtin lists and dicts

Parameters **recursive** (bool) – bool if True (default) all subitems (lists or dicts) are converted into their lockable counterparts

All other args or kwargs will be passed on to initialize the *UserDict*

IMPORTANT NOTE: This is not a direct subclass of dict. So isinstance(a, dict) will be False if a is an LockableDict

freeze()
Freezes the object. This prevents further modifications

Return type None

get_unlocked()
Get copy of object with builtin lists and dicts

Return type dict[~*S*, ~*T*]

property locked: bool
Returns whether the object is locked

Return type bool

class masci_tools.util.lockable_containers.**LockableList**(**args*, *recursive=True*, ***kwargs*)
Subclass of UserList, which can prevent modifications to itself. Raises *RuntimeError* if modification is attempted.

Use *LockableList.freeze()* to enforce. *LockableList.get_unlocked()* returns a copy of the locked object with builtin lists and dicts

Parameters **recursive** (bool) – bool if True (default) all subitems (lists or dicts) are converted into their lockable counterparts

All other args or kwargs will be passed on to initialize the *UserList*

IMPORTANT NOTE: This is not a direct subclass of list. So isinstance(a, list) will be False if a is an LockableList

append(*item*)
S.append(value) – append value to the end of the sequence

Return type None

clear()
Clear the list

Return type None

extend(*other*)
S.extend(iterable) – extend sequence by appending elements from the iterable

Return type None

freeze()
Freezes the object. This prevents further modifications

Return type None

get_unlocked()
Get copy of object with builtin lists and dicts

Return type list[~*T*]

insert(*i*, *item*)
S.insert(index, value) – insert value before index

Return type None

property locked: bool
Returns whether the object is locked

Return type bool

pop(*i=- 1*)
return the value at index i (default last) and remove it from list

Return type ~*T*

remove(*item*)
S.remove(value) – remove first occurrence of value. Raise ValueError if the value is not present.

Return type None

reverse()
S.reverse() – reverse *IN PLACE*

Return type None

masci_tools.util.lockable_containers.**S**
Type variable for the key type of the dictionary

alias of TypeVar('S')

masci_tools.util.lockable_containers.**T**
Type variable for the value type of the dictionary

alias of TypeVar('T')

This module defines a small helper class to make case insensitive dictionary lookups available naturally

class masci_tools.util.case_insensitive_dict.**CaseInsensitiveDict**(**args*, *upper=False*, *recursive=True*, ***kwargs*)

Dict with case insensitive lookup. Used in Schema dicts to make finding paths for tags and attributes easier. Does not preserve the case of the inserted key. Does not support case insensitive lookups in nested dicts Subclass of *masci_tools.util.lockable_containers.LockableDict*. So can be frozen via the`freeze()` method

Parameters **upper** (bool) – bool if True the method *upper()* will be used instead of *lower()* to normalize keys

All other args or kwargs will be passed on to initialize the *UserDict*

IMPORTANT NOTE: This is not a direct subcalss of dict. So isinstance(a, dict) will be False if a is an CaseInsensitiveDict

class masci_tools.util.case_insensitive_dict.**CaseInsensitiveFrozenSet**(*iterable=None*, *upper=False*)

Frozenset (i.e. immutable set) with case insensitive membership tests. Used in Schema dicts in *tag_info* entries to make flexible classification easy Preserves the case of the entered keys (*original_case()* returns the case of the first encounter)

Parameters **iterable** – iterable only containing str

Note: There might be subtle differences to expected behaviour with the methods __radd__, __ror__, and so on

difference(**others*)

Return the difference of two or more sets as a new set.

(i.e. all elements that are in this set but not the others.)

Return type *CaseInsensitiveFrozenSet*[*+T*]

intersection(**others*)

Return the intersection of two sets as a new set.

(i.e. all elements that are in both sets.)

Return type *CaseInsensitiveFrozenSet*[*+T*]

isdisjoint(*other*)

Return True if two sets have a null intersection.

Return type bool

issubset(*other*)

Report whether another set contains this set.

Return type bool

issuperset(*other*)

Report whether this set contains another set.

Return type bool

symmetric_difference(*other*)

Return the symmetric difference of two sets as a new set.

(i.e. all elements that are in exactly one of the sets.)

Return type *CaseInsensitiveFrozenSet*[*+T*]

union(**others*)

Return the union of sets as a new set.

(i.e. all elements that are in either set.)

Return type *CaseInsensitiveFrozenSet*[*+T*]

masci_tools.util.case_insensitive_dict.**S**
Generic Type

alias of TypeVar('S')

masci_tools.util.case_insensitive_dict.**T**
Generic Type

alias of TypeVar('T', covariant=True)

This module defines some aliases used in typing

masci_tools.util.typing.**FileLike: TypeAlias = 'str | bytes | Path | os.PathLike[Any] | IO'**
Type used for functions accepting file-like objects, i.e. handles or file paths

masci_tools.util.typing.**TXPathLike**
Type for xpath expressions

alias of TypeVar('TXPathLike', str, lxml.etree.XPath, masci_tools.util.xml.xpathbuilder.XPathBuilder)

masci_tools.util.typing.**XMLFileLike: TypeAlias = 'etree._ElementTree | etree._Element | FileLike'**
Type used for functions accepting xml-file-like objects, i.e. handles or file paths or already parsed xml objects

masci_tools.util.typing.**XMLLike: TypeAlias = 'etree._Element | etree._ElementTree'**
Type used for functions accepting xml objects from lxml

masci_tools.util.typing.**XPathLike: TypeAlias = 'str | bytes | etree.XPath | XPathBuilder'**
Type for xpath expressions

6.1.5.2 Common XML utility

Common functions for parsing input/output files or XMLschemas from FLEUR

masci_tools.util.xml.common_functions.**abs_to_rel_xpath**(*xpath*, *new_root*)
Convert a given xpath to be relative from a tag appearing in the original xpath.

Parameters

- **xpath** (str) – str of the xpath to convert
- **new_root** (str) – str of the tag from which the new xpath should be relative

Return type str

Returns str of the relative xpath

masci_tools.util.xml.common_functions.**add_tag**(*xpath*, *tag*)
Add tag to xpath

Note: etree.XPath objects could lose context in here, i.e. non-default options passed at init

Parameters

- **xpath** (*~TXPathLike*) – xpath to change
- **tag** (str) – str of the tag to add

Return type *~TXPathLike*

Returns xpath with the form {old_xpath}/tag

masci_tools.util.xml.common_functions.**check_complex_xpath**(*node*, *base_xpath*, *complex_xpath*)
Check that the given complex xpath produces a subset of the results for the simple xpath

Parameters

- **node** – root node of an etree or an etree
- **base_xpath** – str of the xpath without complex syntax
- **complex_xpath** – str of the xpath to check

Raises **ValueError** – If the complex_xpath does not produce a subset of the results of the base_xpath

masci_tools.util.xml.common_functions.**clear_xml**(*tree*)
Removes comments and executes xinclude tags of an xml tree.

Parameters **tree** (*_ElementTree*) – an xml-tree which will be processed

Return type tuple[_ElementTree, set[str]]

Returns cleared_tree, an xmltree without comments and with replaced xinclude tags

masci_tools.util.xml.common_functions.**eval_xpath**(*node*, *xpath*, *logger=None*, *list_return=False*, *namespaces=None*, ***variables*)
Tries to evaluate an xpath expression. If it fails it logs it. If a absolute path is given (starting with '/') and the tag of the node does not match the root. It will try to find the tag in the path and convert it into a relative path

Parameters

- **node** – root node of an etree
- **xpath** – xpath expression (relative, or absolute)
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **list_return** – if True, the returned quantity is always a list even if only one element is in it
- **namespaces** – dict, passed to namespaces argument in xpath call

Returns text, attribute or a node list

masci_tools.util.xml.common_functions.**get_xml_attribute**(*node*, *attributename*, *logger=None*)
Get an attribute value from a node.

Parameters

- **node** – a node from etree
- **attributename** – a string with the attribute name.
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised

Returns either attributevalue, or None

masci_tools.util.xml.common_functions.**reverse_xinclude**(*xmltree*, *schema_dict*, *included_tags*, ***kwargs*)
DEPRECATED ALIAS: Moved to masci_tools.util.schema_dict_util

Split the xmltree back up according to the given included tags. The original xmltree will be returned with the corresponding xinclude tags and the included trees are returned in a dict mapping the inserted filename to the extracted tree

Tags for which no known filename is known are returned under unknown-1.xml, ... The following tags have known filenames:

- *relaxation*: `relax.xml`
- *kPointLists*: `kpts.xml`
- *symmetryOperations*: `sym.xml`
- *atomSpecies*: `species.xml`
- *atomGroups*: `atoms.xml`

Additional mappings can be given in the keyword arguments

Parameters

- **xmltree** – an xml-tree which will be processed
- **schema_dict** – Schema dictionary containing all the necessary information
- **included_tags** – Iterable of str, containing the names of the tags to be excluded

Returns xmltree with the inseerted xinclude tags and a dict mapping the filenames to the excluded trees

Raises `ValueError` – if the tag can not be found in teh given xmltree

masci_tools.util.xml.common_functions.**split_off_attrib**(*xpath*)

Splits off attribute of the given xpath (part after @)

Note: etree.XPath objects could lose context in here, i.e. non-default options passed at init

---

Parameters **xpath** (*~TXPathLike*) – xpath to split up

Return type `tuple`[*~TXPathLike*, `str`]

masci_tools.util.xml.common_functions.**split_off_tag**(*xpath*)

Splits off the last part of the given xpath

Note: etree.XPath objects could lose context in here, i.e. non-default options passed at init

---

Parameters **xpath** (*~TXPathLike*) – xpath to split up

Return type `tuple`[*~TXPathLike*, `str`]

masci_tools.util.xml.common_functions.**validate_xml**(*xmltree*, *schema*, *error_header='File does not validate'*)

Checks a given xmltree against a schema and produces a nice error message with all the validation errors collected

Parameters

- **xmltree** (*_ElementTree*) – xmltree of the file to validate
- **schema** (*XMLSchema*) – etree.XMLSchema to validate against
- **error_header** (`str`) – str to lead a evtl error message with

Raises etree.DocumentInvalid if the schema does not validate

Return type `None`

Common functions for converting types to and from XML files

masci_tools.util.xml.converters.**convert_fleur_electronconfig**(*econfig_element*)
Convert electronConfig tag to eConfig string

Return type str

masci_tools.util.xml.converters.**convert_fleur_lo**(*loelements*)
Converts lo xml elements from the inp.xml file into a lo string for the inpgen

Return type str

masci_tools.util.xml.converters.**convert_from_fortran_bool**(*stringbool*)
Converts a string in this case ('T', 'F', or 't', 'f') to True or False

Parameters **stringbool** – a string ('t', 'f', 'F', 'T')

Returns boolean (either True or False)

masci_tools.util.xml.converters.**convert_from_xml**(*xmlstring*, *schema_dict*, *name*, *text=False*, *constants=None*, *logger=None*, *list_return=False*)
Tries to converts a given string to the types specified in the schema_dict. First succeeded conversion will be returned

If no logger is given and a attribute cannot be converted an error is raised

Parameters

- **stringattribute** – str, Attribute to convert.
- **schema_dict** – Schema dictionary containing all the information
- **name** – name of the attribute or element
- **text** – bool, decides whether to take the definitions for text or attributes
- **constants** – dict, of constants defined in fleur input
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted value of the first successful conversion

masci_tools.util.xml.converters.**convert_from_xml_explicit**(*xmlstring*, *definitions*, *constants=None*, *logger=None*, *list_return=False*)
Tries to converts a given string to the types given in definitions. First succeeded conversion will be returned

If no logger is given and a attribute cannot be converted an error is raised

Parameters

- **stringattribute** – str, Attribute to convert.
- **definitions** – list of *AttributeType* definitions
- **constants** – dict, of constants defined in fleur input
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted value of the first successful conversion

masci_tools.util.xml.converters.**convert_from_xml_single_values**(*xmlstring*, *possible_types*, *constants=None*, *logger=None*)

Tries to converts a given string attribute to the types given in possible_types. First succeeded conversion will be returned

If no logger is given and a attribute cannot be converted an error is raised

Parameters

- **stringattribute** – str, Attribute to convert.
- **possible_types** – list of str What types it will try to convert to
- **constants** – dict, of constants defined in fleur input
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted value of the first successful conversion

masci_tools.util.xml.converters.**convert_str_version_number**(*version_str*)

Convert the version number as a integer for easy comparisons

Parameters **version_str** (str) – str of the version number, e.g. '0.33'

Return type tuple[int, int]

Returns tuple of ints representing the version str

masci_tools.util.xml.converters.**convert_to_fortran_bool**(*boolean*)

Converts a Boolean as string to the format defined in the input

Parameters **boolean** – either a boolean or a string ('True', 'False', 'F', 'T')

Returns a string (either 't' or 'f')

masci_tools.util.xml.converters.**convert_to_xml**(*value*, *schema_dict*, *name*, *text=False*, *logger=None*, *list_return=False*)

Tries to converts a given string to the types specified in the schema_dict. First succeeded conversion will be returned

If no logger is given and a attribute cannot be converted an error is raised

Parameters

- **stringattribute** – str, Attribute to convert.
- **schema_dict** – Schema dictionary containing all the information
- **name** – name of the attribute or element
- **text** – bool, decides whether to take the definitions for text or attributes
- **constants** – dict, of constants defined in fleur input
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted value of the first successful conversion

masci_tools.util.xml.converters.**convert_to_xml_explicit**(*value*, *definitions*, *logger=None*, *float_format='.10'*, *list_return=False*)

Tries to convert a given list of values to str for a xml file based on the definitions (length and type). First succeeded conversion will be returned

Parameters

- **textvalue** – value to convert
- **definitions** – list of *AttributeType* definitions
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted value of the first succesful conversion

masci_tools.util.xml.converters.**convert_to_xml_single_values**(*value*, *possible_types*, *logger=None*, *float_format='.10'*)

Tries to converts a given attributevalue to a string for a xml file according to the types given in possible_types. First succeeded conversion will be returned

Parameters

- **value** – value to convert.
- **possible_types** – list of str What types it will try to convert from
- **logger** – logger object for logging warnings if given the errors are logged and the list is returned with the unconverted values otherwise a error is raised, when the first conversion fails
- **list_return** – if True, the returned quantity is always a list even if only one element is in it

Returns The converted str of the value of the first succesful conversion

This module contains Classes for building complex XPath expressions based on general attribute conditions from simple XPath expressions

class masci_tools.util.xml.xpathbuilder.**XPathBuilder**(*simple_path*, *filters=None*, *compile_path=False*, *strict=False*, ***kwargs*)

Class for building a complex xpath (restricted to adding filters) from a simple xpath expression

---

Note: passing in an etree.XPath object will not respect the options passed into it. Only the kwargs in __init__ are used to compile the path if compile_path=True

---

Note: Filters/Constraints (or predicates like they are called for XPaths) can either be added by providing the `filters` argument in the constructor or by calling the *add_filter()* method.

The `filters` argument is a dictionary with the tag names, where to apply the condition, as keys and the condition as values while the *add_filter()* method takes these as it's two arguments. The tag name has to be a part of the original simple xpath expression. The conditition is a dictionary with one key specifying the kind of condition and the value for the condition. The condition can also be the name of an attribute or path, in which case the

value can be another condition dictionary. The following conditions operators i.e. keys in the dictionary are supported:

- =/==: equal to
- !=: not equal to
- <: less than
- >: greater than
- <=: less than or equal to
- >=: greater than or equal to
- `contains`: attribute/tag contains the given value (case sensitive)
- `not-contains`: attribute/tag does not contains the given value
- `starts-with`: attribute/tag starts with the given value (case sensitive)
- `ends-with`: attribute/tag ends with the given value (case sensitive)
- `index`: Select tags based on their index in the parent tag (either explicit index or another condition)
- `has`: Select tags based on the presence of the given attribute/tag
- `has-not`: Select tags based on the absence of the given attribute/tag
- `number-nodes`: Compute the number of nodes in the previous path and select based on further criteria
- `and`: Provide multiple conditions in a list joined by `and`
- `or`: Provide multiple conditions in a list joined by `or`
- `in`: Select tags if the value of the path is in a given list of values
- `not-in`: Select tags if the value of the path is not in a given list of values
- `<string>`: All other strings are interpreted as paths to attributes/tags specifying conditions on their value
- `<tuple of paths>`: Multiple strings are interpreted as multiple node sets, which are joined with |

Example:

```
from masci_tools.util.xml.xpathbuilder import XPathBuilder

# XPath selecting all lo tags for SCLO type LOs and Iron species
xpath = XPathBuilder('/fleurInput/atomSpecies/species/lo',
                     filters = {'species': {
                                    'name': {'contains': 'Fe'},
                                },
                                'lo': {
                                    'type': 'SCLO'
                                }
                            })
```

Parameters

- **simple_path** – basic simple XPath expression to start from
- **filters** – dictionary with filters
- **compile_path** – bool if True the path property will be compiled as etree.XPath

- **strict** – bool if True the __str__ conversion will raise an error

Other Kwargs will be passed on to the etree.XPath compilation if `compile_path=True`

add_filter(*tag*, *conditions*)
Add a filter to the filters dictionary

Parameters

- **tag** – str name of the tag name to add a filter to
- **conditions** – dictionary specifying the filter

append_tag(*tag*)
Append another tag to the end of the simple xpath expression

Parameters **tag** (str) – str name of the tag to append

Return type None

get_predicate(*tag*, *condition*, *compound=False*, *path='.'*, *process_path=False*)
Construct the predicate for the given tag and condition

Parameters

- **tag** (str) – str name of the tag
- **condition** (Any) – condition specified, either dict or single value
- **compound** (bool) – bool if True the enclosing condition is a compound condition, forbidding any other compound condition
- **path** (str) – path, to which to apply the condition
- **process_path** (bool) – bool if True the path will taken apart into its components and the components will be checked with XPath variables

Return type str

property path: etree._xpath
Property for constructing the complex Xpath

process_condition(*tag*, *operator*, *content*, *path*, *process_path=False*)
Process the condition for the given tag and condition

Parameters

- **tag** (str) – str name of the tag
- **operator** (str) – operator for condition
- **content** (Any) – content of condition
- **path** (str) – path, to which to apply the condition
- **process_path** (bool) – bool if True the path will taken apart into its components and the components will be checked with XPath variables

Return type str

strip_off_tag()
Strip off the last tag of the simple xpath expression

Return type str

6.1.5.3 XML Setter functions

Functions for modifying the xml input file of Fleur utilizing the schema dict and as little knowledge of the concrete xpaths as possible

masci_tools.util.xml.xml_setters_names.**add_number_to_attrib**(*xmltree*, *schema_dict*, *attributename*, *add_number*, *complex_xpath=None*, *filters=None*, *mode='abs'*, *occurrences=None*, ***kwargs*)

Adds a given number to the attribute value in a xmltree specified by the name of the attribute and optional further specification If there are no nodes under the specified xpath an error is raised

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns xmltree with shifted attribute

masci_tools.util.xml.xml_setters_names.**add_number_to_first_attrib**(*xmltree*, *schema_dict*, *attributename*, *add_number*, *complex_xpath=None*, *filters=None*, *mode='abs'*, ***kwargs*)

Adds a given number to the first occurrence of an attribute value in a xmltree specified by the name of the attribute and optional further specification If there are no nodes under the specified xpath an error is raised

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation

- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns xmltree with shifted attribute

masci_tools.util.xml.xml_setters_names.**clone_species**(*xmltree*, *schema_dict*, *species_name*, *new_name*, *changes=None*)

Method to create a new species from an existing one with evtl. modifications

For reference of the changes dictionary look at *set_species()*

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **species_name** – string, name of the specie you want to clone Has to correspond to one single species (no 'all'/'all-<search_string>')
- **new_name** – new name of the cloned species
- **changes** – a optional python dict specifying what you want to change.

Return xmltree xml etree of the new inp.xml

masci_tools.util.xml.xml_setters_names.**create_tag**(*xmltree*, *schema_dict*, *tag*, *complex_xpath=None*, *filters=None*, *create_parents=False*, *occurrences=None*, ***kwargs*)

This method creates a tag with a uniquely identified xpath under the nodes of its parent. If there are no nodes evaluated the subtags can be created with *create_parents=True*

The tag is always inserted in the correct place if a order is enforced by the schema

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag** – str of the tag to create or etree Element with the same name to insert
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create_parents** – bool optional (default False), if True and the given xpath has no results the the parent tags are created recursively
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with created tags

masci_tools.util.xml.xml_setters_names.**delete_att**(*xmltree*, *schema_dict*, *attrib_name*, *complex_xpath=None*, *filters=None*, *occurrences=None*, ***kwargs*)

This method deletes a attribute with a uniquely identified xpath.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag** – str of the attribute to delete
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **occurrences** – int or list of int. Which occurence of the parent nodes to delete a attribute. By default all nodes are used.

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns xmltree with deleted attributes

masci_tools.util.xml.xml_setters_names.**delete_tag**(*xmltree*, *schema_dict*, *tag_name*, *complex_xpath=None*, *filters=None*, *occurrences=None*, ***kwargs*)

This method deletes a tag with a uniquely identified xpath.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag** – str of the tag to delete
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **occurrences** – int or list of int. Which occurence of the parent nodes to delete a tag. By default all nodes are used.

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with deleted tags

masci_tools.util.xml.xml_setters_names.**replace_tag**(*xmltree*, *schema_dict*, *tag_name*, *newelement*, *complex_xpath=None*, *filters=None*, *occurrences=None*, ***kwargs*)

This method deletes a tag with a uniquely identified xpath.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag** – str of the tag to replace
- **newelement** – etree Element to replace the tag
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **occurrences** – int or list of int. Which occurence of the parent nodes to replace a tag. By default all nodes are used.

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with replaced tags

masci_tools.util.xml.xml_setters_names.**set_atomgroup**(*xmltree*, *schema_dict*, *attributedict*, *position=None*, *species=None*, *filters=None*, *create=False*)

Method to set parameters of an atom group of the fleur inp.xml file.

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **attributedict** – a python dict specifying what you want to change.
- **position** – position of an atom group to be changed. If equals to 'all', all species will be changed
- **species** – atom groups, corresponding to the given species will be changed
- **create** – bool, if species does not exist create it and all subtags?
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Returns xml etree of the new inp.xml

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a beta noco parameter it can be done via:

```
'attributedict': {'nocoParams': {'beta': val}}
```

masci_tools.util.xml.xml_setters_names.**set_atomgroup_label**(*xmltree*, *schema_dict*, *atom_label*, *attributedict*, *create=False*)

This method calls *set_atomgroup()* method for a certain atom species that corresponds to an atom with a given label.

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **atom_label** – string, a label of the atom which specie will be changed. 'all' to change all the species
- **attributedict** – a python dict specifying what you want to change.
- **create** – bool, if species does not exist create it and all subtags?

Returns xml etree of the new inp.xml

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a beta noco parameter it can be done via:

```
'attributedict': {'nocoParams': {'beta': val}}
```

masci_tools.util.xml.xml_setters_names.**set_attrib_value**(*xmltree*, *schema_dict*, *attributename*, *attribv*, *complex_xpath=None*, *filters=None*, *occurrences=None*, *create=False*, ***kwargs*)

Sets an attribute in a xmltree to a given value, specified by its name and further specifications. If there are no nodes under the specified xpath a tag can be created with *create=True*. The attribute values are converted automatically according to the types of the attribute with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns xmltree with set attribute

masci_tools.util.xml.xml_setters_names.**set_complex_tag**(*xmltree*, *schema_dict*, *tag_name*, *changes*, *complex_xpath=None*, *filters=None*, *create=False*, ***kwargs*)

Function to correctly set tags/attributes for a given tag. Goes through the attributedict and decides based on the schema_dict, how the corresponding key has to be handled. The tag is specified via its name and evtl. further specification

Supports:

- attributes
- tags with text only
- simple tags, i.e. only attributes (can be optional single/multiple)
- complex tags, will recursively create/modify them

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag_name** – name of the tag to set
- **attributedict** – Keys in the dictionary correspond to names of tags and the values are the modifications to do on this tag (attributename, subdict with changes to the subtag, ...)
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create** – bool optional (default False), if True and the path, where the complex tag is set does not exist it is created

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with changes to the complex tag

masci_tools.util.xml.xml_setters_names.**set_first_attrib_value**(*xmltree*, *schema_dict*, *attributename*, *attribv*, *complex_xpath=None*, *filters=None*, *create=False*, ***kwargs*)

Sets the first occurrence of an attribute in a xmltree to a given value, specified by its name and further specifications. If there are no nodes under the specified xpath a tag can be created with *create=True*. The attribute values are converted automatically according to the types of the attribute with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation

- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create** – bool optional (default False), if True the tag is created if is missing

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns xmltree with set attribute

masci_tools.util.xml.xml_setters_names.**set_first_text**(*xmltree*, *schema_dict*, *attributename*, *attribv*, *complex_xpath=None*, *filters=None*, *create=False*, ***kwargs*)

Sets the text the first occurrence of a tag in a xmltree to a given value, specified by the name of the tag and further specifications. By default the text will be set on all nodes returned for the specified xpath. If there are no nodes under the specified xpath a tag can be created with *create=True*. The text values are converted automatically according to the types with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag_name** – str name of the tag, where the text should be set
- **text** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create** – bool optional (default False), if True the tag is created if is missing

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with set text

masci_tools.util.xml.xml_setters_names.**set_inpchanges**(*xmltree*, *schema_dict*, *change_dict*, *path_spec=None*)

This method sets all the attribute and texts provided in the change_dict.

The first occurrence of the attribute/tag is set

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **path_spec** – dict, with ggf. necessary further specifications for the path of the attribute

Params change_dict dictionary {attrib_name : value} with all the wanted changes.

An example of change_dict:

```
change_dict = {'itmax' : 1,
               'l_noco': True,
               'ctail': False,
               'l_ss': True}
```

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_kpath**(*xmltree*, *schema_dict*, *kpath*, *count*, *gamma=False*)
Sets a k-path directly into inp.xml as a alternative kpoint set with purpose 'bands'

Warning: This method is only supported for input versions before the Max5 release

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **kpath** – a dictionary with kpoint name as key and k point coordinate as value
- **count** – number of k-points
- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_kpath_max4**(*xmltree*, *schema_dict*, *kpath*, *count*, *gamma=False*)
Sets a k-path directly into inp.xml as a alternative kpoint set with purpose 'bands'

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **kpath** – a dictionary with kpoint name as key and k point coordinate as value
- **count** – number of k-points
- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_kpointlist**(*xmltree*, *schema_dict*, *kpoints*, *weights*, *name=None*, *kpoint_type='path'*, *special_labels=None*, *switch=False*, *overwrite=False*)
Explicitely create a kPointList from the given kpoints and weights. This routine will add the specified kPointList with the given name.

Warning: For input versions Max4 and older **all** keyword arguments are not valid (*name*, *kpoint_type*, *special_labels*, *switch* and *overwrite*)

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **kpoints** – list or array containing the **relative** coordinates of the kpoints
- **weights** – list or array containing the weights of the kpoints
- **name** – str for the name of the list, if not given a default name is generated
- **kpoint_type** – str specifying the type of the kPointList ('path', 'mesh', 'spex', 'tria', ...)
- **special_labels** – dict mapping indices to labels. The labels will be inserted for the kpoints corresponding to the given index
- **switch** – bool, if True the kPointlist will be used by Fleur when starting the next calculation
- **overwrite** – bool, if True and a kPointlist with the given name already exists it will be overwritten

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_kpointlist_max4**(*xmltree*, *schema_dict*, *kpoints*, *weights*)
Explicitely create a kPointList from the given kpoints and weights. This routine is specific to input versions Max4 and before and will replace any existing kPointCount, kPointMesh, ... with the specified kPointList

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **kpoints** – list or array containing the **relative** coordinates of the kpoints
- **weights** – list or array containing the weights of the kpoints

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_nkpts**(*xmltree*, *schema_dict*, *count*, *gamma=False*)
Sets a k-point mesh directly into inp.xml

> **Warning:** This method is only supported for input versions before the Max5 release

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **count** – number of k-points
- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_nkpts_max4**(*xmltree*, *schema_dict*, *count*, *gamma=False*)
Sets a k-point mesh directly into inp.xml specific for inputs of version Max4

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **count** – number of k-points

- **gamma** – bool that controls if the gamma-point should be included in the k-point mesh

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**set_simple_tag**(*xmltree*, *schema_dict*, *tag_name*, *changes*, *complex_xpath=None*, *filters=None*, *create_parents=False*, ***kwargs*)

Sets one or multiple *simple* tag(s) in an xmltree. A simple tag can only hold attributes and has no subtags. The tag is specified by its name and further specification If the tag can occur multiple times all existing tags are DELETED and new ones are written. If the tag only occurs once it will automatically be created if its missing.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag_name** – str name of the tag to modify/set
- **changes** – list of dicts or dict with the changes. Elements in list describe multiple tags. Keys in the dictionary correspond to {'attributename': attributevalue}
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **create_parents** – bool optional (default False), if True and the path, where the simple tags are set does not exist it is created

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with set simple tags

masci_tools.util.xml.xml_setters_names.**set_species**(*xmltree*, *schema_dict*, *species_name*, *attributedict*, *filters=None*, *create=False*)

Method to set parameters of a species tag of the fleur inp.xml file.

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **species_name** – string, name of the specie you want to change Can be name of the species, 'all' or 'all-<string>' (sets species with the string in the species name)
- **attributedict** – a python dict specifying what you want to change.
- **create** – bool, if species does not exist create it and all subtags?
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Raises ValueError – if species name is non existent in inp.xml and should not be created. also if other given tags are garbage. (errors from eval_xpath() methods)

Return xmltree xml etree of the new inp.xml

attributedict is a python dictionary containing dictionaries that specify attributes to be set inside the certain specie. For example, if one wants to set a MT radius it can be done via:

```
attributedict = {'mtSphere' : {'radius' : 2.2}}
```

Another example:

```
'attributedict': {'special': {'socscale': 0.0}}
```

that switches SOC terms on a sertain specie. `mtSphere`, `atomicCutoffs`, `energyParameters`, `lo`, `electronConfig`, `nocoParams`, `ldaU` and `special` keys are supported. To find possible keys of the inner dictionary please refer to the FLEUR documentation flapw.de

masci_tools.util.xml.xml_setters_names.**set_species_label**(*xmltree*, *schema_dict*, *atom_label*, *attributedict*, *create=False*)

This method calls *set_species()* method for a certain atom species that corresponds to an atom with a given label

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **atom_label** – string, a label of the atom which specie will be changed. 'all' to change all the species
- **attributedict** – a python dict specifying what you want to change.
- **create** – bool, if species does not exist create it and all subtags?

Returns xml etree of the new inp.xml

masci_tools.util.xml.xml_setters_names.**set_text**(*xmltree*, *schema_dict*, *tag_name*, *text*, *complex_xpath=None*, *filters=None*, *occurrences=None*, *create=False*, ***kwargs*)

Sets the text on tags in a xmltree to a given value, specified by the name of the tag and further specifications. By default the text will be set on all nodes returned for the specified xpath. If there are no nodes under the specified xpath a tag can be created with *create=True*. The text values are converted automatically according to the types with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **tag_name** – str name of the tag, where the text should be set
- **text** – value or list of values to set
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xmltree with set text

masci_tools.util.xml.xml_setters_names.**shift_value**(*xmltree*, *schema_dict*, *change_dict*, *mode='abs'*, *path_spec=None*)

Shifts numerical values of attributes directly in the inp.xml file.

The first occurrence of the attribute is shifted

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **change_dict** – a python dictionary with the keys to shift and the shift values.
- **mode** – 'abs' if change given is absolute, 'rel' if relative
- **path_spec** – dict, with ggf. necessary further specifications for the path of the attribute

Returns a xml tree with shifted values

An example of change_dict:

```
change_dict = {'itmax' : 1, 'dVac': -0.123}
```

masci_tools.util.xml.xml_setters_names.**shift_value_species_label**(*xmltree*, *schema_dict*, *atom_label*, *attributename*, *value_given*, *mode='abs'*, ***kwargs*)

Shifts the value of an attribute on a species by label if atom_label contains 'all' then applies to all species

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **atom_label** – string, a label of the atom which specie will be changed. 'all' if set up all species
- **attributename** – name of the attribute to change
- **value_given** – value to add or to multiply by
- **mode** – 'rel' for multiplication or 'abs' for addition

Kwargs if the attributename does not correspond to a unique path:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns xml etree of the new inp.xml

masci_tools.util.xml.xml_setters_names.**switch_kpointset**(*xmltree*, *schema_dict*, *list_name*)

Switch the used k-point set

> **Warning:** This method is only supported for input versions after the Max5 release

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input

- **list_name** – name of the kPoint set to use

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**switch_kpointset_max4**(*xmltree*, *schema_dict*, *list_name*)
Sets a k-point mesh directly into inp.xml specific for inputs of version Max4

> **Warning:** This method is only supported for input versions after the Max5 release

Parameters

- **xmltree** – xml tree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **list_name** – name of the kPoint set to use

Returns an xmltree of the inp.xml file with changes.

masci_tools.util.xml.xml_setters_names.**switch_species**(*xmltree*, *schema_dict*, *new_species_name*, *position=None*, *species=None*, *filters=None*, *clone=False*, *changes=None*)
Method to switch the species of an atom group of the fleur inp.xml file.

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **new_species_name** – name of the species to switch to
- **position** – position of an atom group to be changed. If equals to 'all', all species will be changed
- **species** – atom groups, corresponding to the given species will be changed
- **clone** – if True and the new species name does not exist and it corresponds to changing from one species the species will be cloned with *clone_species()*
- **changes** – changes to do if the species is cloned
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Returns xml etree of the new inp.xml

masci_tools.util.xml.xml_setters_names.**switch_species_label**(*xmltree*, *schema_dict*, *atom_label*, *new_species_name*, *clone=False*, *changes=None*)
Method to switch the species of an atom group of the fleur inp.xml file based on a label of a contained atom

Parameters

- **xmltree** – xml etree of the inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **atom_label** – string, a label of the atom which group will be changed. 'all' to change all the groups
- **new_species_name** – name of the species to switch to

- **clone** – if True and the new species name does not exist and it corresponds to changing from one species the species will be cloned with *clone_species()*
- **changes** – changes to do if the species is cloned

Returns xml etree of the new inp.xml

This module contains useful methods for initializing or modifying a n_mmp_mat file for LDA+U

masci_tools.util.xml.xml_setters_nmmpmat.**rotate_nmmpmat**(*xmltree*, *nmmplines*, *schema_dict*, *species_name*, *orbital*, *phi*, *theta*, *filters=None*)

Rotate the density matrix with the given angles phi and theta

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **nmmplines** – list of lines in the n_mmp_mat file
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **species_name** – string, name of the species you want to change
- **orbital** – integer, orbital quantum number of the LDA+U procedure to be modified
- **phi** – float, angle (radian), by which to rotate the density matrix
- **theta** – float, angle (radian), by which to rotate the density matrix
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Raises

- **ValueError** – If something in the input is wrong
- **KeyError** – If no LDA+U procedure is found on a species

Returns list with modified nmmplines

masci_tools.util.xml.xml_setters_nmmpmat.**set_nmmpmat**(*xmltree*, *nmmplines*, *schema_dict*, *species_name*, *orbital*, *spin*, *state_occupations=None*, *orbital_occupations=None*, *denmat=None*, *phi=None*, *theta=None*, *filters=None*)

Routine sets the block in the n_mmp_mat file specified by species_name, orbital and spin to the desired density matrix

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **nmmplines** – list of lines in the n_mmp_mat file
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **species_name** – string, name of the species you want to change
- **orbital** – integer, orbital quantum number of the LDA+U procedure to be modified
- **spin** – integer, specifies which spin block should be modified
- **state_occupations** – list, sets the diagonal elements of the density matrix and everything else to zero
- **denmat** – matrix, specify the density matrix explicitely
- **phi** – float, optional angle (radian), by which to rotate the density matrix before writing it

- **theta** – float, optional angle (radian), by which to rotate the density matrix before writing it
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Raises

- **ValueError** – If something in the input is wrong
- **KeyError** – If no LDA+U procedure is found on a species

Returns list with modified nmmplines

masci_tools.util.xml.xml_setters_nmmpmat.**validate_nmmpmat**(*xmltree*, *nmmplines*, *schema_dict*)

Checks that the given nmmp_lines is valid with the given xmltree

Checks that the number of blocks is as expected from the inp.xml and each block does not contain non-zero elements outside their size given by the orbital quantum number in the inp.xml. Additionally the occupations, i.e. diagonal elements are checked that they are in between 0 and the maximum possible occupation

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **nmmplines** – list of lines in the n_mmp_mat file

Raises **ValueError** – if any of the above checks are violated.

Functions for modifying the xml input file of Fleur with explicit xpath arguments These can still use the schema dict for finding information about the xpath

masci_tools.util.xml.xml_setters_xpaths.**eval_xpath_create**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *create_parents=False*, *occurrences=None*, *number_nodes=1*, *list_return=False*)

Evaluates and xpath and creates tag if the result is empty

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to place a new tag
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **create_parents** – bool optional (default False), if True also the parents of the tag are created if they are missing
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag if the tag is missing. By default all nodes are used.
- **list_return** – if True, the returned quantity is always a list even if only one element is in it
- **number_nodes** – how many identical nodes to create

Returns list of nodes from the result of the xpath expression

masci_tools.util.xml.xml_setters_xpaths.**xml_add_number_to_attrib**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *attributename*, *add_number*, *mode='abs'*, *occurrences=None*)

Adds a given number to the attribute value in a xmltree. By default the attribute will be shifted on all nodes returned for the specified xpath. If there are no nodes under the specified xpath an error is raised

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attributes
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.

Raises

- **ValueError** – If the attribute is unknown or cannot be float or int
- **ValueError** – If the evaluation of the old values failed
- **ValueError** – If a float result is written to a integer attribute

Returns xmltree with shifted attribute

masci_tools.util.xml.xml_setters_xpaths.**xml_add_number_to_first_attrib**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *attributename*, *add_number*, *mode='abs'*)

Adds a given number to the first occurrence of a attribute value in a xmltree. If there are no nodes under the specified xpath an error is raised

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attributes
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **attributename** – the attribute name to change
- **add_number** – number to add/multiply with the old attribute value
- **mode** – str (either *rel* or *abs*). *rel* multiplies the old value with *add_number abs* adds the old value and *add_number*

Raises

- **ValueError** – If the attribute is unknown or cannot be float or int
- **ValueError** – If the evaluation of the old values failed
- **ValueError** – If a float result is written to a integer attribute

Returns xmltree with shifted attribute

masci_tools.util.xml.xml_setters_xpaths.**xml_create_tag_schema_dict**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *element*, *create_parents=False*, *number_nodes=1*, *occurrences=None*)

This method evaluates an xpath expression and creates a tag in a xmltree under the returned nodes. If there are no nodes evaluated the subtags can be created with *create_parents=True*

The tag is always inserted in the correct place if a order is enforced by the schema

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to place a new tag
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **element** – a tag name or etree Element to be created
- **create_parents** – bool optional (default False), if True and the given xpath has no results the the parent tags are created recursively
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.
- **number_nodes** – how many identical nodes to create

Raises ValueError – If the nodes are missing and *create_parents=False*

Returns xmltree with created tags

masci_tools.util.xml.xml_setters_xpaths.**xml_set_attrib_value**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *attributename*, *attribv*, *occurrences=None*, *create=False*)

Sets an attribute in a xmltree to a given value. By default the attribute will be set on all nodes returned for the specified xpath. If there are no nodes under the specified xpath a tag can be created with *create=True*. The attribute values are converted automatically according to the types of the attribute with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attributes
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing

Raises

- ValueError – If the conversion to string failed

- **ValueError** – If the tag is missing and *create=False*
- **ValueError** – If the attributename is not allowed on the base_xpath

Returns xmltree with set attribute

masci_tools.util.xml.xml_setters_xpaths.**xml_set_complex_tag**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *attributedict*, *create=False*)

Recursive Function to correctly set tags/attributes for a given tag. Goes through the attributedict and decides based on the schema_dict, how the corresponding key has to be handled.

Supports:

- attributes
- tags with text only
- simple tags, i.e. only attributes (can be optional single/multiple)
- complex tags, will recursively create/modify them

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attributes
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **tag_name** – name of the tag to set
- **attributedict** – Keys in the dictionary correspond to names of tags and the values are the modifications to do on this tag (attributename, subdict with changes to the subtag, ...)
- **create** – bool optional (default False), if True and the path, where the complex tag is set does not exist it is created

Returns xmltree with changes to the complex tag

masci_tools.util.xml.xml_setters_xpaths.**xml_set_first_attrib_value**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *attributename*, *attribv*, *create=False*)

Sets the first occurrence attribute in a xmltree to a given value. If there are no nodes under the specified xpath a tag can be created with *create=True*. The attribute values are converted automatically according to the types of the attribute with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attribute
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set
- **create** – bool optional (default False), if True the tag is created if is missing

Raises

- **ValueError** – If the conversion to string failed
- **ValueError** – If the tag is missing and *create=False*
- **ValueError** – If the attributename is not allowed on the base_xpath

Returns xmltree with set attribute

masci_tools.util.xml.xml_setters_xpaths.**xml_set_first_text**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *text*, *create=False*)

Sets the text on the first occurrence of a tag in a xmltree to a given value. If there are no nodes under the specified xpath a tag can be created with *create=True*. The text values are converted automatically according to the types with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the text
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **text** – value or list of values to set
- **create** – bool optional (default False), if True the tag is created if is missing

Raises

- **ValueError** – If the conversion to string failed
- **ValueError** – If the tag is missing and *create=False*

Returns xmltree with set text

masci_tools.util.xml.xml_setters_xpaths.**xml_set_simple_tag**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *tag_name*, *changes*, *create_parents=False*)

Sets one or multiple *simple* tag(s) in an xmltree. A simple tag can only hold attributes and has no subtags. If the tag can occur multiple times all existing tags are DELETED and new ones are written. If the tag only occurs once it will automatically be created if its missing.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the attributes
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **tag_name** – name of the tag to set
- **changes** – list of dicts or dict with the changes. Elements in list describe multiple tags. Keys in the dictionary correspond to {'attributename': attributevalue}
- **create_parents** – bool optional (default False), if True and the path, where the simple tags are set does not exist it is created

Returns xmltree with set simple tags

masci_tools.util.xml.xml_setters_xpaths.**xml_set_text**(*xmltree*, *schema_dict*, *xpath*, *base_xpath*, *text*, *occurrences=None*, *create=False*)

Sets the text on tags in a xmltree to a given value. By default the text will be set on all nodes returned for the specified xpath. If there are no nodes under the specified xpath a tag can be created with *create=True*. The text values are converted automatically according to the types with *convert_to_xml()* if they are not *str* already.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **schema_dict** – InputSchemaDict containing all information about the structure of the input
- **xpath** – a path where to set the text
- **base_xpath** – path where to place a new tag without complex syntax ([] conditions and so on)
- **text** – value or list of values to set
- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.
- **create** – bool optional (default False), if True the tag is created if is missing

Raises

- **ValueError** – If the conversion to string failed
- **ValueError** – If the tag is missing and *create=False*

Returns xmltree with set text

Basic functions for modifying the xml input file of Fleur. These functions DO NOT have the ability to create missing tags on the fly. This functionality is added on top in *xml_setters_xpaths* since we need the schema dictionary to do these operations robustly

masci_tools.util.xml.xml_setters_basic.**xml_create_tag**(*xmltree*, *xpath*, *element*, *place_index=None*, *tag_order=None*, *occurrences=None*, *correct_order=True*, *several=True*)

This method evaluates an xpath expression and creates a tag in a xmltree under the returned nodes. If there are no nodes under the specified xpath an error is raised.

The tag is appended by default, but can be inserted at a certain index (*place_index*) or can be inserted according to a given order of tags

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path where to place a new tag
- **element** – a tag name or etree Element to be created
- **place_index** – defines the place where to put a created tag
- **tag_order** – defines a tag order
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.
- **correct_order** – bool, if True (default) and a tag_order is given, that does not correspond to the given order in the xmltree (only order wrong no unknown tags) it will be corrected and a warning is given This is necessary for some edge cases of the xml schemas of fleur
- **several** – bool, if True multiple tags od the given name are allowed

Raises ValueError – If the insertion failed in any way (tag_order does not match, failed to insert, ...)

Returns xmltree with created tags

masci_tools.util.xml.xml_setters_basic.**xml_delete_att**(*xmltree*, *xpath*, *attrib*, *occurrences=None*)
Deletes an xml attribute in an xmletree.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path to the attribute to be deleted
- **attrib** – the name of an attribute
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Returns xmltree with deleted attribute

masci_tools.util.xml.xml_setters_basic.**xml_delete_tag**(*xmltree*, *xpath*, *occurrences=None*)
Deletes a xml tag in an xmletree.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path to the tag to be deleted
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Returns xmltree with deleted tag

masci_tools.util.xml.xml_setters_basic.**xml_replace_tag**(*xmltree*, *xpath*, *newelement*, *occurrences=None*)
replaces xml tags by another tag on an xmletree in place

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path to the tag to be replaced
- **newelement** – a new tag
- **occurrences** – int or list of int. Which occurence of the parent nodes to create a tag. By default all nodes are used.

Returns xmltree with replaced tag

masci_tools.util.xml.xml_setters_basic.**xml_set_attrib_value_no_create**(*xmltree*, *xpath*, *attributename*, *attribv*, *occurrences=None*)
Sets an attribute in a xmltree to a given value. By default the attribute will be set on all nodes returned for the specified xpath.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path where to set the attributes
- **attributename** – the attribute name to set
- **attribv** – value or list of values to set (if not str they will be converted with *str(value)*)

- **occurrences** – int or list of int. Which occurence of the node to set. By default all are set.

Raises ValueError – If the lengths of attribv or occurrences do not match number of nodes

Returns xmltree with set attribute

masci_tools.util.xml.xml_setters_basic.**xml_set_text_no_create**(*xmltree*, *xpath*, *text*, *occurrences=None*)

Sets the text of a tag in a xmltree to a given value. By default the text will be set on all nodes returned for the specified xpath.

Parameters

- **xmltree** – an xmltree that represents inp.xml
- **xpath** – a path where to set the text
- **text** – value or list of values to set (if not str they will be converted with *str(value)*)
- **occurrences** – int or list of int. Which occurrence of the node to set. By default all are set.

Raises ValueError – If the lengths of text or occurrences do not match number of nodes

Returns xmltree with set text

6.1.5.4 XML Getter functions

This module provides functions to extract distinct parts of the fleur xml files for easy versioning and reuse

masci_tools.util.xml.xml_getters.**get_cell**(*xmltree*, *schema_dict*, *logger=None*, *convert_to_angstroem=True*)

Get the Bravais matrix from the given fleur xml file. In addition a list determining in, which directions there are periodic boundary conditions in the system.

Warning: Only the explicit definition of the Bravais matrix is supported. Old inputs containing the *latnam* definitions are not supported

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors
- **convert_to_angstroem** – bool if True the bravais matrix is converted to angstroem

Returns numpy array of the bravais matrix and list of boolean values for periodic boundary conditions

masci_tools.util.xml.xml_getters.**get_fleur_modes**(*xmltree*, *schema_dict*, *logger=None*)

Determine the calculation modes of fleur for the given xml file. Calculation modes are things that change the produced files or output in the out.xml files

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors

Returns dictionary with all the extracted calculation modes

The following modes are inspected:

- *jspin*: How many spins are considered in the calculation
- *noco*: Is the calculation non-collinear?
- *soc*: Is spin-orbit coupling included?
- *relax*: Is the calculation a structure relaxation?
- *gw*: Special mode for GW/Spex calculations
- *force_theorem*: Is a Force theorem calculation performed?
- *film*: Is the structure a film system
- *ldau*: Is LDA+U included?
- *dos*: Is it a density of states calculation?
- *band*: Is it a bandstructure calculation?
- *bz_integration*: How is the integration over the Brillouin-Zone performed?

masci_tools.util.xml.xml_getters.**get_kpoints_data**(*xmltree*, *schema_dict*, *name=None*, *index=None*, *only_used=False*, *logger=None*, *convert_to_angstroem=True*)

Get the kpoint sets defined in the given fleur xml file.

Warning: For file versions before Max5 the name argument is not valid

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **name** – str, optional, if given only the kpoint set with the given name is returned
- **index** – int, optional, if given only the kpoint set with the given index is returned
- **only_used** – bool if True only the kpoint list used in the calculation is returned
- **logger** – logger object for logging warnings, errors
- **convert_to_angstroem** – bool if True the bravais matrix is converted to angstroem

Returns tuple containing the kpoint information

The tuple contains the following entries:

1. **kpoints** dict or list (list if there is only one kpoint set), containing the coordinates of the kpoints
2. **weights** dict or list (list if there is only one kpoint set), containing the weights of the kpoints
3. **cell** numpy array, bravais matrix of the given system
4. **pbc** list of booleans, determines in which directions periodic boundary conditions are applicable

masci_tools.util.xml.xml_getters.**get_kpoints_data_max4**(*xmltree*, *schema_dict*, *logger=None*, *convert_to_angstroem=True*, *only_used=False*)

Get the kpoint sets defined in the given fleur xml file.

Note: This function is specific to file version before and including the Max4 release of fleur

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors
- **convert_to_angstroem** – bool if True the bravais matrix is converted to angstroem
- **only_used** – (Has no effect for Max4) bool if True only the kpoint list used in the calculation is returned

Returns tuple containing the kpoint information

The tuple contains the following entries:

1. **kpoints** list containing the coordinates of the kpoints
2. **weights** list containing the weights of the kpoints
3. **cell** numpy array, bravais matrix of the given system
4. **pbc** list of booleans, determines in which directions periodic boundary conditions are applicable

masci_tools.util.xml.xml_getters.**get_nkpts**(*xmltree*, *schema_dict*, *logger=None*)

Get the number of kpoints that will be used in the calculation specified in the given fleur XMl file.

Warning: For file versions before Max5 only kPointList or kPointCount tags will work. However, for kPointCount there is no real guarantee that for every occasion it will correspond to the number of kpoints. So a warning is written out

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors

Returns int with the number of kpoints

masci_tools.util.xml.xml_getters.**get_nkpts_max4**(*xmltree*, *schema_dict*, *logger=None*)

Get the number of kpoints that will be used in the calculation specified in the given fleur XMl file. Version specific for Max4 versions or older

Warning: For file versions before Max5 only kPointList or kPointCount tags will work. However, for kPointCount there is no real guarantee that for every occasion it will correspond to the number of kpoints. So a warning is written out

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree

- **logger** – logger object for logging warnings, errors

Returns int with the number of kpoints

masci_tools.util.xml.xml_getters.**get_parameter_data**(*xmltree*, *schema_dict*, *inpgen_ready=True*, *write_ids=True*, *extract_econfig=False*, *logger=None*)

This routine returns an python dictionary produced from the inp.xml file, which contains all the parameters needed to setup a new inp.xml from a inpgen input file to produce the same input (for parameters that the inpgen can control)

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **inpgen_ready** – Bool, return a dict which can be inputed into inpgen while setting atoms
- **write_ids** – Bool, if True the atom ids are added to the atom namelists
- **logger** – logger object for logging warnings, errors

Returns dict, which will lead to the same inp.xml (in case if other defaults, which can not be controlled by input for inpgen, were changed)

masci_tools.util.xml.xml_getters.**get_relaxation_information**(*xmltree*, *schema_dict*, *logger=None*)

Get the relaxation information from the given fleur XML file. This includes the current displacements, energy and posforce evolution

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors

Returns dict with the relaxation information

Raises ValueError – If no relaxation section is included in the xml tree

masci_tools.util.xml.xml_getters.**get_relaxation_information_pre029**(*xmltree*, *schema_dict*, *logger=None*)

Get the relaxation information from the given fleur XML file. This includes the current displacements, energy and posforce evolution

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors

Returns dict with the relaxation information

Raises ValueError – If no relaxation section is included in the xml tree

masci_tools.util.xml.xml_getters.**get_structure_data**(*xmltree*, *schema_dict*, *include_relaxations=True*, *site_namedtuple=True*, *convert_to_angstroem=True*, *normalize_kind_name=True*, *logger=None*)

Get the structure defined in the given fleur xml file.

Warning: Only the explicit definition of the Bravais matrix is supported. Old inputs containing the *latnam* definitions are not supported

Warning: In versions `0.5.0` or later the output of the atom sites was restructured to be more interoperable with other IO functions (e.g. *write_inpgen_file()*) The new format returns a list of *AtomSiteProperties* instead of the list of tuples (position, symbol)

For better compatibility this output is not default in `0.5.0` but instead is enabled by `site_namedtuple=True` and a DeprecationWarning is given when this argument is `False`.

Note: In versions `0.5.0` or later the returned atom positions correspond to the relaxed structure if a `relaxation` section is present in the xmltree

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **include_relaxations** – bool if True and a relaxation section is included the resulting positions correspond to the relaxed structure
- **logger** – logger object for logging warnings, errors
- **convert_to_angstroem** – bool if True the bravais matrix is converted to angstroem

Returns tuple containing the structure information

The tuple contains the following entries:

1. **atom_data** list of (named)tuples containing the absolute positions and symbols of the atoms
2. **cell** numpy array, bravais matrix of the given system
3. **pbc** list of booleans, determines in which directions periodic boundary conditions are applicable

masci_tools.util.xml.xml_getters.**get_symmetry_information**(*xmltree*, *schema_dict*, *logger=None*)

Get the symmetry information from the given fleur XML file. This includes the rotation matrices and shifts defined in the `symmetryOperations` tag.

Note: Only the explicit definition of the used symmetry operations in the xml file is supported.

Parameters

- **xmltree** – etree representing the fleur xml file
- **schema_dict** – schema dictionary corresponding to the file version of the xmltree
- **logger** – logger object for logging warnings, errors

Returns tuple of the rotations and their respective shifts

Raises `ValueError` – If no symmetryOperations section is included in the xml tree

6.1.5.5 Basic IO helper functions

Here commonly used functions that do not need aiida-stuff (i.e. can be tested without a database) are collected.

class masci_tools.io.common_functions.**AtomSiteProperties**(*position*, *symbol*, *kind*)
namedtuple used for input output of atom sites

kind: str
Alias for field number 2

position: list[float]
Alias for field number 0

symbol: str
Alias for field number 1

masci_tools.io.common_functions.**_TVectorType**
Generic type variable for atom position types

alias of TypeVar('_TVectorType', tuple[float, float, float], list[float], numpy.ndarray)

masci_tools.io.common_functions.**abs_to_rel**(*vector*, *cell*)
Converts a position vector in absolute coordinates to relative coordinates.

Parameters

- **vector** – list or np.array of length 3, vector to be converted
- **cell** – Bravais matrix of a crystal 3x3 Array, List of list or np.array

Returns list of length 3 of scaled vector, or False if vector was not length 3

masci_tools.io.common_functions.**abs_to_rel_f**(*vector*, *cell*, *pbc*)
Converts a position vector in absolute coordinates to relative coordinates for a film system.

Parameters

- **vector** – list or np.array of length 3, vector to be converted
- **cell** – Bravais matrix of a crystal 3x3 Array, List of list or np.array
- **pbc** – Boundary conditions, List or Tuple of 3 Boolean

Returns list of length 3 of scaled vector, or False if vector was not length 3

masci_tools.io.common_functions.**angles_to_vec**(*magnitude*, *theta*, *phi*)
convert (magnitude, theta, phi) to (x,y,z)

theta/phi need to be in radians!

Input can be single number, list of numpy.ndarray data Returns x,y,z vector

masci_tools.io.common_functions.**camel_to_snake**(*name*)
Converts camelCase to snake_case variable names Used in the Fleur parser to convert attribute names from the xml files

Return type str

masci_tools.io.common_functions.**convert_to_fortran**(*val*, *quote_strings=True*)

Parameters **val** (Any) – the value to be read and converted to a Fortran-friendly string.

Return type str

masci_tools.io.common_functions.**convert_to_fortran_string**(*string*)
converts some parameter strings to the format for the inpgen :type string: str :param string: some string :rtype: str :returns: string in right format (extra “” if not already present)

masci_tools.io.common_functions.**convert_to_pystd**(*value*)
Recursively convert numpy datatypes to standard python, needed by aiida-core.

Usage: converted = convert_to_pystd(to_convert)

where *to_convert* can be a dict, array, list, or single valued variable

Return type Any

masci_tools.io.common_functions.**fac**(*n*)
Returns the factorial of n

Return type int

masci_tools.io.common_functions.**filter_out_empty_dict_entries**(*dict_to_filter*)
Filter out entries in a given dict that correspond to empty values. At the moment this is empty lists, dicts and None

Parameters **dict_to_filter** (dict) – dict to filter

Return type dict

Returns dict without empty entries

masci_tools.io.common_functions.**find_symmetry_relation**(*from_pos*, *to_pos*, *rotations*, *shifts*, *cell*, *relative_pos=False*, *film=False*)
Find symmetry relation between the given vectors. This functions assumes that a symmetry relation exists otherwise an error is raised

Parameters

- **from_pos** – vector to rotate
- **to_pos** – vector to rotate to
- **rotations** – list of np.arrays with the given symmetry rotations
- **shifts** – list of np.arrays with the given shifts for the symmetry operations
- **cell** – Bravais matrix of a crystal 3x3 Array, List of list or np.array
- **relative_pos** – bool if True the given vectors are assuemd to be in internal coordinates
- **film** – bool if True the vectors are assumed to be film coordinates

Returns tuple of rotation and shift mapping from_pos to to_pos

Raises ValueError – If no symmetry relation is found

masci_tools.io.common_functions.**get_corestates_from_potential**(*potfile='potential'*)
Read core states from potential file

masci_tools.io.common_functions.**get_ef_from_potfile**(*potfile*)
extract fermi energy from potfile

masci_tools.io.common_functions.**get_highest_core_state**(*nstates*, *energies*, *lmoments*)
Find highest lying core state from list of core states, needed to find and check energy contour

masci_tools.io.common_functions.**get_wigner_matrix**(*l*, *phi*, *theta*)
Produces the wigner rotation matrix for the density matrix

Parameters

- **l** (int) – int, orbital quantum number
- **phi** (float) – float, angle (radian) corresponds to euler angle alpha
- **theta** (float) – float, angle (radian) corresponds to euler angle beta

Return type ndarray

masci_tools.io.common_functions.**interpolate_dos**(*dosfile*, *return_original=False*)
interpolation function copied from complexdos3 fortran code

Principle of DOS here: Two-point contour integration for DOS in the middle of the two points. The input DOS and energy must be complex. Parameter deltae should be of the order of magnitude of eim:

```
      <-2*deltae->   _
           /\        |     DOS=(n(1)+n(2))/2 + (n(1)-n(2))*eim/deltae
          /  \       |
        (1)  (2)   2*i*eim=2*i*pi*Kb*Tk
        /      \     |
       /        \    |
------------------------ (Real E axis)
```

Parameters **input** – either absolute path of 'complex.dos' file or file handle to it

Returns E_Fermi, numpy array of interpolated dos

Note output units are in Ry!

masci_tools.io.common_functions.**is_sequence**(*arg*)
Checks if arg is a sequence

Return type bool

masci_tools.io.common_functions.**open_general**(*filename_or_handle*, *iomode=None*)
Open a file directly from a path or use a file handle if that is given. Also take care of closed files by reopenning them. This is intended to be used like this:

```
with open_general(outfile) as f:
    txt = f.readlines()
```

masci_tools.io.common_functions.**rel_to_abs**(*vector*, *cell*)
Converts a position vector in internal coordinates to absolute coordinates in Angstrom.

Parameters

- **vector** – list or np.array of length 3, vector to be converted
- **cell** – Bravais matrix of a crystal 3x3 Array, List of list or np.array

Returns list of legth 3 of scaled vector, or False if vector was not lenth 3

masci_tools.io.common_functions.**rel_to_abs_f**(*vector*, *cell*)
Converts a position vector in internal coordinates to absolute coordinates in Angstrom for a film structure (2D).

masci_tools.io.common_functions.**skipHeader**(*seq*, *n*)
Iterate over a sequence skipping the first n elements

Args: seq (iterable): Iterable sequence n (int): Number of Elements to skip in the beginning of the sequence

Yields: item: Elements in seq after the first n elements

Return type Generator[Any, None, None]

masci_tools.io.common_functions.**vec_to_angles**(*vec*)
converts vector (x,y,z) to (magnitude, theta, phi)

Small utility functions for inspecting hdf files and converting the complete file structure into a python dictionary

masci_tools.io.hdf5_util.**h5dump**(*file*, *group='/'*)
Shows the overall filestructure of an hdf file Goes through all groups and subgroups and prints the attributes or the shape and datatype of the datasets

Parameters **filepath** – path to the hdf file

masci_tools.io.hdf5_util.**hdfList**(*name*, *obj*)
Print the name of the current object (indented to create a nice tree structure)

Also prints attribute values and dataset shapes and datatypes

Return type None

masci_tools.io.hdf5_util.**read_groups**(*hdfdata*, *flatten=False*)
Recursive function to read a hdf datastructure and extract the datasets and attributes

Parameters

- **hdfdata** (Group) – current hdf group to process
- **flatten** (bool) – bool, if True the dictionary will be flattened (does not check for lost information)

Return type tuple[dict[str, Any], dict[str, Any]]

Returns two dictionaries, one with the datasets the other with the attributes in the file

masci_tools.io.hdf5_util.**read_hdf_simple**(*file*, *flatten=False*)
Reads in an hdf file and returns its context in a nested dictionary

Parameters

- **filepath** – path or filehandle to the hdf file
- **flatten** – bool, if True the dictionary will be flattened (does not check for lost information)

Returns two dictionaries, one with the datasets the other with the attributes in the file

Non unique group attribute or dataset names will be overwritten in the return dict

6.1.5.6 Logging Utility

This module defines useful utility for logging related functionality

class masci_tools.util.logging_util.**DictHandler**(*log_dict*, *ignore_unknown_levels=False*, ***kwargs*)
Custom Handler for the logging module inserting logging messages into a given dictionary.

Messages are grouped into list under the names of the error categories. Keyword arguments can be used to modify the keys for the different levels

emit(*record*)
Emit a record.

Return type None

class masci_tools.util.logging_util.**OutParserLogAdapter**(*logger*, *extra*)
This adapter expects the passed in dict-like object to have a 'iteration' key, whose value is prepended as [Iteration i] to the message

process(*msg*, *kwargs*)

Process the logging message and keyword arguments passed in to a logging call to insert contextual information. You can either manipulate the message itself, the keyword args or both. Return the message and kwargs modified (or not) to suit your needs.

Normally, you'll only need to override this one method in a LoggerAdapter subclass for your specific needs.

Return type tuple[str, dict]

6.1.5.7 Fleur parser utility

This module contains helper functions for extracting information easily from the schema_dicts defined for the Fleur input/output

Also provides convienient functions to use just a attribute name for extracting the attribute from the right place in the given etree

masci_tools.util.schema_dict_util.**attrib_exists**(*node*, *schema_dict*, *name*, *logger=None*, *iteration_path=False*, *filters=None*, ***kwargs*)

Evaluates whether the attribute exists in the xmltree based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

Returns bool, True if any tag with the attribute exists

masci_tools.util.schema_dict_util.**eval_simple_xpath**(*node*, *schema_dict: masci_tools.io.parsers.fleur_schema.schema_dict.SchemaDict*, *name: str*, *logger: Logger | None = None*, *iteration_path: bool = False*, *filters: FilterType | None = None*, *list_return: Literal[True] = ...*, ***kwargs: Any*) → list[lxml.etree._Element]

masci_tools.util.schema_dict_util.**eval_simple_xpath**(*node*, *schema_dict: masci_tools.io.parsers.fleur_schema.schema_dict.SchemaDict*, *name: str*, *logger: Logger | None = None*, *iteration_path: bool = False*, *filters: FilterType | None = None*, *list_return: Literal[False] = ...*, ***kwargs: Any*) → etree._Element | list[etree._Element]

masci_tools.util.schema_dict_util.**eval_simple_xpath**(*node*, *schema_dict*, *name*, *logger=None*, *iteration_path=False*, *filters=None*, *list_return=False*, ***kwargs*)

Evaluates a simple xpath expression of the tag in the xmltree based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details
- **list_return** – bool, if True a list is always returned

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

Returns etree Elements obtained via the simple xpath expression

masci_tools.util.schema_dict_util.**evaluate_attribute**(*node*, *schema_dict*, *name*, *constants=None*, *logger=None*, *complex_xpath=None*, *filters=None*, *iteration_path=False*, ***kwargs*)

Evaluates the value of the attribute based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **constants** – dict, contains the defined constants
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param tag_name str, name of the tag where the attribute should be parsed

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param exclude list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other

param list_return if True, the returned quantity is always a list even if only one element is in it

param optional bool, if True and no logger given none or an empty list is returned

Returns list or single value, converted in convert_xml_attribute

masci_tools.util.schema_dict_util.**evaluate_parent_tag**(*node*, *schema_dict*, *name*, *constants=None*, *logger=None*, *complex_xpath=None*, *iteration_path=False*, *filters=None*, ***kwargs*)

Evaluates all attributes of the parent tag based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **constants** – dict, contains the defined constants
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param only_required bool (optional, default False), if True only required attributes are parsed

param ignore list of str (optional), attributes not to parse

param list_return if True, the returned quantity is always a list even if only one element is in it

param strict_missing_error if True, and no logger is given an error is raised if any attribute is not found

Returns dict, with attribute values converted via convert_xml_attribute

masci_tools.util.schema_dict_util.**evaluate_single_value_tag**(*node*, *schema_dict*, *name*, *constants=None*, *logger=None*, *complex_xpath=None*, ***kwargs*)

Evaluates the value and unit attribute of the tag based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **constants** – dict, contains the defined constants
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param only_required bool (optional, default False), if True only required attributes are parsed

param ignore list of str (optional), attributes not to parse

param list_return if True, the returned quantity is always a list even if only one element is in it

param strict_missing_error if True, and no logger is given an error is raised if any attribute is not found

param iteration_path bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed

param filters Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Returns value and unit, both converted in convert_xml_attribute

masci_tools.util.schema_dict_util.**evaluate_tag**(*node*, *schema_dict*, *name*, *constants=None*, *logger=None*, *subtags=False*, *text=True*, *complex_xpath=None*, *iteration_path=False*, *filters=None*, ***kwargs*)

Evaluates all attributes of the tag based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **constants** – dict, contains the defined constants
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **subtags** – optional bool, if True the subtags of the given tag are evaluated
- **text** – optional bool, if True the text of the tag is also parsed
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation

- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param only_required bool (optional, default False), if True only required attributes are parsed

param ignore list of str (optional), attributes not to parse

param list_return if True, the returned quantity is always a list even if only one element is in it

param strict_missing_error if True, and no logger is given an error is raised if any attribute is not found

Returns dict, with attribute values converted via convert_xml_attribute

masci_tools.util.schema_dict_util.**evaluate_text**(*node*, *schema_dict*, *name*, *constants=None*, *logger=None*, *complex_xpath=None*, *iteration_path=False*, *filters=None*, ***kwargs*)

Evaluates the text of the tag based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **constants** – dict, contains the defined constants
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised
- **complex_xpath** – an optional xpath to use instead of the simple xpath for the evaluation
- **iteration_path** – bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed
- **filters** – Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param list_return if True, the returned quantity is always a list even if only one element is in it

param optional bool, if True and no logger given none or an empty list is returned

Returns list or single value, converted in convert_xml_text

masci_tools.util.schema_dict_util.**get_attrib_xpath**(*schema_dict*, *name*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

DEPRECATED

Tries to find a unique path from the schema_dict based on the given name of the attribute and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *get_tag_xpath()*

Returns str, xpath to the tag with the given attribute

Raises **ValueError** – If no unique path could be found

masci_tools.util.schema_dict_util.**get_number_of_nodes**(*node*, *schema_dict*, *name*, *logger=None*, ***kwargs*)

Evaluates the number of occurences of the tag in the xmltree based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param iteration_path bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed

param filters Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Returns bool, True if any nodes with the path exist

masci_tools.util.schema_dict_util.**get_relative_attrib_xpath**(*schema_dict*, *name*, *root_tag*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

DEPRECATED

Tries to find a unique relative path from the schema_dict based on the given name of the attribute name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute

- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *get_relative_tag_xpath()*

Returns str, xpath for the given tag

Raises ValueError – If no unique path could be found

masci_tools.util.schema_dict_util.**get_relative_tag_xpath**(*schema_dict*, *name*, *root_tag*, *contains=None*, *not_contains=None*)

DEPRECATED

Tries to find a unique relative path from the schema_dict based on the given name of the tag name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises ValueError – If no unique path could be found

masci_tools.util.schema_dict_util.**get_tag_info**(*schema_dict*, *name*, *contains=None*, *not_contains=None*, *path_return=True*, *convert_to_builtin=False*, *multiple_paths=False*, *parent=False*)

DEPRECATED

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications and returns the tag_info entry for this tag

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **path_return** – bool, if True the found path will be returned alongside the tag_info
- **convert_to_builtin** – bool, if True the CaseInsensitiveFrozenSets are converetd to normal sets with the rigth case of the attributes
- **multiple_paths** – bool, if True mulitple paths are allowed to match as long as they have the same tag_info
- **parent** – bool, if True the tag_info for the parent of the tag is returned

Returns dict, tag_info for the found xpath

Returns str, xpath to the tag if *path_return=True*

masci_tools.util.schema_dict_util.**get_tag_xpath**(*schema_dict*, *name*, *contains=None*, *not_contains=None*)

DEPRECATED

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises ValueError – If no unique path could be found

masci_tools.util.schema_dict_util.**read_constants**(*root*, *schema_dict*, *logger=None*)

Reads in the constants defined in the inp.xml and returns them combined with the predefined constants from fleur as a dictionary

Parameters

- **root** – root of the etree of the inp.xml file
- **schema_dict** – schema_dictionary of the version of the file to read (inp.xml or out.xml)
- **logger** – logger object for logging warnings, errors

Returns a python dictionary with all defined constants

masci_tools.util.schema_dict_util.**reverse_xinclude**(*xmltree*, *schema_dict*, *included_tags*, ***kwargs*)

Split the xmltree back up according to the given included tags. The original xmltree will be returned with the corresponding xinclude tags and the included trees are returned in a dict mapping the inserted filename to the extracted tree

Tags for which no known filename is known are returned under unknown-1.xml, ... The following tags have known filenames:

- *relaxation*: `relax.xml`
- *kPointLists*: `kpts.xml`
- *symmetryOperations*: `sym.xml`
- *atomSpecies*: `species.xml`
- *atomGroups*: `atoms.xml`

Additional mappings can be given in the keyword arguments

Parameters

- **xmltree** – an xml-tree which will be processed
- **schema_dict** – Schema dictionary containing all the necessary information
- **included_tags** – Iterable of str, containing the names of the tags to be excluded

Returns xmltree with the inseerted xinclude tags and a dict mapping the filenames to the excluded trees

Raises ValueError – if the tag can not be found in teh given xmltree

masci_tools.util.schema_dict_util.**tag_exists**(*node*, *schema_dict*, *name*, *logger=None*, ***kwargs*)
Evaluates whether the tag exists in the xmltree based on the given name and additional further specifications with the available type information

Parameters

- **node** – etree Element, on which to execute the xpath evaluations
- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **logger** – logger object for logging warnings, errors, if not provided all errors will be raised

Kwargs:

param contains str, this string has to be in the final path

param not_contains str, this string has to NOT be in the final path

param iteration_path bool if True and the SchemaDict is of an output schema an absolute path into the iteration element is constructed

param filters Dict specifying constraints to apply on the xpath. See *XPathBuilder* for details

Returns bool, True if any nodes with the path exist

This module contains the functions necessary to parse mathematical expressions with predefined constants given in the inp.xml file of Fleur

exception masci_tools.util.fleur_calculate_expression.**MissingConstant**
Exception raised when a constant appearing in a expression is not defined

masci_tools.util.fleur_calculate_expression.**calculate_expression**(*expression*, *constants=None*)
Recursively evaluates the given expression string with the given defined constants

Parameters

- **expression** – str containing the expression to be parsed
- **constants** – dict with all defined constants (predefined in the Fleur code or defined in the inp.xml)

Returns float value of the given expression string

masci_tools.util.fleur_calculate_expression.**calculate_expression_partial**(*expression*, *constants=None*, *prevCommand=None*)
Recursively evaluates the given expression string with the given defined constants and returns the unevaluated part of the expression

Parameters

- **expression** – str containing the expression to be parsed
- **constants** – dict with all defined constants (predefined in the Fleur code or defined in the inp.xml)
- **prevCommand** – str, which gives the command before the beginning of the current block if it is given the calculation is stopped, when a command is encountered, which should be exectuted after prevCommand (order of operations)

Returns float value of the given expression string

masci_tools.util.fleur_calculate_expression.**evaluate_bracket**(*expression*, *constants*)
Evaluates the bracket opened at the start of the expression

Parameters

- **expression** – expression to be parsed
- **constants** – dict with defined constants

Returns value of the expression inside the brackets and remaining string of the expression after the corresponding closed bracket

masci_tools.util.fleur_calculate_expression.**get_first_number**(*expression*)
Reads the number in the beginning of the expression string. This number can begin with a sign +-, a number or the decimal point

Parameters **expression** (str) – str of the expression

Return type tuple[float, str]

Returns float value of the number in the beginning and the string of the remaining expression

masci_tools.util.fleur_calculate_expression.**get_first_string**(*expression*)
Reads the letter string in the beginning of the expression string.

Parameters **expression** (str) – str of the expression

Return type tuple[str, str]

Returns letter string in the beginning and the string of the remaining expression

This module contains a class which organizes the known parsing tasks for outxml files and provides fuctionality for adding custom tasks easily

masci_tools.util.parse_tasks.**MigrationDict: TypeAlias = "dict[str, dict[str, Literal['compatible'] | Callable]]"**
Type describing the dictionary defining the migration pathways

class masci_tools.util.parse_tasks.**ParseTasks**(*version*, *task_file=None*, *validate_defaults=False*)
Representation of all known parsing tasks for the out.xml file

When set up it will initialize the known default tasks and check if they work for the given output version

Accesing definition of task example

```
from masci_tools.io.parsers.fleur import ParseTasks

p = ParseTasks('0.33')
totE_definition = p.tasks['total_energy']
```

add_task(*task_name*, *task_definition*, *append=False*, *overwrite=False*)
Add a new task definition to the tasks dictionary

Will first check if the definition has all the required keys

Parameters

- **task_name** (str) – str, key in the tasks dict
- **task_definition** (dict[str, Any]) – dict with the defined tasks
- **overwrite** (bool) – bool (optional), if True and the key is present in the dictionary it will be overwritten with the new definition

- **append** (bool) – bool (optional), if True and the key is present in the dictionary the new defintions will be inserted into this dictionary (inner keys WILL BE OVERWRITTEN). Additionally if an inner key is overwritten with an empty dict the inner key will be removed

The following keys are expected in each entry of the task_definition dictionary:

param parse_type str, defines which methods to use when extracting the information

param path_spec dict with all the arguments that should be passed to tag_xpath or attrib_xpath to get the correct path

param subdict str, if present the parsed values are put into this key in the output dictionary

param overwrite_last bool, if True no list is inserted and each entry overwrites the last

For the allAttribs parse_type there are more keys that can appear:

param base_value str, optional. If given the attribute with this name will be inserted into the key from the task_definition all other keys are formatted as {task_key}_{attribute_name}

param ignore list of str, these attributes will be ignored

param overwrite list of str, these attributes will not create a list and overwrite any value that might be there

param flat bool, if False the dict parsed from the tag is inserted as a dict into the correspondin key if True the values will be extracted and put into the output dictionary with the format {task_key}_{attribute_name}

Return type None

property all_attribs_function: set[str]
Return the registered parse functions for parsing multipl attributes

Return type set[str]

property conversion_functions: dict[str, typing.Callable]
Return the registered conversion functions

Return type dict[str, Callable]

determine_tasks(*fleurmodes*, *optional_tasks=None*, *minimal=False*)
Determine, which tasks to perform based on the fleur_modes

Parameters

- **fleurmodes** – dict with the calculation modes
- **minimal** – bool, whether to only perform minimal tasks

property general_tasks: list[str]
Tasks to perform for the root node

Return type list[str]

property iteration_tasks: list[str]
Tasks to perform for each iteration

Return type list[str]

property migrations: *MigrationDict*
Return the registered migrations

property optional_tasks: set[str]
Return a set of the available optional defined tasks

Return type set[str]

property parse_functions: dict[str, typing.Callable]
Return the registered parse functions

Return type dict[str, Callable]

perform_task(*task_name*, *node*, *out_dict*, *schema_dict*, *constants*, *logger=None*, *use_lists=True*)
Evaluates the task given in the tasks_definition dict

Parameters

- **task_name** – str, specifies the task to perform
- **node** – etree.Element, the xpath expressions are evaluated from this node
- **out_dict** – dict, output will be put in this dictionary
- **schema_dict** – dict, here all paths and attributes are stored according to the outputschema
- **constants** – dict with all the defined mathematical constants
- **logger** – logger object for logging warnings, errors
- **root_tag** – str, this string will be appended in front of any xpath before it is evaluated
- **use_lists** – bool, if True lists are created for each key if not otherwise specified

show_available_tasks(*show_definitions=False*)
Print all currently available task keys. If show_definitions is True also the corresponding defintions will be printed

Return type None

masci_tools.util.parse_tasks.**find_migration**(*start*, *target*, *migrations*)
Tries to find a migration path from the start to the target version via the defined migration functions

Parameters

- **start** – str of the starting version
- **target** – str of the target version
- **migrations** – dict of funcs registered via the register_migration_function decorator

Returns list of migration functions to be called to go from start to target

This module defines decorators for the ParseTasks class to make extending/modifying the parser more convenient

Up till now 3 decorators are defined:

- `register_migration` marks a function of making backwards incompatible changes to the parsing tasks
- `register_parsing_function` gives a mappimg between available parsing functions and the keywords in the parsing tasks
- `conversion_function` makes the decorated function available to be called easily after a certain parsing task has occured

masci_tools.util.parse_tasks_decorators.**F**
Generic Callable type

alias of TypeVar('F', bound=Callable[[...], Any])

masci_tools.util.parse_tasks_decorators.**conversion_function**(*func*)
Marks a function as a conversion function, which can be called after performing a parsing task. The function can be specified via the _conversions control key in the task definitions.

A conversion function has to have the following arguments:

param out_dict dict with the previously parsed information

param parser_info_out dict, with warnings, info, errors, ...

and return only the modified output dict

Return type ~F

masci_tools.util.parse_tasks_decorators.**register_migration**(*base_version*, *target_version*)
Decorator to add migration for task definition dictionary to the ParseTasks class The function should only take the dict of task definitions as an argument

Parameters

- **base_version** (str) – str of the version, from which the migration starts
- **target_version** (Union[str, List[str]]) – str or list of str with the versions that work after the migration has been performed

Return type Callable[[~F], ~F]

masci_tools.util.parse_tasks_decorators.**register_parsing_function**(*parse_type_name*, *all_attribs_keys=False*)
Decorator to add parse type for task definition dictionary.

Parameters

- **parse_type_name** (str) – str, the function can be selected in task defintions via this string
- **all_attribs_keys** (bool) – bool, if True the arguments for parsing multiple attributes are valid

The decorated function has to have the following arguments:

param node etree Element, on which to execute the xpath evaluations

param schema_dict dict, containing all the path information and more

param name str, name of the tag/attribute

param parser_info_out dict, with warnings, info, errors, ...

param kwargs here all other keyword arguments are collected

Return type Callable[[~F], ~F]

This module contains custom conversion functions for the outxml_parser, which cannot be handled by the standard parsing framework

masci_tools.io.parsers.fleur.outxml_conversions.**calculate_total_magnetic_moment**(*out_dict*, *logger*)
Calculate the the total magnetic moment per cell

Parameters **out_dict** (dict[str, Any]) – dict with the already parsed information

Return type dict[str, Any]

masci_tools.io.parsers.fleur.outxml_conversions.**calculate_walltime**(*out_dict*, *logger*)
Calculate the walltime from start and end time

Parameters

- **out_dict** (dict[str, Any]) – dict with the already parsed information

- **logger** (Logger) – logger object for logging warnings, errors, if not provided all errors will be raised

Return type dict[str, Any]

masci_tools.io.parsers.fleur.outxml_conversions.**convert_forces**(*out_dict*, *logger*)
Convert the parsed forces from a iteration

Parameters **out_dict** (dict[str, Any]) – dict with the already parsed information

Return type dict[str, Any]

masci_tools.io.parsers.fleur.outxml_conversions.**convert_ldau_definitions**(*out_dict*, *logger*)
Convert the parsed information from LDA+U into a more readable dict

ldau_info has keys for each species with LDA+U ({species_name}/{atom_number}) and this in turn contains a dict with the LDA+U definition for the given orbital (spdf)

Parameters **out_dict** (dict[str, Any]) – dict with the already parsed information

Return type dict[str, Any]

masci_tools.io.parsers.fleur.outxml_conversions.**convert_relax_info**(*out_dict*, *logger*)
Convert the general relaxation information

Parameters **out_dict** (dict[str, Any]) – dict with the already parsed information

Return type dict[str, Any]

masci_tools.io.parsers.fleur.outxml_conversions.**convert_total_energy**(*out_dict*, *logger*)
Convert total energy to eV

Return type dict[str, Any]

Functions for expanding/splitting or converting electron configuration strings

masci_tools.util.econfig.**convert_fleur_config_to_econfig**(*fleurconf_str*, *keep_spin=False*)
'[Kr] (4d3/2) (4d5/2) (4f5/2) (4f7/2)' -> '[Kr] 4d10 4f14', or '[Kr] 4d3/2 4d5/2 4f5/2 4f7/2'

for now only use for coreconfig, it will fill all orbitals, since it has no information on the filling.

Parameters

- **fleurconf_str** (str) – string of the electron config like it is read from the inp.xml
- **keep_spin** (bool) – bool if True the spin indices will be kept in the converted string

Return type str

Returns string of the electron config to be used in the inpgen

masci_tools.util.econfig.**get_coreconfig**(*element*, *full=False*)
returns the econfiguration as a string of an element.

Parameters

- **element** – element string
- **full** – a bool if True the econfig without [He]... is returned

Returns coreconfig string

masci_tools.util.econfig.**get_econfig**(*element*, *full=False*)
returns the econfiguration as a string of an element.

Parameters

- **element** – element string

- **full** – a bool if True the econfig without [He]… is returned

Returns a econfig string

masci_tools.util.econfig.**rek_econ**(*econfigstr*)
recursive routine to return a full econfig '[Xe] 4f14 | 5d10 6s2 6p4' -> '1s 2s … 4f14 | 5d10 6s2 6p4'

Parameters **econfigstr** – electron config string to expand

Returns expanded econfig string

6.1.6 Basic Fleur Schema parser functions

Load all fleur schema related functions

class masci_tools.io.parsers.fleur_schema.**AttributeType**(*base_type*, *length*)
Type for describing the types of attributes/text

base_type: str
Alias for field number 0

length: int | Literal['unbounded'] | None
Alias for field number 1

class masci_tools.io.parsers.fleur_schema.**InputSchemaDict**(**args*, *xmlschema=None*, ***kwargs*)
This class contains information parsed from the FleurInputSchema.xsd

The keys contain the following information:

inp_version Version string of the input schema represented in this object

tag_paths simple xpath expressions to all valid tag names Multiple paths or ambiguous tag names are parsed as a list

_basic_types Parsed definitions of all simple Types with their respective base type (int, float, …) and evtl. length restrictions (Only used in the schema construction itself)

attrib_types All possible base types for all valid attributes. If multiple are possible a list, with 'string' always last (if possible)

simple_elements All elements with simple types and their type definition with the additional attributes

unique_attribs All attributes and their paths, which occur only once and have a unique path

unique_path_attribs All attributes and their paths, which have a unique path but occur in multiple places

other_attribs All attributes and their paths, which are not in 'unique_attribs' or 'unique_path_attribs'

omitt_contained_tags All tags, which only contain a list of one other tag

tag_info For each tag (path), the valid attributes and tags (optional, several, order, simple, text)

classmethod **fromPath**(*path*)
load the FleurInputSchema dict for the specified FleurInputSchema file

Parameters **path** (PathLike) – path to the input schema file

Return type *InputSchemaDict*

Returns InputSchemaDict object with the information for the provided file

classmethod fromVersion(*version*, *logger=None*, *no_cache=False*)
load the FleurInputSchema dict for the specified version

Parameters

- **version** – str with the desired version, e.g. '0.33'
- **logger** – logger object for warnings, errors and information, ...

Returns InputSchemaDict object with the information for the provided version

property inp_version: tuple[int, int]
Returns the input version as an integer for comparisons (> or <)

Return type tuple[int, int]

exception masci_tools.io.parsers.fleur_schema.**NoPathFound**
Exception raised when no path is found for a given tag/attribute

exception masci_tools.io.parsers.fleur_schema.**NoUniquePathFound**
Exception raised when no unique path is found for a given tag/attribute

class masci_tools.io.parsers.fleur_schema.**OutputSchemaDict**(**args*, *xmlschema=None*, ***kwargs*)
This object contains information parsed from the FleurOutputSchema.xsd

The keys contain the following information:

out_version Version string of the output schema represented in this class

input_tag Name of the element containing the fleur input

iteration_tags Names of the elements that can contain all iteration tags

tag_paths simple xpath expressions to all valid tag names not in an iteration Multiple paths or ambiguous tag names are parsed as a list

iteration_tag_paths simple relative xpath expressions to all valid tag names inside an iteration. Multiple paths or ambiguous tag names are parsed as a list

_basic_types Parsed definitions of all simple Types with their respective base type (int, float, ...) and evtl. length restrictions (Only used in the schema construction itself)

_input_basic_types Part of the parsed definitions of all simple Types with their respective base type (int, float, ...) and evtl. length restrictions from the input schema (Only used in the schema construction itself)

attrib_types All possible base types for all valid attributes. If multiple are possible a list, with 'string' always last (if possible)

simple_elements All elements with simple types and their type definition with the additional attributes

unique_attribs All attributes and their paths, which occur only once and have a unique path outside of an iteration

unique_path_attribs All attributes and their paths, which have a unique path but occur in multiple places outside of an iteration

other_attribs All attributes and their paths, which are not in 'unique_attribs' or 'unique_path_attribs' outside of an iteration

iteration_unique_attribs All attributes and their relative paths, which occur only once and have a unique path inside of an iteration

iteration_unique_path_attribs All attributes and their relative paths, which have a unique path but occur in multiple places inside of an iteration

iteration_other_attribs All attributes and their relative paths, which are not in 'unique_attribs' or 'unique_path_attribs' inside of an iteration

omitt_contained_tags All tags, which only contain a list of one other tag

tag_info For each tag outside of an iteration (path), the valid attributes and tags (optional, several, order, simple, text)

iteration_tag_info For each tag inside of an iteration (relative path), the valid attributes and tags (optional, several, order, simple, text)

classmethod fromPath(*path*, *inp_path=None*, *inpschema_dict=None*)
load the FleurOutputSchema dict for the specified paths

Parameters

- **path** – path to the FleurOutputSchema file
- **inp_path** – path to the FleurInputSchema file (defaults to same folder as path)

Returns OutputSchemaDict object with the information for the provided files

classmethod fromVersion(*version*, *inp_version=None*, *logger=None*, *no_cache=False*)
load the FleurOutputSchema dict for the specified version

Parameters

- **version** – str with the desired version, e.g. '0.33'
- **inp_version** – str with the desired input version, e.g. '0.33' (defaults to version)
- **logger** – logger object for warnings, errors and information, ...

Returns OutputSchemaDict object with the information for the provided versions

property inp_version: tuple[int, int]
Returns the input version as an integer for comparisons (> or <)

Return type tuple[int, int]

iteration_attrib_xpath(*name*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*, *iteration_tag='iteration'*)
Tries to find a unique path from the schema_dict based on the given name of the attribute and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the attribute
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *iteration_tag_xpath()*
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath to the tag with the given attribute

Raises

- ***NoPathFound*** – If no path matching the criteria could be found
- ***NoUniquePathFound*** – If multiple paths matching the criteria are found

iteration_tag_xpath(*name*, *contains=None*, *not_contains=None*, *iteration_tag='iteration'*)
Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

property out_version: tuple[int, int]
Returns the output version as an integer for comparisons (> or <)

Return type tuple[int, int]

relative_iteration_attrib_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*, *iteration_tag='iteration'*)
Tries to find a unique relative path from the schema_dict based on the given name of the attribute name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *relative_iteration_tag_xpath()*
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

relative_iteration_tag_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *iteration_tag='iteration'*)
Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications in the iteration section of the out.xml and returns the absolute path to it

Parameters

- **name** – str, name of the tag

- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **iteration_tag** – name of the tag containing the iteration information

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

class masci_tools.io.parsers.fleur_schema.**SchemaDict**(**args*, *xmlschema=None*, ***kwargs*)

Base class for schema dictionaries. Is locked on initialization with *freeze()*. Holds a reference to the xmlSchema for validating files.

Also provides interfaces for utility functions

Parameters **xmlschema** – etree.XMLSchema object for validating files

All other arguments are passed on to *LockableDict*

attrib_xpath(*name*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

Tries to find a unique path from the schema_dict based on the given name of the attribute and additional further specifications

Parameters

- **name** – str, name of the attribute
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *tag_xpath()*

Returns str, xpath to the tag with the given attribute

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

classmethod clear_cache()

Remove all stored entries in the schema dictionary cache

Return type None

relative_attrib_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*, *exclude=None*, *tag_name=None*)

Tries to find a unique relative path from the schema_dict based on the given name of the attribute name of the root, from which the path should be relative and additional further specifications

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the attribute
- **root_tag** – str, name of the tag from which the path should be relative

- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **exclude** – list of str, here specific types of attributes can be excluded valid values are: settable, settable_contains, other
- **tag_name** – str, if given this name will be used to find a path to a tag with the same name in *relative_tag_xpath()*

Returns str, xpath for the given tag

Raises

- ***NoPathFound*** – If no path matching the criteria could be found
- ***NoUniquePathFound*** – If multiple paths matching the criteria are found

relative_tag_xpath(*name*, *root_tag*, *contains=None*, *not_contains=None*)

Tries to find a unique relative path from the schema_dict based on the given name of the tag name of the root, from which the path should be relative and additional further specifications

Parameters

- **name** – str, name of the tag
- **root_tag** – str, name of the tag from which the path should be relative
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises **ValueError** – If no unique path could be found

tag_info(*name*, *contains=None*, *not_contains=None*, *parent=False*, ***kwargs*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications and returns the tag_info entry for this tag

Parameters

- **schema_dict** – dict, containing all the path information and more
- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path
- **parent** – bool, if True the tag_info for the parent of the tag is returned

Returns dict, tag_info for the found xpath

tag_xpath(*name*, *contains=None*, *not_contains=None*)

Tries to find a unique path from the schema_dict based on the given name of the tag and additional further specifications

Parameters

- **name** – str, name of the tag
- **contains** – str or list of str, this string has to be in the final path
- **not_contains** – str or list of str, this string has to NOT be in the final path

Returns str, xpath for the given tag

Raises

- *NoPathFound* – If no path matching the criteria could be found
- *NoUniquePathFound* – If multiple paths matching the criteria are found

masci_tools.io.parsers.fleur_schema.**list_available_versions**(*output_schema*)
List the available versions for the schema

Parameters **output_schema** (bool) – bool, if True search for FleurOutputSchema.xsd otherwise FleurInputSchema.xsd

Return type list[str]

Returns list version string of the available versions

masci_tools.io.parsers.fleur_schema.**schema_dict_version_dispatch**(*output_schema=False*)
Decorator for creating variations of functions based on the inp/out version of the schema_dict. All functions here need to have the signature:

```
def f(node, schema_dict, *args, **kwargs):
    pass
```

So schema_dict is the second positional argument

Inspired by singledispatch in the functools module

Return type Callable[[~F], *SchemaDictDispatch*]

functions to extract information about the fleur schema input or output

class masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**AttributeType**(*base_type*, *length*)
Type for describing the types of attributes/text

base_type: str
Alias for field number 0

length: int | Literal['unbounded'] | None
Alias for field number 1

class masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**TagInfo**
Dict representing the entries for the tag information.

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**convert_str_version_number**(*version_str*)
Convert the version number as a integer for easy comparisons

Parameters **version_str** (str) – str of the version number, e.g. '0.33'

Return type tuple[int, int]

Returns tuple of ints representing the version str

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**extract_attribute_types**(*xmlschema_evalu*, ***kwargs*)
Determine the required type of all attributes

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveDict*[str, list[*AttributeType*]]

Returns possible types of the attributes in a dictionary, if multiple types are possible a list is inserted for the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**extract_text_types**(*xmlschema_evaluator*, ***kwargs*)

Determine the required type of all elements with text

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveDict*[str, list[*AttributeType*]]

Returns possible types of the attributes in a dictionary, if multiple types are possible a list is inserted for the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_basic_types**(*xmlschema_evaluator*, ***kwargs*)

find all types, which can be traced back directly to a base_type

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type dict[str, list[*AttributeType*]]

Returns dictionary with type names and their corresponding type_definition meaning a dicationary with possible base types and evtl. length restriction

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_input_tag**(*xmlschema_evaluator*, ***kwargs*)

Returns the tag for the input type element of the outxmlschema

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type str

Returns name of the element with the type 'FleurInputType'

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_iteration_tags**(*xmlschema_evaluator*, ***kwargs*)

Returns the tags that can contain the information from a SCF iteration

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveFrozenSet*[str]

Returns set of tag names that contain elements from the group 'GeneralIterationType'

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_omittable_tags**(*xmlschema_evaluator*, ***kwargs*)

find tags with no attributes and, which are only used to mask a list of one other possible tag (e.g. atomSpecies)

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type list[str]

Returns list of tags, containing only a sequence of one allowed tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_other_attribs**(*xmlschema_evaluator*, ***kwargs*)

Determine all other attributes not contained in settable or settable_contains

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveDict*[str, list[str]]

Returns dictionary with all attributes and the corresponding list of paths to the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_root_tag**(*xmlschema_evaluator*, ***kwargs*)

Returns the tag for the root element of the xmlschema

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type str

Returns name of the single element defined in the first level of the schema

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_tag_info**(*xmlschema_evaluator*, ***kwargs*)

Get all important information about the tags

- allowed attributes
- contained tags (simple (only attributes), optional (with default values), several, order, text tags)

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type dict[str, *TagInfo*]

Returns dictionary with the tag information

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_tag_paths**(*xmlschema_evaluator*, ***kwargs*)

Determine simple xpaths to all possible tags

Parameters **xmlschema_evaluator** – etree.XPathEvaluator for the schema

Returns possible paths of all tags in a dictionary, if multiple paths are possible a list is inserted for the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_text_tags**(*xmlschema_evaluator*, ***kwargs*)

find all elements, who can contain text

Parameters **xmlschema** – xmltree representing the schema

Return type *CaseInsensitiveFrozenSet*[str]

Returns dictionary with tags and their corresponding type_definition meaning a dicationary with possible base types and evtl. length restriction

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_unique_attribs**(*xmlschema_evaluator*, ***kwargs*)

Determine all attributes, which can be set through set_inpchanges in aiida_fleur Meaning ONE possible path and no tags in the path with maxOccurs!=1

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveDict*[str, str]

Returns dictionary with all settable attributes and the corresponding path to the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**get_unique_path_attribs**(*xmlschema_evalu*
***kwargs*)

Determine all attributes, with multiple possible path that do have at least one path with all contained tags maxOccurs!=1

Parameters **xmlschema_evaluator** (XPathDocumentEvaluator) – etree.XPathEvaluator for the schema

Return type *CaseInsensitiveDict*[str, list[str]]

Returns dictionary with all attributes and the corresponding list of paths to the tag

masci_tools.io.parsers.fleur_schema.fleur_schema_parser_functions.**type_order**(*type_def*)

Key function for sorting the type definitions to avoid conflicts

Sorted by base_type first (bool before int, string at the end) and then by length in ascending order (unbounded last)

Parameters **type_def** (*AttributeType*) – definition to be sorted

Return type tuple[int, float]

6.1.7 Defined constants

Here we collect physical constants which are used throughout the code. That way we ensure consistency.

Note: For masci-tools versions after v0.4.6, the constants values used in the KKR functions for conversion between Angstrom and Bohr radius, and electron Volt and Rydberg, have been replaced by the NIST values by default. Prior to that, two different versions had been in use. If you need to work with KKR calculations / `aiida-kkr` workchains performed with these constants versions, you can switch to these older KKR constants versions by setting the environment variable `MASCI_TOOLS_USE_OLD_CONSTANTS` prior to loading masci-tools. During interpreter runtime, the chosen version cannot be switched.

- For KKR constants versions used starting from masci-tools v0.4.7, more specifically starting from commit 66953f8, Apr 28, 2021, do not set `MASCI_TOOLS_USE_OLD_CONSTANTS`.
- For KKR constants versions used in masci-tools v0.4.0-dev7 - v0.4.6, more specifically starting from commit c171563, Feb 16, 2021, to prior to commit 66953f8, Apr 28, 2021, set `MASCI_TOOLS_USE_OLD_CONSTANTS` to `'interim'`.
- For KKR constants versions used prior to masci-tools v0.4.0-dev7, more specifically prior to commit c171563, Feb 16, 2021, set `MASCI_TOOLS_USE_OLD_CONSTANTS` to `'old'` or `'True'`.

```
   :language: python
   :lines: 28-
   :linenos:

"""
import numpy as np
import os

# NIST https://physics.nist.gov/cgi-bin/cuu/Value?hrev
HTR_TO_EV = 27.211386245988  #(53)
RY_TO_EV = 13.605693122994  #(26)
BOHR_A = 0.5291772108
HTR_TO_KELVIN = 315_775.02480407
```

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```
#Scipy bohr 5.29177210903e-11 m
#Scipy htr 27.211386245988 eV
# NIST BOHR 0.529177210903 #(80)
#https://physics.nist.gov/cgi-bin/cuu/Value?bohrrada0

#KKR constants versions. See module docstring for details.
_MASCI_TOOLS_USE_OLD_CONSTANTS = os.environ.get('MASCI_TOOLS_USE_OLD_CONSTANTS', None)
if _MASCI_TOOLS_USE_OLD_CONSTANTS and _MASCI_TOOLS_USE_OLD_CONSTANTS.lower() in ['old',
↪'true']:
    ANG_BOHR_KKR = 1.8897261254578281
    RY_TO_EV_KKR = 13.605693009
elif _MASCI_TOOLS_USE_OLD_CONSTANTS and _MASCI_TOOLS_USE_OLD_CONSTANTS.lower() in [
↪'interim']:
    ANG_BOHR_KKR = 1.8897261249935897
    RY_TO_EV_KKR = RY_TO_EV
else:
    #Set the constants to the NIST values
    ANG_BOHR_KKR = 1.8897261246257702
    RY_TO_EV_KKR = RY_TO_EV

#Fleur
#htr_eV   = 27.21138602
#bohr=0.5291772108
#bohrtocm=0.529177e-8
#pymatgen uses scipy.constants
#ase: Bohr 0.5291772105638411
#Hartree 27.211386024367243
#Rydberg 13.605693012183622
#1/Bohr
#1.8897261258369282
#aiida-core units:
#bohr_to_ang = 0.52917720859

#Predefined constants in the Fleur Code (These are accepted in the inp.xml)
FLEUR_DEFINED_CONSTANTS = {
    'Pi': np.pi,
    'Deg': 2 * np.pi / 360.0,
    'Ang': 1.8897261247728981,
    'nm': 18.897261247728981,
    'pm': 0.018897261247728981,
    'Bohr': 1.0,
    'Htr': 1.0,
    'eV': 1.0 / HTR_TO_EV,
    'Ry': 0.5
}

PERIODIC_TABLE_ELEMENTS = {
    0: {  # This is for empty spheres etc.
        'mass': 1.00000,
        'name': 'Unknown',
        'symbol': 'X'
    },
```

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```
    1: {
        'mass': 1.00794,
        'name': 'Hydrogen',
        'symbol': 'H',
        'econfig': '1s1',
        'fleur_default_econfig': '| 1s1',
        'lo': '',
        'rmt': 0.65,
        'lmax': '',
        'jri': 981,
        'soc': False,
        'mag': False
    },
    2: {
        'mass': 4.002602,
        'name': 'Helium',
        'symbol': 'He',
        'econfig': '1s2',
        'fleur_default_econfig': '| 1s2',
        'lo': '',
        'rmt': 1.2,
        'lmax': '',
        'jri': 981
    },
    3: {
        'mass': 6.941,
        'name': 'Lithium',
        'symbol': 'Li',
        'econfig': '1s2 | 2s1',
        'fleur_default_econfig': '1s2 | 2s1',
        'lo': '',
        'rmt': 2.13,
        'lmax': '',
        'jri': 981
    },
    4: {
        'mass': 9.012182,
        'name': 'Beryllium',
        'symbol': 'Be',
        'econfig': '1s2 | 2s2',
        'fleur_default_econfig': '1s2 | 2s2',
        'lo': '',
        'rmt': 1.87,
        'lmax': '',
        'jri': 981
    },
    5: {
        'mass': 10.811,
        'name': 'Boron',
        'symbol': 'B',
        'econfig': '1s2 | 2s2 2p1',
        'fleur_default_econfig': '1s2 | 2s2 2p1',
```

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```
        'lo': '',
        'rmt': 1.4,
        'lmax': '',
        'jri': 981
    },
    6: {
        'mass': 12.0107,
        'name': 'Carbon',
        'symbol': 'C',
        'econfig': '[He] 2s2 | 2p2',
        'fleur_default_econfig': '[He] 2s2 | 2p2',
        'lo': '',
        'rmt': 1.2,
        'lmax': '',
        'jri': 981
    },
    7: {
        'mass': 14.0067,
        'name': 'Nitrogen',
        'symbol': 'N',
        'econfig': '[He] 2s2 | 2p3',
        'fleur_default_econfig': '[He] 2s2 | 2p3',
        'lo': '',
        'rmt': 1.0,
        'lmax': '',
        'jri': 981
    },
    8: {
        'mass': 15.9994,
        'name': 'Oxygen',
        'symbol': 'O',
        'econfig': '[He] 2s2 | 2p4',
        'fleur_default_econfig': '[He] 2s2 | 2p4',
        'lo': '',
        'rmt': 1.1,
        'lmax': '',
        'jri': 981
    },
    9: {
        'mass': 18.9984032,
        'name': 'Fluorine',
        'symbol': 'F',
        'econfig': '[He] 2s2 | 2p5',
        'fleur_default_econfig': '[He] 2s2 | 2p5',
        'lo': '',
        'rmt': 1.2,
        'lmax': '',
        'jri': 981
    },
    10: {
        'mass': 20.1797,
        'name': 'Neon',
```

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```
        'symbol': 'Ne',
        'econfig': '[He] 2s2 | 2p6',
        'fleur_default_econfig': '[He] 2s2 | 2p6',
        'lo': '',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    11: {
        'mass': 22.98977,
        'name': 'Sodium',
        'symbol': 'Na',
        'econfig': '[He] 2s2 | 2p6 3s1',
        'fleur_default_econfig': '[He] | 2s2 2p6 3s1',
        'lo': '2s 2p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    12: {
        'mass': 24.305,
        'name': 'Magnesium',
        'symbol': 'Mg',
        'econfig': '[He] 2s2 | 2p6 3s2',
        'fleur_default_econfig': '[He] 2s2 | 2p6 3s2',
        'lo': '2p',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    13: {
        'mass': 26.981538,
        'name': 'Aluminium',
        'symbol': 'Al',
        'econfig': '[He] 2s2 2p6 | 3s2 3p1',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p1',
        'lo': '',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    14: {
        'mass': 28.0855,
        'name': 'Silicon',
        'symbol': 'Si',
        'econfig': '[He] 2s2 2p6 | 3s2 3p2',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p2',
        'lo': '',
        'rmt': 2.0,
        'lmax': '',
        'jri': 981
    },
```

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```
    15: {
        'mass': 30.973761,
        'name': 'Phosphorus',
        'symbol': 'P',
        'econfig': '[He] 2s2 2p6 | 3s2 3p3',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p3',
        'lo': '',
        'rmt': 1.9,
        'lmax': '',
        'jri': 981
    },
    16: {
        'mass': 32.065,
        'name': 'Sulfur',
        'symbol': 'S',
        'econfig': '[He] 2s2 2p6 | 3s2 3p4',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p4',
        'lo': '',
        'rmt': 1.7,
        'lmax': '',
        'jri': 981
    },
    17: {
        'mass': 35.453,
        'name': 'Chlorine',
        'symbol': 'Cl',
        'econfig': '[He] 2s2 2p6 | 3s2 3p5',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p5',
        'lo': '',
        'rmt': 1.7,
        'lmax': '',
        'jri': 981
    },
    18: {
        'mass': 39.948,
        'name': 'Argon',
        'symbol': 'Ar',
        'econfig': '[He] 2s2 2p6 | 3s2 3p6',
        'fleur_default_econfig': '[He] 2s2 2p6 | 3s2 3p6',
        'lo': '',
        'rmt': 1.8,
        'lmax': '',
        'jri': 981
    },
    19: {
        'mass': 39.0983,
        'name': 'Potassium',
        'symbol': 'K',
        'econfig': '[Ne] 3s2 | 3p6 4s1',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s1',
        'lo': '3s 3p',
        'rmt': 2.0,
```

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```
        'lmax': '',
        'jri': 981
    },
    20: {
        'mass': 40.078,
        'name': 'Calcium',
        'symbol': 'Ca',
        'econfig': '[Ne] 3s2 | 3p6 4s2',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2',
        'lo': '3s 3p',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    21: {
        'mass': 44.955912,
        'name': 'Scandium',
        'symbol': 'Sc',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d1',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2 3d1',
        'lo': '3s 3p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    22: {
        'mass': 47.867,
        'name': 'Titanium',
        'symbol': 'Ti',
        'econfig': '[Ne] | 3s2 3p6 4s2 3d2',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2 3d2',
        'lo': '3s 3p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    23: {
        'mass': 50.9415,
        'name': 'Vanadium',
        'symbol': 'V',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d3',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2 3d3',
        'lo': '3s 3p',
        'rmt': 1.9,
        'lmax': '',
        'jri': 981
    },
    24: {
        'mass': 51.9961,
        'name': 'Chromium',
        'symbol': 'Cr',
        'econfig': '[Ne] 3s2 3p6 | 4s1 3d5',
```

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```
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s1 3d5',
        'lo': '3s 3p',
        'rmt': 1.8,
        'lmax': '',
        'jri': 981
    },
    25: {
        'mass': 54.938045,
        'name': 'Manganese',
        'symbol': 'Mn',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d5',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2 3d5',
        'lo': '3s 3p',
        'rmt': 2.0,
        'lmax': '',
        'jri': 981
    },
    26: {
        'mass': 55.845,
        'name': 'Iron',
        'symbol': 'Fe',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d6',
        'fleur_default_econfig': '[Ne] | 3s2 3p6 4s2 3d6',
        'lo': '3s 3p',
        'rmt': 2.00,
        'lmax': '',
        'jri': 981
    },
    27: {
        'mass': 58.933195,
        'name': 'Cobalt',
        'symbol': 'Co',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d7',
        'fleur_default_econfig': '[Ne] 3s2 | 3p6 4s2 3d7',
        'lo': '3p',
        'rmt': 1.9,
        'lmax': '',
        'jri': 981
    },
    28: {
        'mass': 58.6934,
        'name': 'Nickel',
        'symbol': 'Ni',
        'econfig': '[Ne] 3s2 3p6 | 4s2 3d8',
        'fleur_default_econfig': '[Ne] 3s2 | 3p6 4s2 3d8',
        'lo': '3p',
        'rmt': 1.9,
        'lmax': '',
        'jri': 981
    },
    29: {
        'mass': 63.546,
```

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```
        'name': 'Copper',
        'symbol': 'Cu',
        'econfig': '[Ne] 3s2 3p6 |4s1 3d10',
        'fleur_default_econfig': '[Ne] 3s2 | 3p6 4s1 3d10',
        'lo': '3p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    30: {
        'mass': 65.38,
        'name': 'Zinc',
        'symbol': 'Zn',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2',
        'lo': '3d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    31: {
        'mass': 69.723,
        'name': 'Gallium',
        'symbol': 'Ga',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p1',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p1',
        'lo': '3d',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    32: {
        'mass': 72.64,
        'name': 'Germanium',
        'symbol': 'Ge',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p2',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p2',
        'lo': '3d',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    33: {
        'mass': 74.9216,
        'name': 'Arsenic',
        'symbol': 'As',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p3',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p3',
        'lo': '3d',
        'rmt': 2.0,
        'lmax': '',
        'jri': 981
```

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```
    },
    34: {
        'mass': 78.96,
        'name': 'Selenium',
        'symbol': 'Se',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p4',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p4',
        'lo': '3d',
        'rmt': 2.0,
        'lmax': '',
        'jri': 981
    },
    35: {
        'mass': 79.904,
        'name': 'Bromine',
        'symbol': 'Br',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p5',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p5',
        'lo': '3d',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    36: {
        'mass': 83.798,
        'name': 'Krypton',
        'symbol': 'Kr',
        'econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p6',
        'fleur_default_econfig': '[Ne] 3s2 3p6 | 3d10 4s2 4p6',
        'lo': '3d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    37: {
        'mass': 85.4678,
        'name': 'Rubidium',
        'symbol': 'Rb',
        'econfig': '[Ar] 3d10 4s2 | 4p6 5s1',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s1',
        'lo': '4s 4p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    38: {
        'mass': 87.62,
        'name': 'Strontium',
        'symbol': 'Sr',
        'econfig': '[Ar] 3d10 4s2 | 4p6 5s2',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s2',
        'lo': '4s 4p',
```

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```
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    39: {
        'mass': 88.90585,
        'name': 'Yttrium',
        'symbol': 'Y',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s2 4d1',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s2 4d1',
        'lo': '4s 4p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    40: {
        'mass': 91.224,
        'name': 'Zirconium',
        'symbol': 'Zr',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s2 4d2',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s2 4d2',
        'lo': '4s 4p',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    41: {
        'mass': 92.90638,
        'name': 'Niobium',
        'symbol': 'Nb',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s1 4d4',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s1 4d4',
        'lo': '4s 4p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    42: {
        'mass': 95.96,
        'name': 'Molybdenum',
        'symbol': 'Mo',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s1 4d5',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s1 4d5',
        'lo': '4s 4p',
        'rmt': 2.0,
        'lmax': '',
        'jri': 981
    },
    43: {
        'mass': 98.0,
        'name': 'Technetium',
        'symbol': 'Tc',
```

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```
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s2 4d5',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s2 4d5',
        'lo': '4s 4p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    44: {
        'mass': 101.07,
        'name': 'Ruthenium',
        'symbol': 'Ru',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s1 4d7',
        'fleur_default_econfig': '[Ar] 4s2 3d10 | 4p6 5s1 4d7',
        'lo': '4p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    45: {
        'mass': 102.9055,
        'name': 'Rhodium',
        'symbol': 'Rh',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s1 4d8',
        'fleur_default_econfig': '[Ar] 4s2 3d10 | 4p6 5s1 4d8',
        'lo': '4p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    46: {
        'mass': 106.42,
        'name': 'Palladium',
        'symbol': 'Pd',
        'econfig': '[Ar] 4s2 3d10 4p6 | 4d10',
        'fleur_default_econfig': '[Ar] 4s2 3d10 | 4p6 4d10',
        'lo': '4p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    47: {
        'mass': 107.8682,
        'name': 'Silver',
        'symbol': 'Ag',
        'econfig': '[Ar] 4s2 3d10 4p6 | 5s1 4d10',
        'fleur_default_econfig': '[Ar] 3d10 | 4s2 4p6 5s1 4d10',
        'lo': '4s 4p',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    48: {
```

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```
        'mass': 112.411,
        'name': 'Cadmium',
        'symbol': 'Cd',
        'econfig': '[Ar] 4s2 3d10 4p6 | 4d10 5s2',
        'fleur_default_econfig': '[Ar] 4s2 3d10 4p6 | 4d10 5s2',
        'lo': '4d',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    49: {
        'mass': 114.818,
        'name': 'Indium',
        'symbol': 'In',
        'econfig': '[Ar] 4s2 3d10 4p6 | 4d10 5s2 5p1',
        'fleur_default_econfig': '[Ar] 4s2 3d10 4p6 | 4d10 5s2 5p1',
        'lo': '4d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    50: {
        'mass': 118.71,
        'name': 'Tin',
        'symbol': 'Sn',
        'econfig': '[Kr] 4d10 | 5s2 5p2',
        'fleur_default_econfig': '[Kr] | 4d10 5s2 5p2',
        'lo': '4d',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    51: {
        'mass': 121.76,
        'name': 'Antimony',
        'symbol': 'Sb',
        'econfig': '[Kr] 4d10 | 5s2 5p3',
        'fleur_default_econfig': '[Kr] | 4d10 5s2 5p3',
        'lo': '4d',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    52: {
        'mass': 127.6,
        'name': 'Tellurium',
        'symbol': 'Te',
        'econfig': '[Kr] 4d10 | 5s2 5p4',
        'fleur_default_econfig': '[Kr] | 4d10 5s2 5p4',
        'lo': '4d',
        'rmt': 2.3,
        'lmax': '',
```

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```
        'jri': 981
    },
    53: {
        'mass': 126.90447,
        'name': 'Iodine',
        'symbol': 'I',
        'econfig': '[Kr] 4d10 | 5s2 5p5',
        'fleur_default_econfig': '[Kr] | 4d10 5s2 5p5',
        'lo': '4d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    54: {
        'mass': 131.293,
        'name': 'Xenon',
        'symbol': 'Xe',
        'econfig': '[Kr] 4d10 | 5s2 5p6',
        'fleur_default_econfig': '[Kr] | 4d10 5s2 5p6',
        'lo': '4d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    55: {
        'mass': 132.9054519,
        'name': 'Caesium',
        'symbol': 'Cs',
        'econfig': '[Kr] 4d10 5s2 | 5p6 6s1',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s1',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    56: {
        'mass': 137.327,
        'name': 'Barium',
        'symbol': 'Ba',
        'econfig': '[Kr] 4d10 5s2 | 5p6 6s2',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    57: {
        'mass': 138.90547,
        'name': 'Lanthanum',
        'symbol': 'La',
        'econfig': '[Kr] 4d10 5s2 | 5p6 6s2 5d1',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 5d1',
```

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```
        'lo': '5s 5p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    58: {
        'mass': 140.116,
        'name': 'Cerium',
        'symbol': 'Ce',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f1 5d1',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f1 5d1',
        'lo': '5s 5p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    59: {
        'mass': 140.90765,
        'name': 'Praseodymium',
        'symbol': 'Pr',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f3',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6  6s2 4f3',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    60: {
        'mass': 144.242,
        'name': 'Neodymium',
        'symbol': 'Nd',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f4',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f4',
        'lo': '5s 5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    61: {
        'mass': 145.0,
        'name': 'Promethium',
        'symbol': 'Pm',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f5',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f5',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    62: {
        'mass': 150.36,
        'name': 'Samarium',
```

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```
        'symbol': 'Sm',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f6',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f6',
        'lo': '5s 5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    63: {
        'mass': 151.964,
        'name': 'Europium',
        'symbol': 'Eu',
        'econfig': '[Kr] 4d10 | 4f7 5s2 5p6 6s2',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 4f7 6s2',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    64: {
        'mass': 157.25,
        'name': 'Gadolinium',
        'symbol': 'Gd',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f7 5d1',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f7 5d1',
        'lo': '5s 5p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    65: {
        'mass': 158.92535,
        'name': 'Terbium',
        'symbol': 'Tb',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f9',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f8 5d1',
        'lo': '5s 5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    66: {
        'mass': 162.5,
        'name': 'Dysprosium',
        'symbol': 'Dy',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f10',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f9 5d1',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
```

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```
    67: {
        'mass': 164.93032,
        'name': 'Holmium',
        'symbol': 'Ho',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f11',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f10 5d1',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    68: {
        'mass': 167.259,
        'name': 'Erbium',
        'symbol': 'Er',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f12',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f11 5d1',
        'lo': '5s 5p',
        'rmt': 2.5,
        'lmax': '',
        'jri': 981
    },
    69: {
        'mass': 168.93421,
        'name': 'Thulium',
        'symbol': 'Tm',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f13',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f12 5d1',
        'lo': '5s 5p',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    70: {
        'mass': 173.054,
        'name': 'Ytterbium',
        'symbol': 'Yb',
        'econfig': '[Kr] 4d10 5s2 5p6 | 6s2 4f14',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 6s2 4f13 5d1',
        'lo': '5s 5p',
        'rmt': 2.6,
        'lmax': '',
        'jri': 981
    },
    71: {
        'mass': 174.9668,
        'name': 'Lutetium',
        'symbol': 'Lu',
        'econfig': '[Kr] 4d10 | 4f14 5s2 5p6 5d1 6s2',
        'fleur_default_econfig': '[Kr] 4d10 | 5s2 5p6 4f14 6s2 5d1',
        'lo': '5s 5p',
        'rmt': 2.5,
```

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```
        'lmax': '',
        'jri': 981
    },
    72: {
        'mass': 178.49,
        'name': 'Hafnium',
        'symbol': 'Hf',
        'econfig': '[Kr] 4d10 | 4f14 5s2 5p6 5d2 6s2',
        'fleur_default_econfig': '[Kr] 4d10 4f14 | 5s2 5p6 6s2 5d2',
        'lo': '5s 5p',
        'rmt': 2.3,
        'lmax': '',
        'jri': 981
    },
    73: {
        'mass': 180.94788,
        'name': 'Tantalum',
        'symbol': 'Ta',
        'econfig': '[Kr] 4d10 4f14 | 5s2 5p6 5d3 6s2',
        'fleur_default_econfig': '[Kr] 4d10 4f14 | 5s2 5p6 6s2 5d3',
        'lo': '5s 5p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    74: {
        'mass': 183.84,
        'name': 'Tungsten',
        'symbol': 'W',
        'econfig': '[Kr] 5s2 4d10 4f14 | 5p6 6s2 5d4',
        'fleur_default_econfig': '[Kr] 4d10 4f14 | 5s2 5p6 6s2 5d4',
        'lo': '5s 5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    75: {
        'mass': 186.207,
        'name': 'Rhenium',
        'symbol': 'Re',
        'econfig': '[Kr] 4d10 4f14 5p6 | 5s2 6s2 5d5',
        'fleur_default_econfig': '[Kr] 4d10 4f14 | 5s2 5p6 6s2 5d5',
        'lo': '5s 5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    76: {
        'mass': 190.23,
        'name': 'Osmium',
        'symbol': 'Os',
        'econfig': '[Kr] 4d10 4f14 5p6 | 5s2 6s2 5d6',
```

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```
        'fleur_default_econfig': '[Kr] 5s2 4d10 4f14 | 5p6 6s2 5d6',
        'lo': '5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    77: {
        'mass': 192.217,
        'name': 'Iridium',
        'symbol': 'Ir',
        'econfig': '[Kr] 4d10 4f14 5p6 | 5s2 6s2 5d7',
        'fleur_default_econfig': '[Kr] 5s2 4d10 4f14 | 5p6 6s2 5d7',
        'lo': '5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    78: {
        'mass': 195.084,
        'name': 'Platinum',
        'symbol': 'Pt',
        'econfig': '[Kr] 4d10 4f14 5p6 | 5s2 6s2 5d8',
        'fleur_default_econfig': '[Kr] 5s2 4d10 4f14 | 5p6 6s2 5d8',
        'lo': '5p',
        'rmt': 2.1,
        'lmax': '',
        'jri': 981
    },
    79: {
        'mass': 196.966569,
        'name': 'Gold',
        'symbol': 'Au',
        'econfig': '[Kr] 4d10 4f14 5p6 | 5s2 6s2 5d9',
        'fleur_default_econfig': '[Kr] 4d10 4f14 | 5s2 5p6 6s2 5d9',
        'lo': '5s 5p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    80: {
        'mass': 200.59,
        'name': 'Mercury',
        'symbol': 'Hg',
        'econfig': '[Kr] 5s2 4d10 4f14 | 5p6 5d10 6s2',
        'fleur_default_econfig': '[Kr] 5s2 4d10 4f14 5p6 | 5d10 6s2',
        'lo': '5d',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    81: {
        'mass': 204.3833,
```

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```
        'name': 'Thallium',
        'symbol': 'Tl',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p1',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p1',
        'lo': '5d',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    82: {
        'mass': 207.2,
        'name': 'Lead',
        'symbol': 'Pb',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p2',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p2',
        'lo': '5d',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    83: {
        'mass': 208.9804,
        'name': 'Bismuth',
        'symbol': 'Bi',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p3',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p3',
        'lo': '5d',
        'rmt': 2.4,
        'lmax': '',
        'jri': 981
    },
    84: {
        'mass': 209.0,
        'name': 'Polonium',
        'symbol': 'Po',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p4',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p4',
        'lo': '5d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    85: {
        'mass': 210.0,
        'name': 'Astatine',
        'symbol': 'At',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p5',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p5',
        'lo': '5d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
```

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```
    },
    86: {
        'mass': 222.0,
        'name': 'Radon',
        'symbol': 'Rn',
        'econfig': '[Xe] 4f14 | 5d10 6s2 6p6',
        'fleur_default_econfig': '[Xe] 4f14 | 5d10 6s2 6p6',
        'lo': '5d',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },  # TODO: after wards not rigth
    87: {
        'mass': 223.0,
        'name': 'Francium',
        'symbol': 'Fr',
        'econfig': '[Xe] 4f14 5d10 6s2 | 6p6 7s1',
        'fleur_default_econfig': '[Xe] 4f14 5d10 | 6s2 6p6 7s1',
        'lo': '6s 6p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    88: {
        'mass': 226.0,
        'name': 'Radium',
        'symbol': 'Ra',
        'econfig': '[Xe] 4f14 5d10 6s2 | 6p6 7s2',
        'fleur_default_econfig': '[Xe] 4f14 5d10 | 6s2 6p6 7s2',
        'lo': '6s 6p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    89: {
        'mass': 227.0,
        'name': 'Actinium',
        'symbol': 'Ac',
        'econfig': '[Xe] 4f14 5d10 6s2 | 6p6 7s2 6d1',
        'fleur_default_econfig': '[Xe] 4f14 5d10 | 6s2 6p6 7s2 6d1',
        'lo': '6s 6p',
        'rmt': 2.2,
        'lmax': '',
        'jri': 981
    },
    90: {
        'mass': 232.03806,
        'name': 'Thorium',
        'symbol': 'Th',
        'econfig': '[Xe] 4f14 5d10 6s2 | 6p6 7s2 6d1 5f1',
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1364 }
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CHAPTER

SEVEN

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PYTHON MODULE INDEX

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