Simulation Science Laboratory 2018

An Analysis Tool for Materials Design

Students:
Praneeth Katta Venkatesh Babu
Christian Partmann
Johannes Wasmer

Supervisors:
Stefan Blügel Prof. Dr.
Stefan Rost MSc
Quantum Theory of Materials PGI-1
Forschungszentrum Jülich

Abstract — The electronic band structure and the density of states of a material can help to explain many of it's electrical, magnetical and optical properties. Real-world materials band structures are quite complex. One way to obtain them is numerical simulation using density functional theory (DFT) and high-performance computing. Still, the raw numerical data output by itself is not much help. Interactive visualization as a post-processing step can help to explore that space and find the important features. This work presents such a freely availabe post-processing pipeline for band structure calculations of Fleur, a full potential linearized augmented planewave code based on DFT. It features a generalized Python interface for processing and visualizing data in the hierarchical data format HDF5. Two interactive graphical user interfaces (GUIs) built on that interface are introduced. Simulations of $\mathrm{MoSe_2}$ and Co materials are examined using using those GUIs, helping to deduce some of their properties.

Keywords band structure, density of states, visualization, DFT simulation, Fleur, HDF5

AICES
Schinkelstr. 2
Rogowski Building
4th Floor
52062 Aachen

Acknowledgments

The authors would like to thank the following members of the section Quantum Theory of Materials in the Peter-Grünberg Institute at the Forschungszentrum Jülich: our supervisors Prof. Dr. Stefan Blügel and Stefan Rost for their helpful input, their time and commitment; Dr. Gregor Michalicek and Dr. Jens Bröder for their inspiring ideas.

Contents

List of Figures

Chapter 1

Introduction

Problem Statement

Solid-state physics deals with the study of large-scale properties of solid materials resulting from the atomic scale properties. A solid state physicist can deduce atomic scale properties from the experiments conducted on the material. Another way to elucidate physical properties is numerical simulation by means of Density Function Theory (DFT). This is a computational quantum mechanical modeling method for investigating the electronic structure of many-body systems. Some example properties that are made amenable via DFT simulations include the electron density, charge transfer excitations, a material's band gap or the intermolecular forces in a molecule.

Fleur is a freely available full potential linearized augmented planewave (FLAPW) code that is based on DFT[Blü+18]. It is developed by physicists at the Forschungzentrum Jülich. Like any other kind of numerical simulation, DFT simulations produce a lot of data. It is not a trivial task for a solid-state physicist to understand and determine the electronic strucure of a material, and through that understand and determine the physical properties. Fleur is run specifying the crystal structure of a material and so can be used on any type of crystal cell, to obtain the characteristics of same. Often it is used to simulate and find properties of solids with impurities in the cell structure.

Fleur outputs the data of the DFT simulation. It gives the data of ground state and excited state properties of solids. These data are raw and are generally not accessible directly. They have to be processed in several steps for any solid-state physicist to understand. This becomes a major problem which is addressed in this project. The goal of this project was to implement a complete data analysis pipeline for this application. The steps include preprocessing followed by data exploration through visualization.

Motivation and Requirements

One project goal was a software library or 'backend' with which solves the physicist's problem of understanding the simulation data. The backend transforms raw data to useful data such that it is processed and can be visualized. This backend has to process the output files from Fleur directly so that it is easier for physicists to get the data processed without manual effort. Having said this, modularization and easy maintainability of the code also matters since the format and structure of simulation results keeps varying over time with the development of the simulation code, when more and more data may be collected from the simulation.

This backend should not only be solving the physicist's problem but also should be fast enough in terms of computation. A problem that may arise when only offering a library with an application programming interface though is that potential domain expert users may not use it because they lack the specific programming knowledge or time to learn it. So a graphical user interface (GUI) or 'frontend' is needed such that a physicist can use the GUI to input the parameters and to present the data in a visual manner. As this is used for research purposes, the produced plots and images should be of high quality and resolution such that they can be shared with others.

Project Steps

The project was organized into several steps with the supervisors.

- Understanding the problem: the theory and practice of DFT simulation, band theory including density of states, the output file formats produced by Fleur, and other necessary theory needed are learnt and the requirement of the problem to process the data in different steps is understood.
- Pre-Processing: Once the problem is clearly understood, the first step of the project comes to preprocessing the data. Reading the data, transforming the data and aggregating it which so that it can be used in further stages of the implementation.
- Exploring the data: From the raw data, not just band plots but other features as well can be extracted. Finding out the features through exploring the data and trying to understand and extract those features is accomplished.
- Visualization: The data which is pre-processed and extracted need to be visualized into plots such that any user with a solid-state physics background can understand it.
- Frontend: A GUI is developed so that it is easier in future for any physicist to just run the GUI and get the plots and other visualization instead going through hassle of manual coding.
- Results and lookup: Getting to know the features extracted, studying it, reporting the

same.

Chapter 2

Theoretical Background

...some introduction scentence depending on intro chapter...

Fleur computes the electronic structure in crystals using the Density Functional Theory approach (DFT), which is the state of the art method for this problem. The many-body Schrödinger equation, that can be used to describe electrons in solids, is almost impossible to solve directly, because the storage of the wavefunctions of each of the N electrons in the system at each spatial coordinate exceeds the memory of any currently available computer for even quite small N. This motivates the DFT approach, that uses two fundamental theorems to reduce the computational complexity of the many-body problem significantly: The Hohenberg-Kohn theorem allows to use the electron density instead of the N-electron wavefunctions to uniquely characterize the ground state of a system. With the Kohn-Sham equations, the interacting Hamiltonian of the system can be replaced by non-interacting equations with an effective potential. This approach reduces the dimensionality of the problem from N^3 to 3 and trades the interacting Hamiltonian for a set of non-interacting equations that have to be solved self-consistently. In general, the DFT approach is not just limited to computations of electrons in crystals, but is also for example used in chemistry to compute nonperiodic molecules. The output of a DFT calculation includes various physical quantities (for example the 3-dimensional spatial electron density, which is the central quantity in DFT calculations), but for this project we focus on two quantities that are easy to interpret, already reduced in dimensionality and frequently used in both experimental and theoretical physics.

The band structure $E(\mathbf{k})$ represents the eigenenergies of the eigenfunctions of the Hamiltonian for each crystal momentum $\mathbf{k}$. It is the dispersion relation of electrons in the crystal and relates allowed momenta and energies. In general, $E(\mathbf{k})$ is defined at any point inside the Brillouin zone, which is a special choice of the unit cell in the reciprocal lattice of the crystal. Both, the real-space lattice and the reciprocal lattice are shown for a face centered cubic (fcc) crystal in figure 2.1. For larger unit cells with fewer symmetries, the Brillouin zone can be much more complicated than in the shown example. In order to reduce the dimensionality of $E(\mathbf{k})$ with

$k \in \mathbb{R}^3$, the dispersion relation is only sampled along a discrete one-dimensional path between high symmetry points in the Brillouin zone. This path still contains most of the relevant physical features.

(a) Lattice in real space

(b) Brillouin zone

Figure 2.1: Brillouin zone of a fcc lattice. The red curve in the reciprocal lattice represents a possible sampling path of $E(\mathbf{k})$ in the reciprocal lattice.

The second central quantity in this project is the Density of States (DOS) $D(E)$, which describes the number of states per energy interval that is independent from the crystal momentum. In this sense, the DOS is also derived from $E(\mathbf{k})$, but instead of just selecting a subset, the $\mathbf{k}$ dependency is summed out. Both complementary quantities together are a common choice for comprehensive visualizations of electronic structure data while still capturing most of the important physics.

For applications, it is useful to investigate where the contributions to $E(\mathbf{k})$ and $D(E)$ come from. Therefore, the data contains the weights of each basis function of the DFT calculation belonging to the individual atom groups and the orbitals. This means, spatial information about the system can be restored by considering only contributions from certain atom groups. (An atom group contains all atoms that are equivalent with respect to symmetries of the real space lattice.) On the other hand, the projection on the hydrogen orbitals s, p, d, f encode information about the shape of the wavefunction at each atom. These contributions are stored in the form of relative weights that can be summed to include contributions for multiple groups and orbitals. In case of distinct spins in the crystal, $E(\mathbf{k})$, $D(E)$ and the weights can be different for both spins and are therefore stored individually.

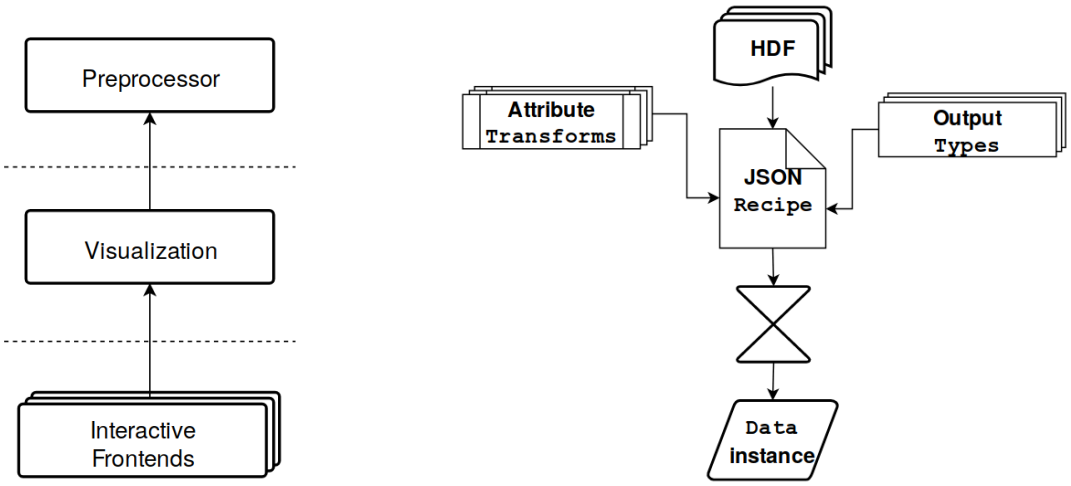
Chapter 3

Implementation

As per the requirements expounded upon in the introduction, the deliverable of the project should be a finished software product. The software is written in Python so as to integrate easily with the research group's ongoing software projects around the Fleur code [Blü+18]. These are chiefly the group's materials science tool collection `masci-tools` [RBR18] , where also this project's code is hosted, and the 'Automated Interactive Infrastructure and Database for Computational Science' (AiiDA) [Piz+16]. The product stakeholders split into frontend users and code developers. In order to accommodate this, the product is organized into three unidirectionally dependent subpackages or -modules, see Figure 3.1a.

An important design consideration was to account for unknown use cases. This has been realized in each submodule by the decoupling of **interface** and **implementation**. The interfaces do not rely on any specific input file format, visualization method or library, unlike the implementations for a specific task or **application**. In this chapter, the word 'application' denotes the band structure and density of states visualization, and for these applications, implementations are provided.

This design choice was also one reason why the product does not reuse any of the `masci-tools` routines which partly solve quite similar problems, but seemed to be too specialized in a cursory code review. For these developers, one added value of the project product could be to inspire the hopefully easy integration into a common interface, where the current abstraction level could serve as a starting point.



(a) Submodules (b) Preprocessor

Figure 3.1: Module Design.

HDF Preprocessor Module

Interface

This is the 'backend' of the tool. It is basically a file reader for the input data, for example a Fleur simulation output. Supported formats are the Hierarchical Data Format (HDF) [Kor11] for the band structure, and a simple Fleur-specific comma-separated values (CSV) format for the density of states (DOS).

The HDF format is a flexible binary container for all kinds of common binary and text file formats. Each file which constitutes a `Dataset` inside the HDF file. The format supports metadata annotation and high-throughput input/output (I/O). As a consequence, it is considered by some developers in some application domains that rely on numerical simulation codes, to be one possible base for the establishment of common domain-specific rich data exchange standards in order to increase code interoperability. These developers are in the process of extending their codes' I/O capabilities towards that end. However, HDF's flexibility comes at the price of a relatively complex Application Programming Interface (API) as the keyhole for all operations.

The preprocessor module tries to hide that complexity by introducing the concept of `Recipes`, see Figure 3.1b. A specific application `Recipe` is a dictionary that aims to describe a complete Extract-Transform-Load (ETL) pipeline for one specific application of the original data. The 'extract' is the reading of a dataset from HDF, the 'transform' a sequence of once-through functions applied to the the dataset, and the 'load' the aggregation of all transformed datasets into one runtime object which has all the methods for operations on the data that are going to

be used later on in the intended application.

The 'transform' and 'output' type methods are defined in hierarchical `Transform` and `Output_Type` classes. Multiple inheritance is used to sort them from general to application-specific applicability. This structure is built using Python's `AbstractBaseClass` (`ABC`). The advantages of the 'recipes approach' are:

- All ETL processes for one application are collected in one simple list (the recipe), not locked in different code locations with conflicting contexts. In this list, entries can be sorted in any manner, e.g. alphabetical for perusal. Thus a recipe also serves as a concise documentation of how an application-domain HDF format should be handled.
- Recipes are de/serializable (can be read from and saved to disk) and thus be machine-created and manipulated, for instance in a workflow pipeline.
- The ETL processes, when declared in this interface, can be easily reused across applications. A recipe can combine different output types into a new type.

The feature that enables this flexibility is **type introspection**: the preprocessor processes the datasets listed in the recipe in the order of their mutual dependencies as found in the introspected listed transform and output methods. When all transformed datasets have been added to the object, all specified output types are searched and all their methods and attributes added. Thus the output object's type is defined at runtime, when the preprocessing is finished.

Implementation for Band Structure Visualization

The frontend has to draw three kinds of plots: a 3D atom plot of the unit cell or supercell, and a combined band structure and DOS plot sharing the same vertical energy axis. If no DOS data is present, the DOS part of the plot shall be omitted. All three plots are controlled by one set of graphical frontend control elements (widgets) for varying the parameters. In the current implementation, the data for the first two plots come from a HDF file, while the data for the DOS plot come from CSV files.

The band structure plot is a scatter plot. It plots discrete $E(\mathbf{k})$ data from the simulation. Firstly, the plotter needs the k-path (where $|\mathbf{k}| = k$) for the horizontal axis. The preprocessor, having received the recipe `FleurBands`, computes it from the k-points in the HDF in a transform. Secondly, the plotter needs the eigenergies for every point on the k-path, labeled by the band index ν, and its associated l-like charge $n_{s,k,\nu,g,l}$. This dataset is fivedimensional, and represents the contribution of spin s, point k point on k-path, band index ν, atom group g, and character or orbital l (here: only s,p,d,f) to the specific eigenergy. So plotting must involve a dimension reduction. The preprocessor resolves the processed data into the like-named output type `FleurBands`. This type has a data selection method. The respective `BandPlot` type calls this selector with a user selection of subsets of all (s, k, ν, g, l). The method then computes the according **effective weight** shown in Equation 3.1. The plotter uses that for the dot size

of each $E(k)$ in the plot. Before rendering, the plotter normalizes the energies to the Fermi Level.

$$W^{\text{eff}}_{s,k,\nu} = \left(\frac{\sum\limits_{\substack{g \in \text{groups} \\ l \in \text{characters}}} n_{s,k,\nu,g,l} \, N_g}{\sum\limits_{\substack{g \in \text{all groups} \\ l \in \text{all characters}}} n_{s,k,\nu,g,l} \, N_g} \right) \left(W^{\text{unf}}_{s,k,\nu} \right)^{\alpha} \tag{3.1}$$

N_g denotes the number of atoms in a group. $W^{\text{unf}}_{s,k,\nu}$ is the unfolding weight and α its exponent. In the frontends, the latter is also a user control. The effect of unfolding is illustrated in Figure 3.2 for a toy example of a monatomic chain, with a two-atom supercell of size a' representing $\alpha = 0$ and a one-atom unit cell of size a representing $\alpha = 1$. A use-case is discussed in the Application Chapter 5.

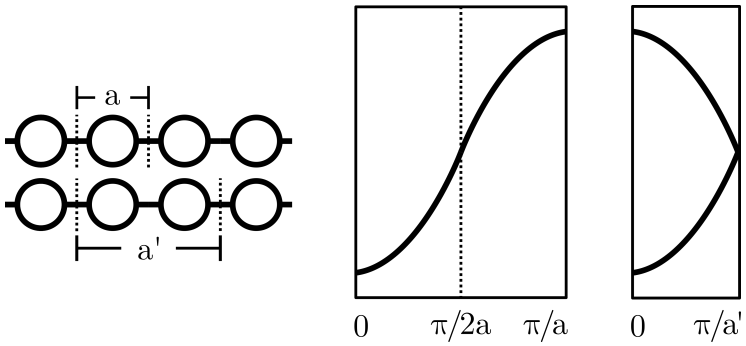


Figure 3.2: Band unfolding: example for a simple monatomic chain [Hof87].

Even for small band structures, the selector has to access on the order 10^7 individual data points for every selection change. Optimizations were introduced which included:

- a cutoff filter that skips effective weights too small to show up on the plot,
- use of optimized Numpy functions like `np.tensor` for the effective weight summation,
- buffering of unchanged data between two selections,
- array reshaping.

Together, these tweaks achieve a speedup of approximately 10^2 in plotting speed. Thanks to that, the tool remains usable even when the input HDF is in the 10^2 MB range.

Visualization Module & Interactive Graphical Frontends

Visualization Module

The Python visualization landscape abounds with a rapidly evolving plethora of plotting libraries for different application contexts and technology stacks [VR17]. Thus the project's visualization module's first design objective was to account for that fact by decoupling it from any specific library use, and modularizing it for intended applications. This structure again is built using Python's `AbstractBaseClass` (`ABC`) interface and multiple inheritance. Each application is represented by an abstract base class that contains the common plotting method signatures. Likewise, each plotting library is represented by an abstract base class that contains library-specifics. An *implementation* inherits both from one library base class and one or more application base classes. See Fig. 3.3 for an impression. Thus switching the library in a use context should require minimal adjustment, and a new application (base class) can be be built from existing ones.

The second design objective was for the plotting methods to hide all interactions with the actual plotting library used under the hood. The application's base class' method arguments should only be tied to the data, not the plotting library. Thus different frontend implementations need no or minimal individual setup beforey they can call the same method for one specific plot and receive the identical visualization with identical interactive behavior.

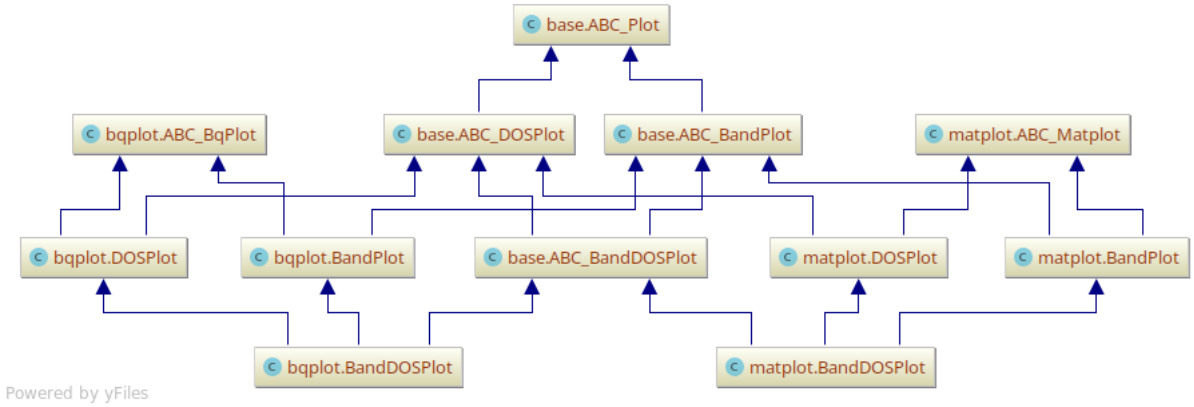


Figure 3.3: Visualization Module Design: Example Structure for two applications `BandPlot` and `DOSPlot`, and two plotting libraries `matplotlib` and `bqplot`.

Desktop Frontend

A Desktop Frontend is always a helping hand for the physicists to just execute it on the computer when one wants to go through the plots of the raw data that is already in the computer.

Since the reading of HDF files and preprocessing of the data is done using Python, it is decided that it would be better to use Python for frontend development. Considering various packages for frontend in python such as PyQt, Tkinter and other libraries available for Desktop GUIs, Tkinter is selected, as it is bundled with Python and thus meets the requirement of easy maintainability best. It is a package where every button can be designed and can be assigned to a function. GUI types like `Label`, `Button`, `CheckButton`, `ListBox`, `Canvas` for plots, `Tab` for viewing each plot in different tab have been used to make a simple Desktop front end. It is simple to use with limited options for what the end-user, the solid-state physicist, needs. It is also easy to convert the Desktop frontend code into a executable software and run in any system without any installation.

Web Frontend

As Web Frontends continue to replace traditional Desktop Frontends in many application domains [Dou+08], so Python-based Frontends and visualizations are increasingly moving towards the browser, too. There, GUIs with interactive visualizations are often called **Dashboards**. For this project, a survey was undertaken to find the most suitable technology stack for a Web Frontend. The full survey is documented in [Was19]. The requirements for the solution, on top of those stated in the introduction, were defined as follows: The solution...

1. **openness**: relies solely on Open-Source-Software (OSS) with licensing suitable for academic use, sports a stable release cycle, developer base and documentation,
2. **dashboarding**: features graphical control elements (widgets) that interact with InfoVis[1] plotting libraries,
3. **deployment**: ideally works like any web service, i.e. only a modern web browser is required to use it,
4. **maintenance**: requires only Python and no Web Development knowledge like e.g. Javascript, with respect to the product stakeholders.

The last point implies a client-server model where the dashboard app is hosted on a remote machine. This model requires a communication framework and protocol between the Python interpreter running on the server and the JavaScript interpreter running in the client browser. As per requirement no. 4, unlike a generic Python web framework like e.g. Flask, the framework should take care of that communication by itself. Four major frameworks were identified which fulfill the first three requirements: Project Jupyter, PyViz, Bokeh, and Dash by Plotly. The last two only partially fulfilled the requirement no. 4, so they were discarded. PyViz is the newest contender among these four. Its expressed goal is to untangle the Python visualization

[1] InfoVis libraries: visualizations of information in arbitrary spaces, not necessarily the three-dimensional physical world. Example: matplotlib. SciVis libraries: visualizing physically situated data. Example: VTK [Bed18].

jungle by providing one high-level API that ties together all major Python InfoVis libraries and data formats, including support for dashboarding. That ambitious goal comes at the price of sacrificing support for 3D plotting [aut18], which was needed in this project for the atoms plot. So PyViz had to be discarded.

That left Project Jupyter. By now, a wide variety of popular plotting libraries have made their tools capable of working with Jupyter's widget library `ipywidgets`. However, Jupyter only partially fulfills requirement no. 3 – a Jupyter notebook (app) cannot, by itself, be published (deployed) as a stand-alone website outside a live Jupyter environment [Bed18]:

> [...] "However, despite their web-based interactivity, the ipywidgets-based libraries (ipyleaflet, pythreejs, ipyvolume, bqplot) are difficult to deploy as public-facing apps because the Jupyter protocol allows arbitrary code execution" [...].

To avoid requiring users to setup a working Jupyter environment on their machine, the go-to solution for this problem is to setup a JupyterHub multi-user server. This still requires users to register an account there, so it's not completely open. Fortunately though, the intended users are contributors to the AiiDA project, and so should have access to the JupyterHub-based AiiDaLab service where the app can be registered. Details on this procedure and alternative hosting solutions can be found in the developer section of the manual 4 on page 19.

Chapter 4

Manual

The project code and documentation is hosted on the `masci-tools` repository [RBR18] under the branch `studentproject18ws`. All of the project code resides in the folders `binder` (for the Web Frontend Demo) and `studentproject18w` (all code and documentation). The `README.md` in the latter folder serves as the manual. Therefore, the remaining part of this chapter is a TEX-ified version of that `README.md` commit `5a0f3541f1d8505e528a8c87d23ef5070dc5d9d2`.

SiScLab 2018 Student Project **Analysis Tool for Materials Design**. Written in Python3.

Authors: Johannes Wasmer, Christian Partmann, and Praneeth Katta.

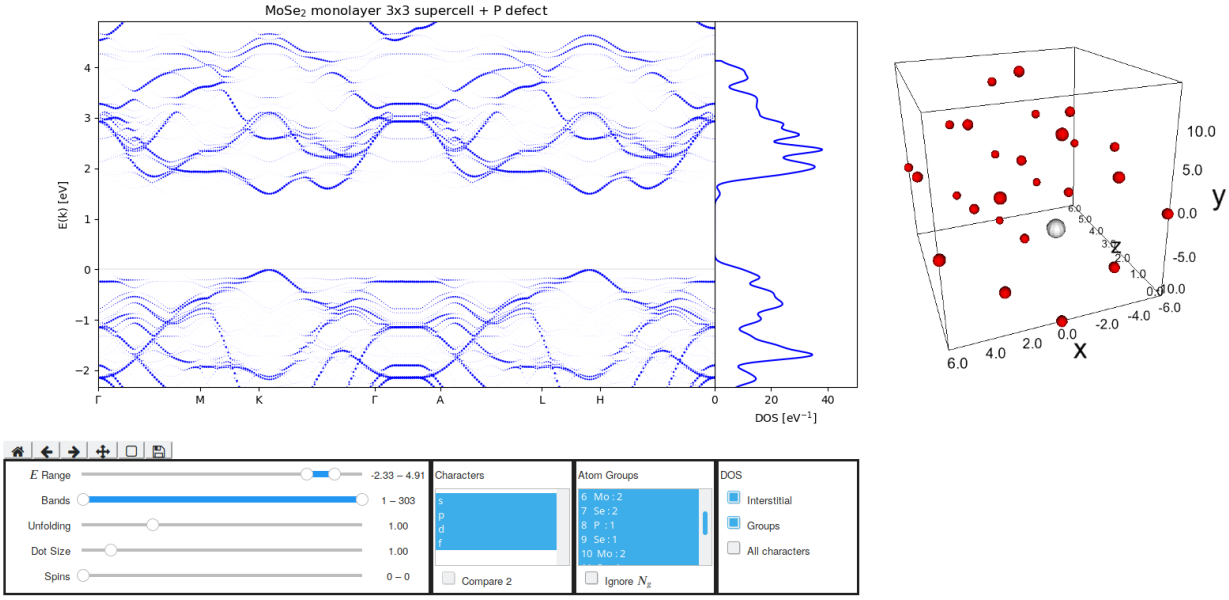
Overview

This subfolder `studentproject18ws` is currently a largely independent side-project accompanying the main module `masci-tools`. It was created in a student project at FZJ PGI-1, and consists of three submodules:

- preprocessor: a general HDF5 reader interface, and one implementation for band structure simulation output of the DFT code Fleur
- visualization: a plotting interface, and one implementation for Fleur band structure + DOS plots
- frontends: a Desktop GUI and a Web Dashboard (Tk and Jupyter) for interactive Fleur bandDOS plots.

A more thorough description and example use cases can be found in the project report and

presentation.



For Frontend Users

General Remarks

These remarks apply to all frontends.

Though the Desktop and Web Frontend are functionally identical, there might be small differences in how the controls are used and how they are labeled.

File Input

The frontends currently expect band structure data in the HDF output format of Fleur. The density of states data is expected to be in the CSV output format of Fleur, one file per spin. If no density of states files are supplied, the frontend will just draw a band structure plot (BandPlot) and omit the adjoined density of states plot (DOSPlot). Thus, in the following BandDOSPlot stands for both kinds of plot.

Desktop Frontend

Access

A windows executable file (.exe) is made by packing all the required packages into the file. Any modern PC running on windows can run the frontend without any installation process. You don't need Python or specific packages installed.

The executable for Windows (or other operating systems) can be obtained from the developers upon request.

Usage

The Desktop-based GUI is easy to use. Running the .exe file will open up the frontend with all packages loaded. The GUI consists of three tab windows. In the first tab window, absolute paths to the input data files must be entered in this order: HDF and (optional) DOS file for spin '0' and '1'. Tab 2 shows the BandDOSPlot, and Tab 3 the 3D atoms plot. After loading the files, the controls must be initialized. Finally, clicking the 'Update' button produces the plots.

Controls for all plots:

- **Atom Groups**: draw the BandDOSPlot only for the selected symmetry groups.
- **Character**: select one or more band Characters (orbitals) 'S','P','D','F'.
- **Spin**: select any one spin or both spins.
- **Marker size**: Default marker size of 1.0 is selected. How ever, user have a choice to increase the marker size of the dots (eigenenergies) plotted in the BandPlot.
- **Ymin, Ymax**: This control is used to limit the range energy range of the BandDOSPlot.
- **BandMin, BandMax**: This control is used to limit the band range of the BandDOSPlot.
- **Update, SaveButton**: Update the BandDOSPlot to the newly selected data by user. Save the the plot as a PDF on disk.
- **Exponential weight**: The unfolding exponent for supercell calculations (see report). Value 0.0 means no unfolding. If the calculation is done with a unit cell, this control has no effect.
- **Compare 2Characters**: When a user wants to compare 2 characters, this button makes the BandPlot show the influence of each character to each eigenergy using a sequential (2) colormap. The control is disabled if other than two characters are selected.
- **Ignore Atom group**: This button allows an option to ignore the atom groups.

Controls for the DOSPlot only:

- **Select groups**: include selected atom groups in the DOS
- **Interstitial**: include the interstitial in the DOS
- **All characters**: include all characters in the DOS regardless of character selection. In

the DOS CSV file, different input data is used (a summed column).

Troubleshooting

If the BandPlot is not visible:

- Click update two to three times.
- Check if the three input files (if any) are belonging to the same Fleur calculation and selected appropriately.
- Check if at least one Atom Group, one Character, one Spin is selected.
- Check if Ymin is less than Ymax and similarly BandMin is less than BandMax such that software is able to plot.

If the DOSPlot is not visible:

- Make sure either Select Groups or Interstitial is selected.

If the problem persists, try restarting the GUI. If that fails, please open an issue to contact the developers.

Web Frontend

Access

The Web Frontend is a Jupyter Dashboard. It is in experimental state (no fileupload yet). You can try it out here on Binder. You can also run it locally (see developer section). If you have an AiiDaLab account: the dashboard is planned to be published as an app there.

Usage

Using the Dashboard should be self-explanatory to the domain user. Some tips:

- If the plot window is not on startup or gets stuck, reload/rerun once.
- Plot updates are instantaneous.
- Empty selections are impossible.
- Only shows controls for data that is present in the input.
- Multi-selection boxes: use ctrl or shift to select multiple items.
- Slider values can also be typed into the adjoining text box.
- Try out the zoom and pan tools below the plot, they're useful.

For Developers

Installation

Clone this repo (branch). Then create a virtual environment for the project.

With conda (recommended): - Install Anaconda (3 recommended) - Install the environment `masci-stupro` with the necessary and recommended dependencies:

```
conda create -f environment.yml
source activate masci-stupro
```

With virtualenv (untested):

```
virtualenv masci-stupro
source masci-stupro/bin/activate
pip install -r requirements_pip.txt # install requirements
```

Programmatic use

Though `masci-tools` is (planned to be) availabe via PyPI, there is currently no plan to integrate `studentproject18ws`. If you want to use it in your code, use it in an IDE, or append the path to your `sys.path`:

```
import sys
if path_repo not in sys.path:
    sys.path.append(path_repo)

# now import works
from studentproject18w.hdf.reader import Reader
# ...
```

In this example, a Fleur HDF file is preprocessed using the Recipe `FleurBands`. The resulting output `data` with the extracted and transformed HDF datasets and attached load methods (Extract-Transform-Load) is then passed to a plotter, alongside some DOS CSV files for a bandstructure plot using `matplotlib` as backend library.

```
from studentproject18w.hdf.reader import Reader
from studentproject18w.hdf.recipes import Recipes
from studentproject18w.plot.matplot import BandDOSPlot
import matplotlib.pyplot as plt

data = None
reader = Reader(filepath=filepath_hdf)
```

```
with reader as h5file:
    data = reader.read(recipe=Recipes.FleurBands)
    #
    # Note:
    # Inside the with statement (context manager),
    # all data attributes that are type h5py Dataset are available
    # (on-disk access). When the statement is left, the HDF5 file
    # gets closed and the datasets are closed.
    #
    # Use data outside the with-statement (in-memory access: all
    # HDF5 datasets converted to numpy ndarrays):
    data.move_datasets_to_memory()

plotter = BandDOSPlot(plt, data, filepaths_dos)
(fig, ax_bands, ax_dos) = plter.setup_figure()

data_selection = some_selection_process()
plotter.plot_bandDOS(*data_selection)
plt.show()
```

Try out the Web Frontend locally

The demo notebook with the Dashboard is `studentproject18w/frontend/jupyter/demo/demo.ipynb`.

If using Jupyter Notebook

On Windows, omit keyword `source`.

```
source activate masci-stupro
cd mypath/masci-tools/studentproject18ws/
jupyter-notebook .
# if Home is not set to this dir, try this instead:
# /home/you/anaconda3/envs/myenv/bin/python /home/you/anaconda3/envs/myenv/bin/
    ↪jupyter-notebook .
```

If using Jupyter Lab

Additional installation step needed:

```
source activate masci-stupro
```

```
jupyter labextension install @jupyter-widgets/jupyterlab-manager jupyter-matplotlib ipyvolume
cd mypath/masci-tools/studentproject18ws/
jupyter-lab
```

Frontend Deployment

Desktop Frontend

To create executables for different operating systems, use PyInstaller. The target file is `frontend/tkinter/gui.py`.

```
source activate masci-stupro
conda install -c conda-forge pyinstaller
# if not using conda: pip install pyInstaller
cd mypath/masci-tools/studentproject18ws/
pyinstaller --onefile frontend/tkinter/gui.py
```

Web Frontend

The Web Frontend is currently a single Jupyter Notebook. In order to publish it as a usable standalone app, additional work has to be done.

- Create `frontend/jupyter/Dashboard.py` and put code of demo_backend.ipynb notebook inside it. This will become the widget. Use aiidalab-widgets-base > StructureUploadWidget as a template. Create `frontend/jupyter/Dashboard.ipynb` notebook. This will become the app. Use StructureUploadWidget Demo Notebook as a template.
- Add fileupload buttons (for HDF, DOS) to widget (again, like in StructureUploadWidget. See binder_fileupload_test.ipynb notebook for a demo that works with binder.)
- Now the Web Frontend should work on Binder.
- For publishing the app on AiiDA Lab, it has to be registered in the aiidalab-registry.
  - Create a skeleton using the aiidalab-app-cutter.
  - The project code is in Python3, but aiidalab requires Python2. So the code has to first be backported by hand using the `future` package. If this takes too long, maybe try the tool 3to2.
  - Use the simplest app in the registry, aiidalab-units as a template. Adapt code.
  - Try it out first in the Quantum Mobile Virtual Machine, which has aiidalab installed and configured. Else try it in a virtual environment with aiidalab installed from PyPI.
  - Register the app.

Note: other publishing options besides Binder and AiiDALab are listed here. For instance, Google Colaboratory is a free Notebook hosting service that allows environment creation and file upload.

Extending the code

Use Case: HDF format that includes DOS data

The Fleur output HDF format is expected to change and incorporate more data. In turn, this project's code has to be extended as well. The procedure is outlined for a an example use case: the incorporation of DOS data into the band structure HDF (thus eliminating the need for separate DOS CSV files). The instructions show how to extend the preprocessor, the visualization and frontend submodules to that scenario.

- Add a new output type to `hdf/output_types`, say `FleurBandDOS`. Let it inherit from output type `FleurBands`. If you want an output type just for the DOS as well, add a type `FleurDOS` and let `FleurBandDOS` inherit it.
- Add a new recipe to `hdf/recipes` e.g. `FleurBandDOS`. Copy unchanged things from recipe `FleurBands`.
- If needed, add new transforms to `hdf/input_transforms`. Adhere to the transform function standard there. If there are mutual dependencies, add them to the list in the top of the file.
- Add a DOS data selection method to the output type `FleurBands`. The `DOSPlot` in `plot/base` types will need those to plot the DOS plot. Simply adapt from the function in `dos/reader` for the DOS CSV files, adopt the identical signature.
- In the `DOSPlot` types in submodule `plot`, add a switch to the constructor that can distinguish the three cases (bands, bands+CSV DOS, bands+HDF DOS). Use the switch in the `plotDOS` methods, and for the case bands+HDF DOS, call your new `FleurBandDOS` function.

Extending the Visualization (Plots)

- In addition to the inheritance scheme based on Python `AbstractBaseClass` (ABC) detailed in the report, the `Plot` types in `plot` have an additional facility that helps to keep the appearance of different Frontends synchronized: each type has an attribute `icdv` of type `InteractiveControlDisplayValues`. This is an ABC with the same inheritance as the application Plot types. For every plot control argument that an application type's Plot type exposes in it's methods' signatures, this attribute describes the parameters of the accompanying control widget in the Frontend (text label, default values, value ranges, and so on). In the current code, only the Web Frontend uses this

facility, so the labels in the Desktop Frontend differ slightly.

- It is worth pointing out that unlike other languages, Python does not enforce implemented abstract methods to have the same method signature. However, when a new implementation for a different plotting library/backend is added, it is recommended to adopt the `abstractmethod` signature. That way, changing the backend in a use case only requires to change the import.

Open Issues

- The`FleurBands` data selection method could be optimized even more by replacing *all* numerical operations with `numpy` routines.
- Running the Frontends in a debugger or with a counter reveals: on a plot selection change or update, the plot seems to be redrawn not once but several times. The cause could not be found so far.
- In the Desktop Frontend, the Update Button has to be clicked several times.
- In the Web Frontend, on startup, the plot is only visible after two loads/cell runs.

Chapter 5

Applications

To illustrate the use of the graphical user interface, two different physical applications are shown in the desktop and the web frontend, respectively. From the physics point of view, the example in the desktop version focuses more on the density of states and the visualization of spin contributions, while the dataset in web frontend focuses on the band structure $E(\mathbf{k})$ and the visualization of defect states in supercells.

Web Frontend: $\mathrm{MoSe_2}$ Crystal

Figure 5.2 shows the visualization of a band structure calculation of a three-dimensional Molybdenum diselenide ($\mathrm{MoSe_2}$ bulk) crystal using the default settings of the GUI. Even with the default settings the band structure plots clearly indicate, that $\mathrm{MoSe_2}$ is a semiconductor, since there are no states at the Fermi level. Because the minimum of the conduction band is located at an other k as the maximum of the valence band, the plot shows that $\mathrm{MoSe_2}$ has an indirect band gap. This indicates that for the transition with the smallest energy difference between valence and the conduction band, both, energy and momentum have to change.

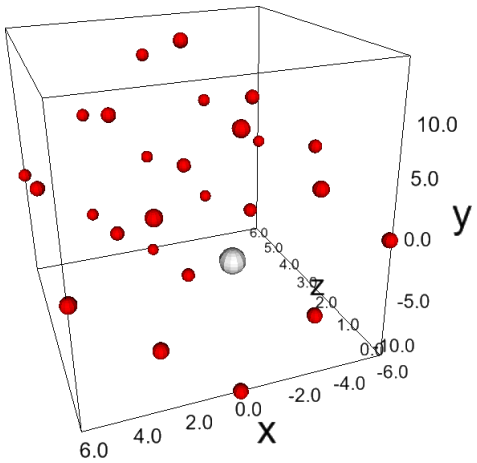


Figure 5.1: Atom Plot of a $\mathrm{MoSe_2}$ monolayer with the defect atom selected in the web frontend

In contrast to the three-dimensional extended $\mathrm{MoSe_2}$ crystal, a $\mathrm{MoSe_2}$ monolayer (see Fig. 5.3) has a direct band gap but is still a semiconductor. Furthermore, the $\mathrm{MoSe_2}$ monolayer has a defect atom in every 9th unit cell and the DFT computation is therefore done in a 3×3 supercell to restore periodicity. This is the reason for the much greater number of states

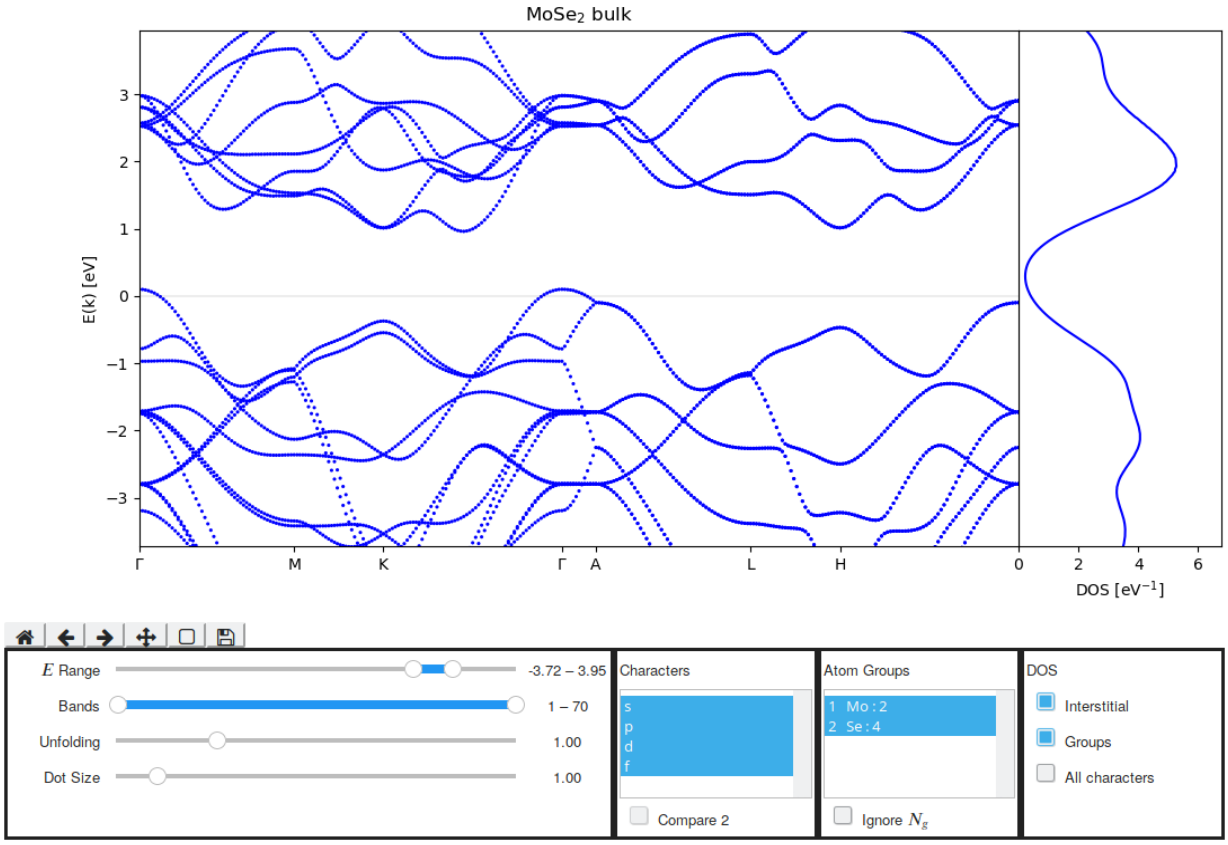


Figure 5.2: Bandstructure of a $MoSe_2$ crystal using the default settings of the web frontend

in the band structure plot.

Since the Brillouin zone of the supercell is smaller than the Brillouin zone of the same crystal without the defect, the supercell Brillouin zone is unfolded to the same size as the Brillouin zone of the unperturbed lattice. To account for the fact that the defect is only present in every 9th cell and its relative importance for the spectrum is therefore degraded, an unfolding weight is introduced to visualize the relative importance of bands in the unfolded Brillouin zone. By default, the unfolding weight is used by our visualization tool, but it can gradually be turned off in order to highlight the impact of defect states. This is shown in figure 5.4. To even better visualize the defect state, it would also be possible to select the atom group belonging the defect atoms only. In this example, the analysis with reduced band unfolding shows, that there are many more direct band gaps origination from the defect state.

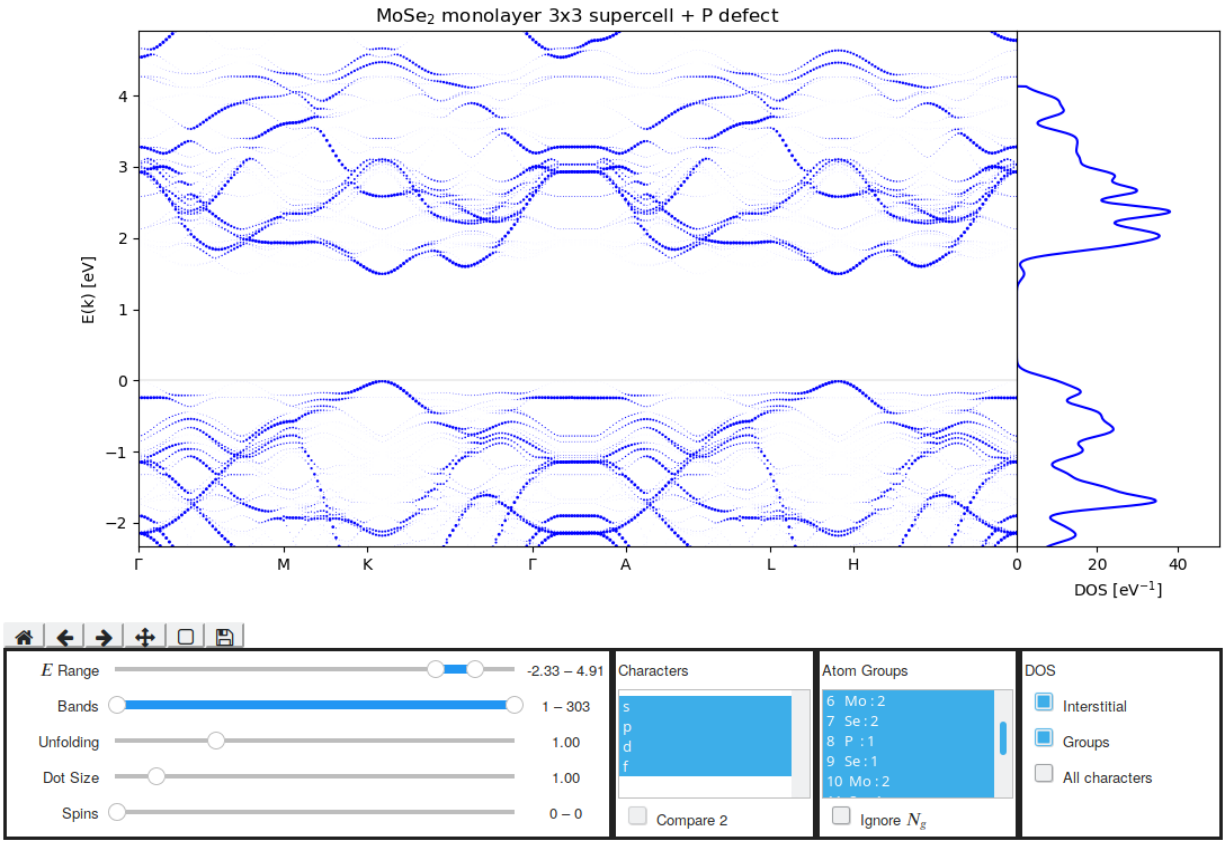


Figure 5.3: Bandstructure of a $MoSe_2$ monolayer using the default settings of the web frontend

Desktop Frontend: Co Crystal

Figure 5.5 shows the visualization of a band structure calculation of a three-dimensional Co crystal with the selection: both spins, one atom group (since there are only two, and each contains one Co atom) with all characters and all bands, and unfolding exponent being at 0.0 (the unfolding exponent has no effect here since the simulation is not done with a supercell). We can see in the figure that the bands for both spins intersect with the Fermi energy level. This means that many electrons excite to the valence band which is a characteristic of a conductor. Hence the Co crystal can be considered as a conductor material.

One more physical property of the Co crystal can be determined by considering and reading the density of states (DOS) files and plotting the density of states along with the band plots. In the figure 5.5, on the right one can see the density of states for both of the spins. If the area covered under the density curve is considered, it is clear that below the Fermi level, electrons of one spin covers more area than for the other spin in the density of states plot. This means there are more electrons with positive spin under the Fermi level. This is the character exhibited by a ferromagnetic substance, so it can be considered and concluded that this Co crystal is a

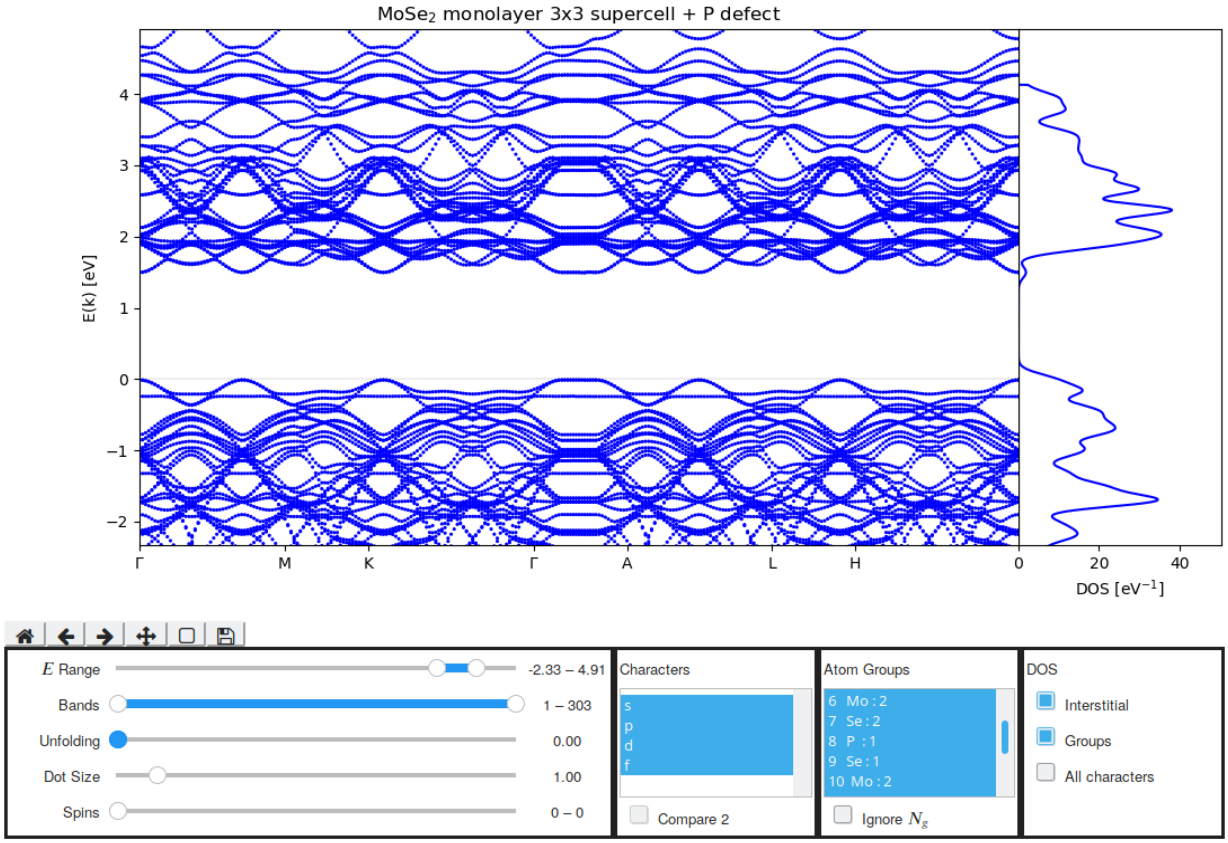


Figure 5.4: Bandstructure of a $\mathrm{MoSe_2}$ monolayer without unfolding weights

ferromagnet.

These are two properties which were deduced by observing the band-DOS plot, but depending on the material and band-DOS plot many properties can be extracted and derived.

Derived physical Quantities: Differentiation

The kind of datasets handled in the scope of the project did not lend themselves readily to applications of automatic differentiation techniques. Nevertheless, it is possible to derive meaningful physical quantities from the band structure using numerical differentiation techniques.

The effective mass m^* represents the mass, that an electron appears to have due to the interatomic forces in the crystal. At every $\mathbf{k}_0$, where $E(\mathbf{k})$ has a local extremum, $E(\mathbf{k})$ can be expanded in a Taylor series with a vanishing first order term $E(\mathbf{k}) = E_0 + \frac{\partial E(\mathbf{k})}{\partial \mathbf{k}} \cdot (\mathbf{k} - \mathbf{k}_0)^2$. Comparing this to the dispersion relation of a free electron $E(\mathbf{k})_{free} = \frac{\hbar^2 \mathbf{k}^2}{2m_e}$ motivates the

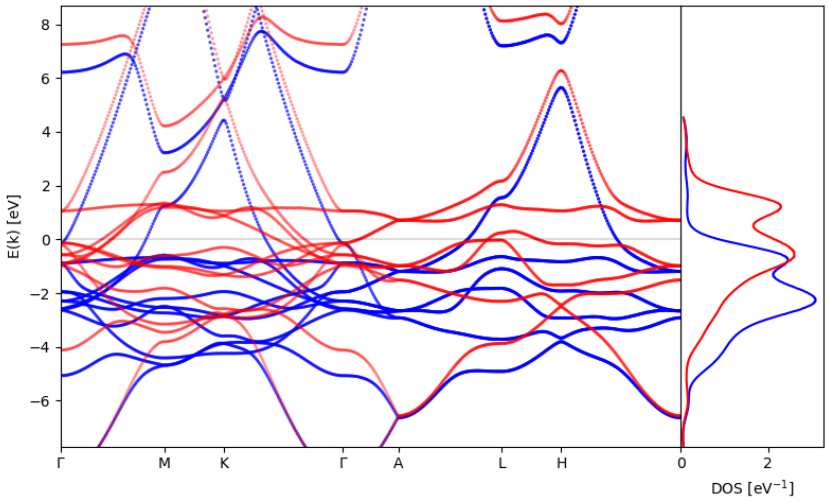


Figure 5.5: Bandstructure of a Co in the Desktop frontend. The plot settings are described in the text.

general definition

$$m^*_{k_i,k_j} = \hbar^2 \left(\frac{\partial^2 E(\mathbf{k})}{\partial k_i \partial k_j} \right)^{-1} \tag{5.1}$$

Since $\frac{\partial^2 E(\mathbf{k})}{\partial \mathbf{k}_i \partial \mathbf{k}_j}$ depends on the direction of the partial derivatives, $m^*_{k_i,k_j}$ is a tensor. Because the band structure files only contain a discrete sampled path in the Brillouin zone, only the derivatives that correspond to the direction from one high-symmetry point to the next can be computed. We are only interested in the diagonal terms of $m^*\big|_{i,j}$.

A second potentially interesting quantity is the group velocity $v_G(\mathbf{k})$ associated to each band. The group velocity $v_G(\mathbf{k})$ at the Fermi energy $E = E_F$ is called Fermi velocity.

$$v_G(\mathbf{k})_{k_i} = \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial \mathbf{k_i}} \tag{5.2}$$

Differentiation

Since the k-mesh in DFT calculations is potentially very sparse, low order finite difference schemes are not expected to work well. Alternatively, one way to exploit all data points efficiently is to use fast Fourier transform methods, which are equivalent to the derivation of a truncated Fourier series. This method is expected be well-suited for the problem since the graph of the band structure $(k, E(|k|))$ with $k \in \{-\Gamma, ..., H, ..., \Gamma\}$ is periodic, where Γ and H are arbitrary representatives of the high symmetry points. This periodicity in the reciprocal space is a direct

consequence of the periodicity of the crystal.

In Fourier space, spatial derivatives transform into multiplications, which can easily be shown by partial integration.

$$f^{(n)}(x) = \mathcal{F}^{-1}\left((ik)^n \mathcal{F}(f(x))\right) \tag{5.3}$$

To test the FFT differentiation method, a band was selected that did not have intersections with other bands within the interval between two high symmetry points and a stationary point at the high symmetry points. Then a resolution study was done to investigate the impact of the number of points within the interval.

The comparison between the FFT and a first-order central difference approximation of the second derivative (FD) is shown in Fig. 5.6, where different k-mesh resolutions are compared to a derivative that is almost fully converged. The comparison indicates that for small N, the error of the FFT method is significantly smaller than the error of the FD derivative. This is especially striking in the vicinity of the high symmetry points, where the error of the differentiation is required to be small in order to get good approximations for m^*, which is only meaningful close to the high symmetry points.

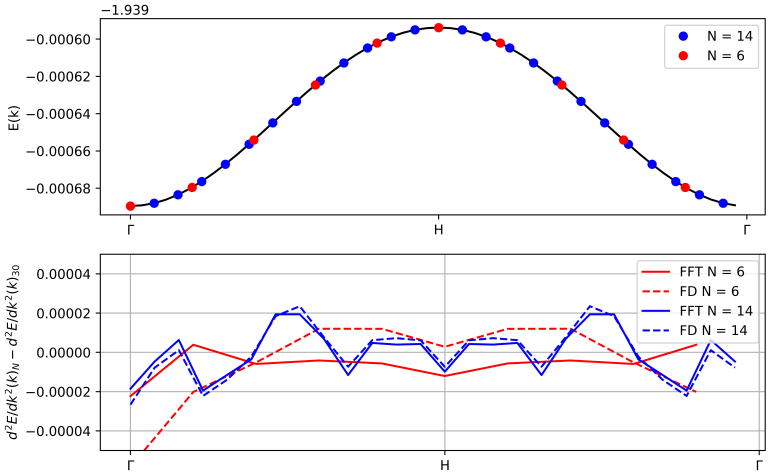


Figure 5.6: Comparison between FFT differentiation method and central finite difference method

When using more points, the difference between both approximation schemes is not significant. It is interesting to note, that the FFT method does not work anymore in the limit of extremely many points. In this case the derivative is dominated by Gibbs oscillations. These are most likely caused by small discontinuities in $E(\mathbf{k})$, due to basis changes inside the DFT computation.

At the current state the question remains to be answered weather the computation of m^* and v_g is useful. The number of bands, which the computation can be applied to is extremely limited. Since the bands in the data files are not labeled according to their corresponding eigenfunction but sorted by value, there are discontinuities at each point, where two bands intersect. This problem might be solved in the future.

Chapter 6

Conclusion

Outlook

- A package to developed to visualize DFT data in an appropriate way. The data is read, extracted and visualized using the package.
- An API and GUI are developed which are easy to use, easy to get the visualization output and visually appealing.
- The API is used and studies data to external physical feature such as effective mass (m), Fermi Velocity(v_{fermi}) using numerical differentiation techniques which is helpful in analyzing materials characteristics.
- Fluer output data are now easily accesible to non-experts since processing and visualization done by this API.
- Integrating of API and GUI into AiiDA workflow makes it easier for anyone to access this and understand the simulation much faster.
- Features extracted through the simulation data can also be saved for further research and analysis.
- A directly executable GUI which makes it easier to use in any computer just by copying the GUI.

TODO Module design:

- Preprocessor module: dataset dependencies for new recipes have to be explicitly stated. This could also be automatically resolved by type inspection.
- Frontends:
  - PyViz Param [Ste+19] makes it possible to decouple the formal description of a particular GUI from the GUI library used. This would serve to separate interface and

implementation like it is done in the preprocessor and visualization submodules.

Bibliography

[aut18] PyViz authors. *PyViz FAQ*. http://pyviz.org/FAQ.html. PyViz team. 2018.

[Bed18] James Bednar. *Python Data Visualization 2018*. Blog. https://www.anaconda.com/python-data-visualization-2018-why-so-many-libraries/ and https://www.anaconda.com/python-data-visualization-2018-moving-toward-convergence/ and https://www.anaconda.com/python-data-visualization-2018-where-do-we-go-from-here/. 2018.

[Blü+18] Stefan Blügel et al. *Fleur: full potential linearized augmented planewave code*. http://www.judft.de. 2018.

[Dou+08] John R Douceur et al. "Leveraging Legacy Code to Deploy Desktop Applications on the Web." In: *OSDI*. Vol. 8. 2008, pp. 339–354.

[Hof87] Roald Hoffmann. "How chemistry and physics meet in the solid state". In: *Angewandte Chemie International Edition in English* 26.9 (1987), pp. 846–878.

[Kor11] Sandeep Koranne. "Hierarchical Data Format 5 : HDF5". In: *Handbook of Open Source Tools*. Boston, MA: Springer US, 2011, pp. 191–200. ISBN: 978-1-4419-7719-9. DOI: 10.1007/978-1-4419-7719-9_10. URL: https://doi.org/10.1007/978-1-4419-7719-9_10.

[Piz+16] Giovanni Pizzi et al. "AiiDA: automated interactive infrastructure and database for computational science". In: *Computational Materials Science* 111 (2016), pp. 218–230. ISSN: 0927-0256. DOI: https://doi.org/10.1016/j.commatsci.2015.09.013. URL: http://www.sciencedirect.com/science/article/pii/S0927025615005820.

[RBR18] Philipp Rüßmann, Jens Bröder, and Stefan Rost. *masci-tools*. https://github.com/JuDFTteam/masci-tools. 2018.

[Ste+19] Jean-Luc Stevens et al. *PyViz Param*. https://github.com/pyviz/param. 2019.

[VR17] Jake VanderPlas and Nicolas Rougier. *Python Visualization Landscape*. https://github.com/rougier/python-visualization-landscape. 2017.

[Was19] Johannes Wasmer. *Software Development Notes*. https://github.com/Irratzo/notes. 2019.