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ADFT-VEX: An Automated Density Functional Theory–based Parameter Visualization and Extraction Tool

by Mahesh Raj Neupane and Protik Das

NOTICES

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14. ABSTRACT

First-principle simulation of nanomaterials and nanostructures involves generation of large-scale materials properties and device-specific parameters in nontrivial, hard-to-interpret data format. In order to analyze these parameters and utilize them in predictive device modeling, an automated tool that can read raw simulation data, analyze them, and extract device-specific parameters, such as work-function, mobility, band alignment, and electronic properties, is required. This report presents a modular tool for streamlining the visualization of density functional theory calculations: Automated Density Functional Theory–based Parameter Visualization and Extraction (ADFT-VEX). ADFT-VEX can visualize different aspects of band structure and the density of states, and it exports publication-quality plots. Effective mass calculation of homogeneous and heterogeneous materials from their band structure is also supported.

15. SUBJECT TERMS

density functional theory, DFT, visualization, python, MATLAB, VASP, ADFT-VEX

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Contents

List of Figures

List of Tables

1. Introduction

Density functional theory (DFT) is a well-known method used to investigate intrinsic material properties at 0 K. To identify potential applications for any new material, the first step is to conduct DFT calculations. Most DFT tools are written for systems running in a Linux environment. As a result, output data generated by these tools are written in plain ASCII text format. There is no agreed-upon convention for writing the data. Each DFT tool has its own format for outputting data, making the visualization and parameter extraction process cumbersome. These varying formats also slow down the throughput of the research, as one needs to develop a separate tool to visualize the data. Enhancements in high-performance computing have improved calculation time drastically over the last few years, but because of the ambiguity involved in the output data for each tool, data visualization and decision-making are still time-consuming.

Automated Density Functional Theory–based Parameter Visualization and Extraction (ADFT-VEX) is a visualization and parameter extraction tool for DFT calculations. This code closes the gap between the output data and the decision-making process. The first version of the code can plot band structure, ionic and orbital composition of the electronic band structure, and various features of density of states (DOS). The exported visualizations are publication quality. In addition, it can extract effective mass from the band structure. The tool is modularized and object oriented. As a result, this code can be extended to any DFT tool. Currently, the code is capable of visualization and parameter extraction using the Vienna Ab initio Simulation Package (VASP).

2. Motivation

The Wikipedia page for quantum chemistry and solid-state physics software[*] listed 88 DFT tools at the time of this report. There is no standard format for the data outputted by these tools. As a result, data analysis involves developing a stand-alone visualization tool for each of the DFT calculation tools.

A few years back, the bottleneck for DFT calculations was due to limited computational resources. With continuous improvements in processor speed and efficiency, and innovations of very high-throughput networking technology like Infiniband, the DFT calculations of a periodic crystal are considered trivial. Unfortunately, now the bottleneck is the lack of appropriate tools for visualization and parameter extraction from the available data. Some packages such as Quantum

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[*] https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

Espresso[1] and Abinit[2] come with their own postprocessing utilities, but they are limited in terms of the operating system they can run on.

The data outputted by the DFT tools are usually electronic band structure and associated projections of the band structures. Some tools are provided with additional features that can be used for relaxation of atomic structures or Nudged Elastic Band calculations. These features can vary widely depending on the tool being discussed.

The data outputted by the DFT tools can be used differently based on the field of application. For example, for a device physicist, the slope of the conduction or valance band of a semiconductor is quite important. Hence, the visualization needed for a scientist focusing on materials with device applications can be quite different from that of a scientist focusing on chemical properties of a material. A field- and specialization-agnostic tool is still not available.

3. Input Parameters

A DFT calculation requires several input parameters, such as the description of the material along with parameters that incorporate physics into the calculation. For Quantum Espresso, all of these parameters are incorporated into one file. For VASP, the input parameters are divided into separate files. A summary of the input files for VASP is shown in Table 1.

Table 1 Input files for a VASP simulation

File name	Description
INCAR	Input parameters for the simulation
POSCAR	Structure information of the material
POTCAR	Pseudopotentials for the material
KPOINTS	K-points scheme for the calculation

The INCAR file contains the keywords that are needed for a calculation. The POSCAR file contains the description of a unit cell and the position of the atoms of a material. The POTCAR file contains the pseudopotentials for the elements of the material. The VASP official website contains a library of pseudopotentials for all the elements. The user needs to create a pseudopotential file from the library of pseudopotentials. The sequence of the pseudopotentials needs to be same as the sequence of the POSCAR file. The KPOINTS file contains the grid of k-points for which the integration is done.

4. Data Collection

For any calculation, VASP outputs its data in two formats. In one case, the different data is outputted in separate text files. For example, the band structure, orbital contribution, and the density of states are written into files named EIGENVAL, PROCAR, and DOSCAR, respectively. Parameters such as the Fermi level are written into a file named OUTCAR, whereas in the second case, all the data for a calculation is written to an XML file named vasprun.xml. While the outputs are scattered in multiple output files, the XML file contains all the necessary data. An XML file is easier to process programmatically for further postprocessing.

When reading the data for visualization and parameter extraction purposes, one can use any of the files to read the data. In terms of data collection, using the vasprun.xml file has some advantages:

- All the data for a calculation can be read from one file.
- An XML file is a structured format, which makes the file more readable compared with a plain text file.
- Reading an XML file programmatically is much easier compared to reading an ASCII file, as almost all languages have a dedicated optimized XML reader.

The primary language used to develop the tool was MATLAB. For calculations involving large structures, MATLAB can run into memory problems due to the limitation of memory within the virtual Java system on which MATLAB runs. To circumvent this problem, a separate XML reader written in Python has been developed. MATLAB can be used to call a Python script from its own environment. ADFT-VEX calls the appropriate Python functions to read the data. The Python script is dependent on libraries numpy and scipy. Often the numpy and scipy code execution fails due to the failure in the native execution of C code. If calling the Python library fails, the code falls back to the XML reader written using MATLAB. In terms of performance, the MATLAB reader is slower compared to its Python counterpart, but it enables graceful execution of the code when Python fails. The programmatic details are discussed in the Appendix.

The data read using code is stored in a predefined dimension. The stored data takes advantage of MATLAB's ability to store higher-dimensional matrices. For example, the eigenvalues are stored in a dimension that is (spin × number of k-points × number of bands). Due to the modular nature of the tool, data read from any other DFT can be visualized using the tool if the data are stored using the same dimension. The convention used to store data is provided in Table 2.

Table 2 Dimensions of the read data within ADFT-VEX

Data	Dimension
Eigenvalue matrix	Spin × bands × k-points
DOS data matrix	Atoms × spin × energy × orbital
Orbital composition matrix	K-points × bands × spin × atoms × orbital
Effective mass matrix	Spin × band × degree

The code uses a caching algorithm to store data. When an XML file is read for the first time, the read data is stored in a data file. For the consequent execution of the code for data processing, a mat file is used. Since reading a mat file is much faster than reading an XML file, data processing is much faster after the mat file is created. ADFT-VEX recognizes if there is a newer XML file; it reads the XML file from scratch and creates a new mat data file. This caching can be manually controlled from the menu.

Features of the ADFT-VEX can be categorized into two parts: visualization and parameter extraction. The visualization part of the code can be used to generate and export publication-quality figures of different properties available within DFT codes. The parameter extraction part of the code can calculate effective mass for both homogeneous and heterogeneous materials within different levels of fidelity.

5. Visualization

The visualization part of the library can plot electronic band structure; orbital and ionic contribution of the atoms to the band structure; and total, ionic, and orbital contribution of density of states. We discuss each feature separately.

5.1 Band Structure

5.1.1 Electronic Band Structure

The electronic band structure calculation proceeds the structure optimization and charge calculation steps within the DFT code. The structure optimization step involves optimizing the atomic geometry of a given system, as shown in Fig. 1. Following the structure optimization, self-consistent charge calculation steps are performed by benchmarking various charge integration–related parameters such as K-points, smearing parameter, and cutoff energy for the wave function. Consequently, the converged charge is used to evaluate eigenvalues around the high symmetry points of the Brillouin zone (BZ). Finally, the eigenvalues are plotted in the band structure form. An example band structure for a monolayer PtSe2 system (Fig. 1) is illustrated in Fig. 2. Plotting the band structure is the very basic visualization for DFT-based calculation data. While the plotting may seem trivial, the data can be in different formats based on the theory applied during the calculation. To read the data properly, one needs to identify the level of theory used to generate the data. Several cases should be considered, such as

- Band structure without any spin degeneracy or spin orbit coupling (SOC),
- Band structure with spin degeneracy,
- Band structure with SOC, and
- Band structure with Heyd–Scuseria–Ernzerhof (HSE) correction applied.

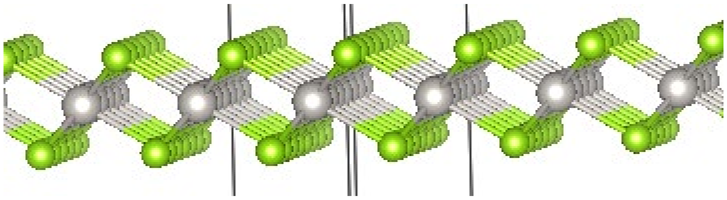


Fig. 1 Atomic structure of a $PtSe_2$ monolayer

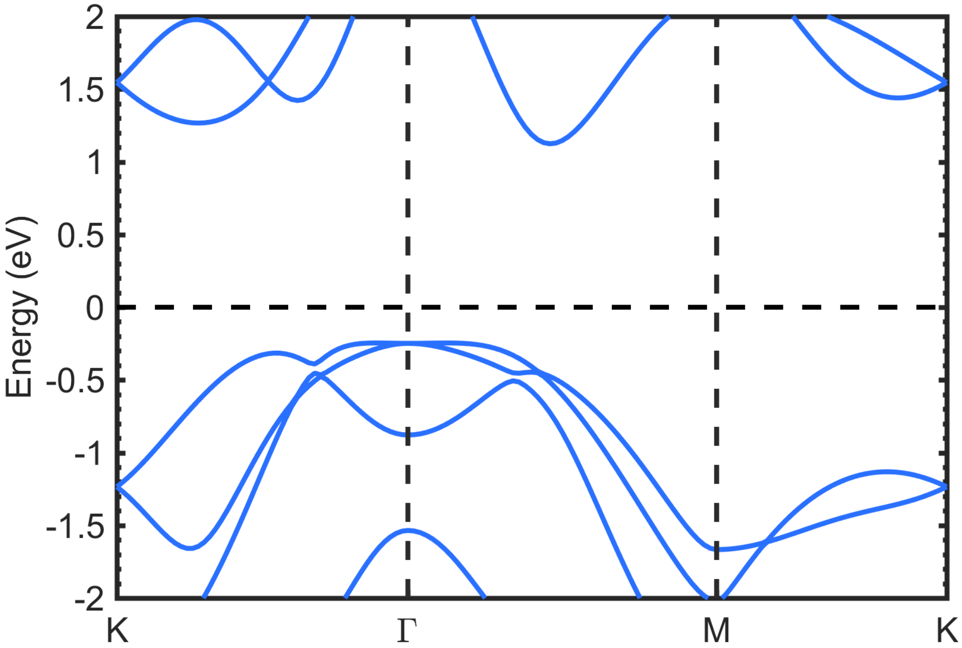


Fig. 2 Band structure of monolayer $PtSe_2$ plotted using ADFT-VEX

ADFT-VEX tries to determine the use case from the input tags, which are provided in the XML file, and read the data accordingly. For example, for the spin degeneracy case, the spin-up and spin-down cases are plotted side by side. For band structures calculated using HSE, the k-points of the irreducible Brillouin zone (IBZ) are also included in the calculation. To plot the data according to the path, the k-points of the IBZ need to be removed. ADFT-VEX removes these k-points and the associated bands from the data and plots the band structure.

5.1.2 Atom-Projected Band Structure

Electronic band structure calculated using DFT can be projected into atoms or orbitals from where information about atomic or orbital contribution can be retrieved. These data can be an important tool for analyzing the material properties. VASP writes the atomic and orbital-projected data in both PROCAR and a vasprun.xml file. Depending on the level of physics that is included, the dimension of the data can be different. Also, with number of atoms, the size of the data is increased linearly. ADFT-VEX identifies the dimension of the data from the input tags and reads the data from the XML file. Figure 3 shows the atom-projected band structure of a monolayer $PtSe_2$ using ADFT-VEX.

For the atom-projected band structure, ADFT-VEX calculates the contribution between different elements and assigns a color to the maximally contributing element for each k-point of each band.

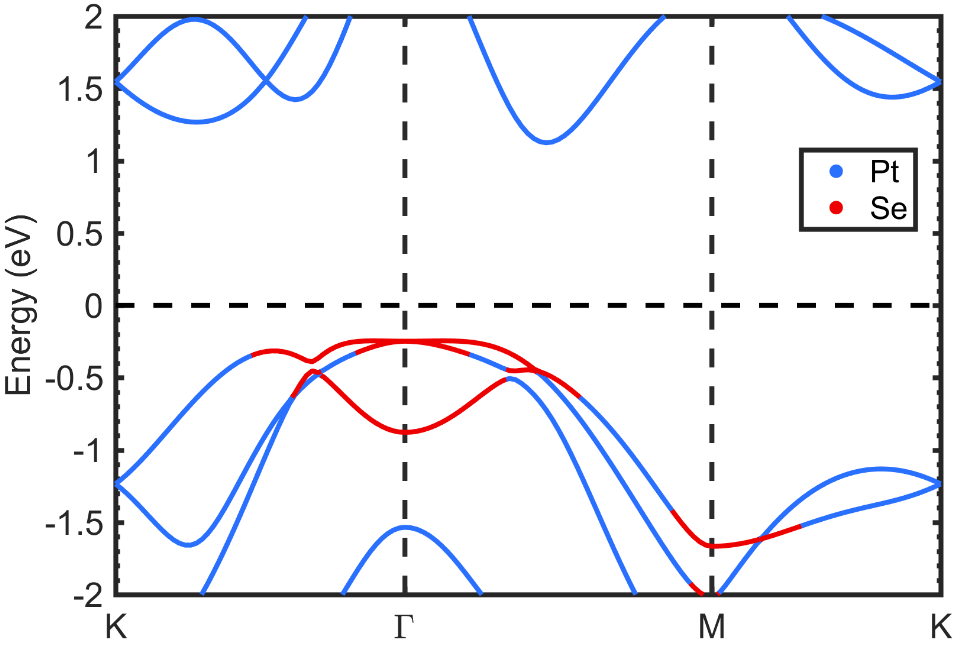


Fig. 3 Atom-projected band structure of monolayer $PtSe_2$ using ADFT-VEX. The figure shows a major contribution from an element at each k-point of the band structure.

While visualizing some generalizations are assumed. This results in two limitations. One, ADFT-VEX cannot identify the contribution from each element. Rather, it sums the contribution for all atoms of an element and plots the data. There is not a general use case for which this may be useful. Two, the color assigned for an element can be misleading. For example, in a k-point for a certain band, for a material AB, the elements A and B can contribute 60% and 40%. ADFT-VEX will assign a color to A and plot that as the maximum contribution coming from element A. In reality, element B has a substantial contribution for that point as well.

The first limitation can be solved by a gradient plot. For a material system with many elements, this scheme will require one gradient plot per atom, which can be difficult to understand.

5.1.3 Orbital-Projected Band Structure

The orbital-projected band structure is calculated and plotted using the same methodology as the atom-projected band structure. In this case the sum is calculated over the orbitals. Several other options can be used for the visualization. The orbital-projected band structure can be visualized as a contribution from s, p, and d orbitals. Also, ADFT-VEX can break down the contribution from p and d orbitals and visualize the data separately. For the p orbital, the contribution of p_x and p_y orbitals or σ-bonds are plotted in one color, and the contribution of p_z or π-bonds are plotted in another color. For the d orbital, the t_{2g} and e_g states are plotted in different colors.

As in the case of the atom-projected plots, for the orbital-projected plots, the orbitals with the maximum contribution to the bands are plotted. For example, Fig. 4 shows the orbital-projected density of states of $PtSe_2$. Furthermore, to understand the real contribution, a separate plot with gradients is needed.

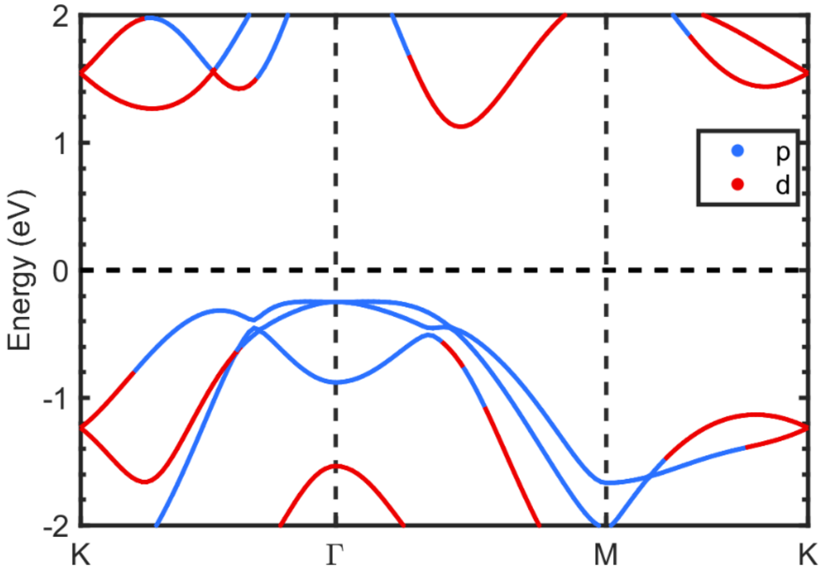


Fig. 4 Orbital-projected band structure of monolayer $PtSe_2$ using ADFT-VEX. Like the atomic projection, the orbital projection shows a major contribution from an orbital at each k-point of the band structure.

5.2 Density of States

5.2.1 Total Density of States

ADFT-VEX can visualize the total DOS of a given system. From the inputs, the ADFT-VEX can identify the physics included in the calculation and read the data accordingly. For example, if the calculation is spin-polarized, ADFT-VEX can plot the spin-up and spin-down differently, as shown in Fig. 5. DOS calculations are usually done separately from a band structure calculation. The DOS calculation needs to be done on the whole BZ, and the convergence as a function of k-points needs to be checked carefully. Figure 5 shows the total DOS of bulk CrSb. The magnetic nature of CrSb is apparent from the DOS difference of spin-up and spin-down DOS.

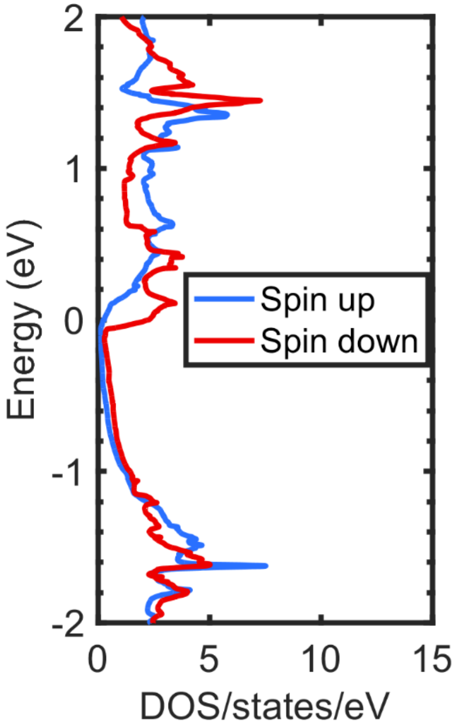


Fig. 5 Total DOS of an antiferromagnetic CrSb plotted by ADFT-VEX. The spin-up and spin-down components of the DOS are plotted with different colors.

5.2.2 Atom-Projected Density of States

ADFT-VEX can also visualize atom-projected DOS. Compared to the atom-projected band structure, atom-projected DOS contains more insight as the calculation is done on the whole BZ rather than a path along the BZ. Figure 6 shows an example of spin-resolved atom-projected DOS plotted using ADFT-VEX.

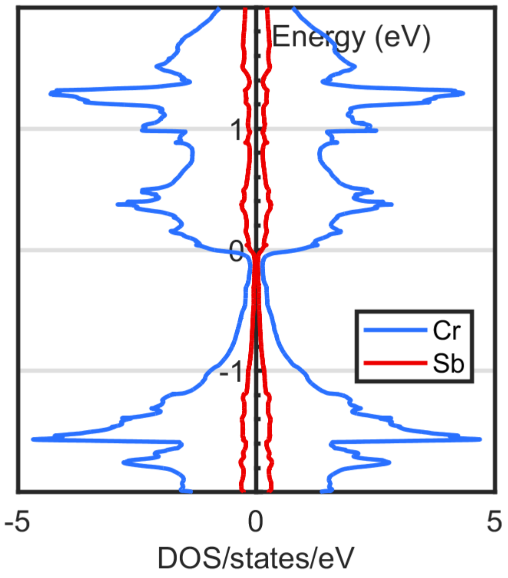


Fig. 6 **Spin-resolved atom-projected DOS of an antiferromagnetic CrSb plotted using ADFT-VEX. The contributions of each atom to the DOS as a function of energy are shown separately.**

5.2.3 Orbital-Projected Density of States

ADFT-VEX can also visualize spin-resolved orbital-projected DOS as shown in Fig. 7. For now, the orbital-projected DOS plots the contribution of the s, p, and d orbitals separately. ADFT-VEX also offers a feature to plot the contribution from the d-orbital in a separate plot. This feature is useful in analyzing the orbital hybridization in metal/semiconductor heterostructures.

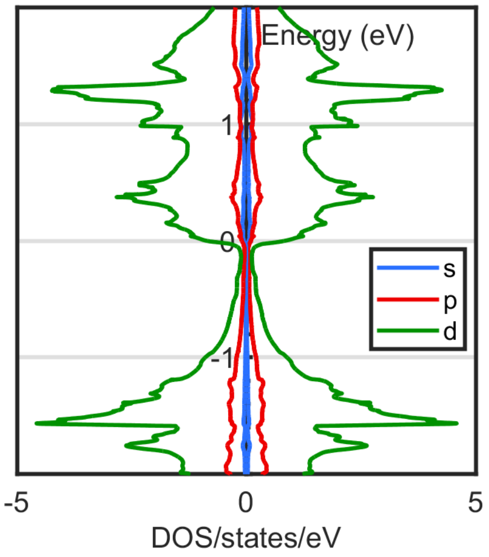


Fig. 7 **Spin-resolved orbital-projected DOS of antiferromagnetic CrSb plotted using ADFT-VEX. The contributions of s, p, and d orbitals to the DOS as a function of energy are shown with separate colors.**

5.3 Effective Mass

Effective mass (m*) is an intrinsic property of a material that defines the slope of the conduction or valance band minima. Electronic transport within a material is strongly dependent on the effective mass of a material because this parameter is inversely proportional to the carrier mobility responsible for the charge transport. Effective mass can be determined from the band structure. The band edge of a semiconducting material is usually parabolic. This parabolic dispersion can be fitted to a second-order polynomial to extract the effective mass. The effective mass can be defined as $\frac{1}{m^8} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial^2 k}$. To verify the order of the fitted polynomial, the dispersion can be fitted to a fourth- or sixth-order polynomial. If the residuals are close to zero, then the dispersion is parabolic.

Effective mass is a tensor for a material. In a band minima (or maxima), the effective mass is calculated in the longitudinal and transverse directions. Usually the longitudinal direction is along k_x and the transverse direction is perpendicular to k_x. If the mass along the longitudinal and transverse directions for the conduction or valance band is the same, the mass for that band is called “isotropic”. For an isotropic material, the transport along either direction is same. If the masses are not the same along the longitudinal and transverse directions, then the material is “anisotropic” and the transport along the directions will be different.

Within ADFT-VEX, the effective mass can be calculated in two ways: 1) directly from the band structure or 2) perform a dense E-k calculation along the longitudinal and transverse directions.

5.3.1 Generic Effective Mass

The generic effective mass is calculated from a band structure calculation. For the generic calculation of effective mass, three inputs are required. One is the threshold to cut off the band—usually it is in order of room temperature thermal energy (i.e., kT), 35 meV. The band minima will be fitted to second-, fourth-, and sixth-order polynomials to ensure there are no residues for higher-order fits. For some cases, the band minima or maxima are split due to the SOC effect. If the splitting is higher than a given threshold value, then ADFT-VEX calculates effective mass for both bands. If the SOC splitting is less than the kT, the polynomial fitting operation might lead to overestimation of the effective mass.

While the effective mass from the band structure can be useful, the results should be interpreted with caution. The calculation is done not necessarily on a straight path of k-points. Hence, if the minima is at a corner, the effective mass calculation may yield the wrong result. Also, for an anisotropic dispersion, the curvature along different high-symmetry points can be different, which can affect effective mass output.

5.3.2 Accurate, Effective Mass Calculation

5.3.2.1 Generate k-Points

For an accurate, effective mass calculation, a separate band structure calculation is needed. ADFT-VEX can be used to generate the line of k-points. In this mode, ADFT-VEX identifies the band minima and generates k-points along the longitudinal and transverse directions. For this mode, a threshold cutoff can be given. ADFT-VEX fits the dispersion up to the threshold energy. ADFT-VEX can write the k-point path in two formats. The default format is to write the file as a KPOINTS file as required for VASP calculations. The other is to write it as a mat file, which can be read later programmatically. This mat file can be used to set the band structure path using Python tools like Atomic Simulation Environment.[3]

5.3.2.2 Calculate Effective Mass

In this mode, ADFT-VEX reads the calculation output done for KPOINTS provided by the earlier mode and calculates the effective mass. The functionality of this mode is similar to the generic calculation. As the dispersion path is along the longitudinal and transverse directions with dense k-points along those directions, the calculation output is more accurate. Figure 8 shows the published band structure of GaN. Figure 9 shows the band structure calculated using VASP and plotted using ADFT-VEX. An example output for the in-plane and out-of-plane effective mass calculation is shown in Figs. 10 and 11. When compared to the available published effective masses for the zinc-blend GaN, the ADFT-VEX effective masses are within 10% root mean square error, which is within the experimental error of margin.

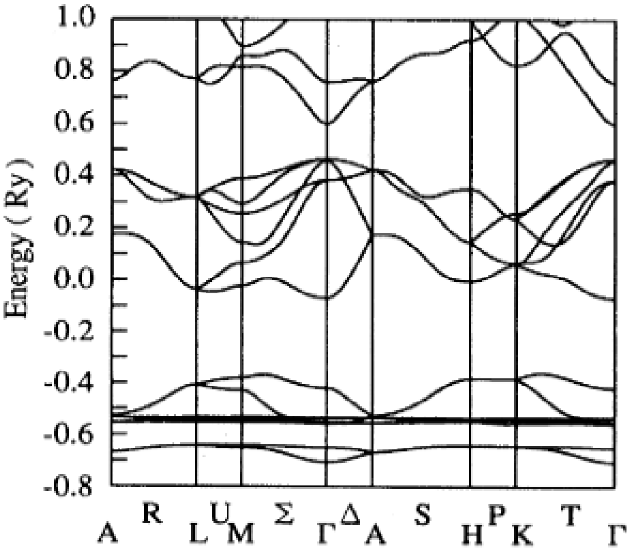


Fig. 8 Band structure of zinc blend bulk GaN[4]

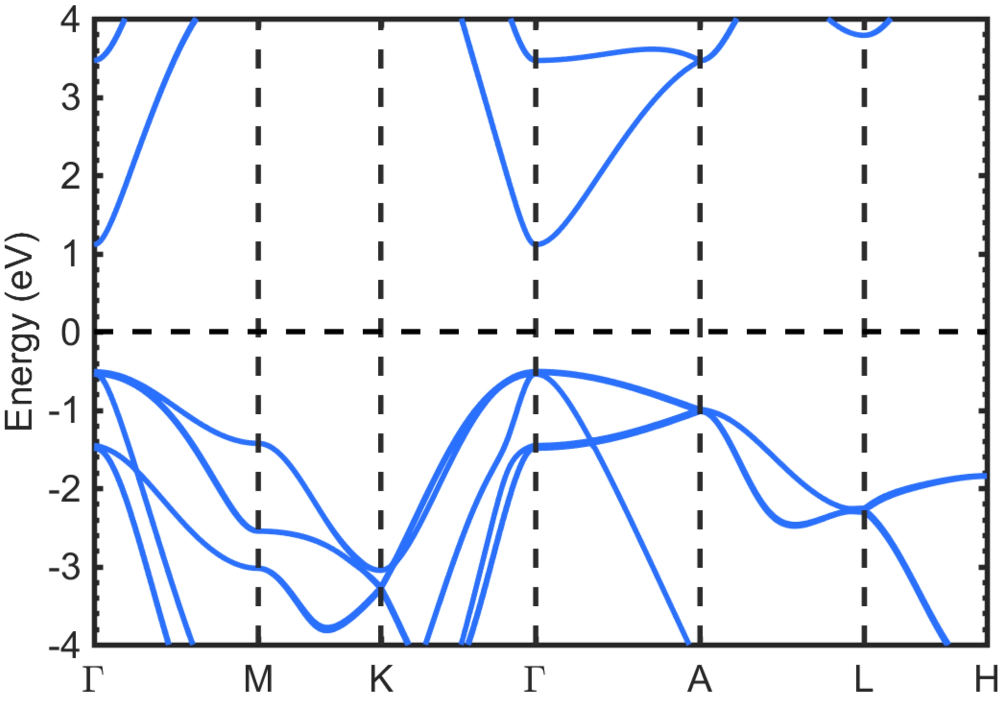
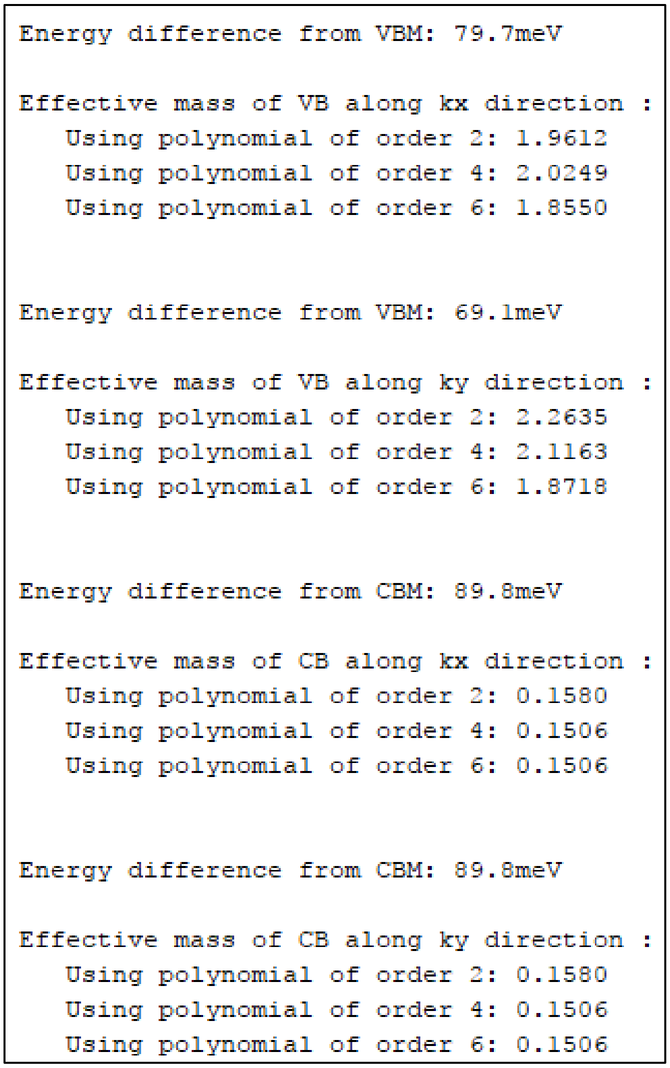
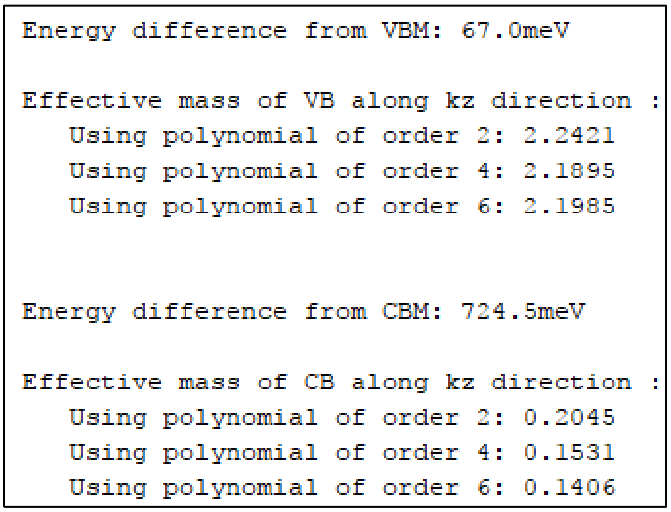


Fig. 9 Calculated band structure of zinc blend bulk GaN as plotted using ADFT-VEX



```
Energy difference from VBM: 79.7meV

Effective mass of VB along kx direction :
   Using polynomial of order 2: 1.9612
   Using polynomial of order 4: 2.0249
   Using polynomial of order 6: 1.8550


Energy difference from VBM: 69.1meV

Effective mass of VB along ky direction :
   Using polynomial of order 2: 2.2635
   Using polynomial of order 4: 2.1163
   Using polynomial of order 6: 1.8718


Energy difference from CBM: 89.8meV

Effective mass of CB along kx direction :
   Using polynomial of order 2: 0.1580
   Using polynomial of order 4: 0.1506
   Using polynomial of order 6: 0.1506


Energy difference from CBM: 89.8meV

Effective mass of CB along ky direction :
   Using polynomial of order 2: 0.1580
   Using polynomial of order 4: 0.1506
   Using polynomial of order 6: 0.1506
```

Fig. 10 **A screenshot of the output of calculated in-plane effective mass using ADFT-VEX**



```
Energy difference from VBM: 67.0meV

Effective mass of VB along kz direction :
   Using polynomial of order 2: 2.2421
   Using polynomial of order 4: 2.1895
   Using polynomial of order 6: 2.1985


Energy difference from CBM: 724.5meV

Effective mass of CB along kz direction :
   Using polynomial of order 2: 0.2045
   Using polynomial of order 4: 0.1531
   Using polynomial of order 6: 0.1406
```

Fig. 11 **A screenshot of out-of-plane effective mass calculated by ADFT-VEX**

5.3.3 Effective Mass of Semiconducting Material of a Heterostructure

A heterostructure is formed when two materials are stacked. In a field-effect transistor a metallic material is stacked over a semiconducting material to form a contact. This can be done in DFT to observe changes in the material properties. The curvature of the valance band maximum or conduction band minimum of a semiconducting material can be affected when stacked with a metallic layered material. This can be quantified by calculating the effective mass of the pristine material and the mass of the semiconducting material in a heterostructure.

As a case study, a $MoTe_2$-$TaSe_2$ heterostructure is created. Band structure and effective mass calculations are conducted using VASP. Figure 12 shows the atom-projected band structure of the heterostructure. Table 3 shows the effective mass of the $MoTe_2$ and $MoTe_2$-$TaSe_2$ heterostructure.

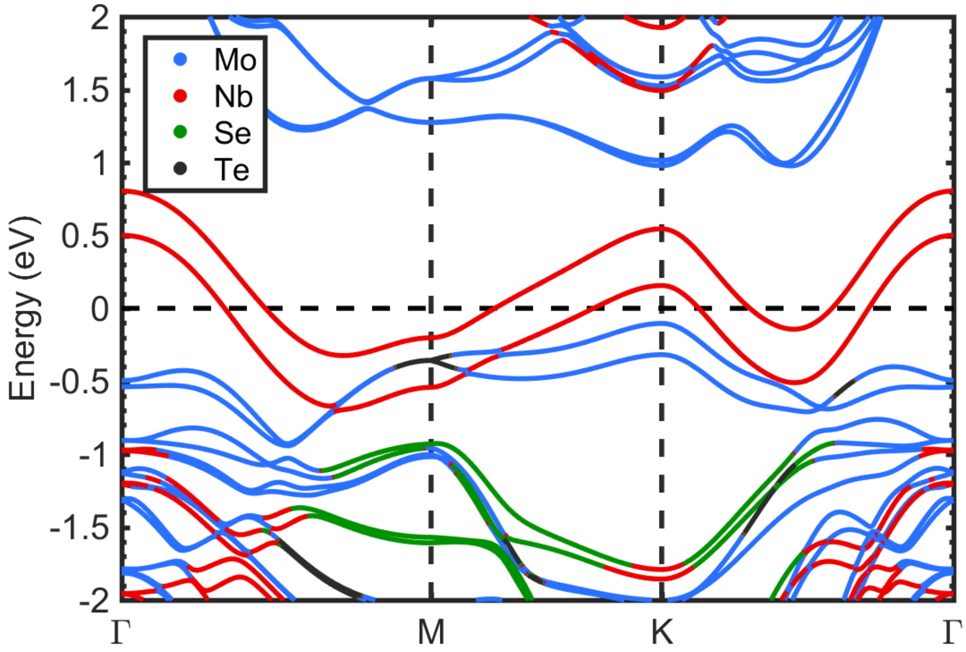


Fig. 12 **Atom-projected band structure of a $MoTe_2$-$TaSe_2$ heterostructure using ADFT-VEX**

Table 3 **Effective masses of an isolated monolayer $MoTe_2$ and that of a $NbSe_2$-$MoTe_2$ heterostructure calculated using ADFT-VEX**

Material	Valence Band		Conduction Band	
	m^*_l	m^*_t	m^*_l	m^*_t
$MoTe_2$	0.6333	0.6332	0.5394	0.5381
$NbSe_2$-$MoTe_2$	0.6670	0.6661	0.8484	0.6989
% change	5.32	5.19	57.29	29.88

5.3.3.1 Generate k-Points

In this mode, ADFT-VEX identifies the minima and maxima contributed from the material that is provided by the user. From the minima or maxima, ADFT-VEX generates k-points along the longitudinal and transverse direction within the threshold provided by the user.

5.3.3.2 Calculate Effective Mass

In this mode, ADFT-VEX reads the calculation output done for KPOINTS provided by the earlier mode and calculates the effective mass. For example, the calculated effective masses for the $MoTe_2$-$TaSe_2$ are tabulated in Table 3. The functionality of this mode is similar to the accurate calculation. In this case, ADFT-VEX calculates the effective mass for the band contributed by the material provided by the user.

6. Conclusion

In summary, we have created a modular tool for visualization and parameter extraction from DFT calculations. ADFT-VEX can visualize data generated by a DFT tool. The tool supports the visualization of band structure, projected band structure, and density of states. In terms of parameter extraction, the tool can calculate the effective mass from the band structure data of the given material. This can be done in a generic way from a band structure and also in a more precise way by performing a separate calculation. For such a precise calculation of effective mass, the necessary input files can be generated using ADFT-VEX. Furthermore, the effective mass of both homogenous and heterogeneous material systems can be calculated using this tool. In summary, at this point, the library supports visualization and parameter extraction from only VASP calculations. However, due to the modular nature of the tool, it can be easily ported and extended to be applicable to other DFT tools.

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Appendix. Installation, Sample Run and Code Snippets[*]

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[*] DFT-VEX in this appendix refers to ADFT-VEX.

A.1 Installation

The installation of the Automated Density Functional Theory–based Parameter Visualization and Extraction (ADFT-VEX) tool is trivial. The user needs to extract the package in a convenient directory and then add the directory to the path. Version-specific instruction for adding a directory to the MATLAB path can be found here: https://www.mathworks.com/help/matlab/ref/addpath.html. Adding the folder to the path ensures that the top-level script DFT_VEX.m and other required scripts are accessible to MATLAB.

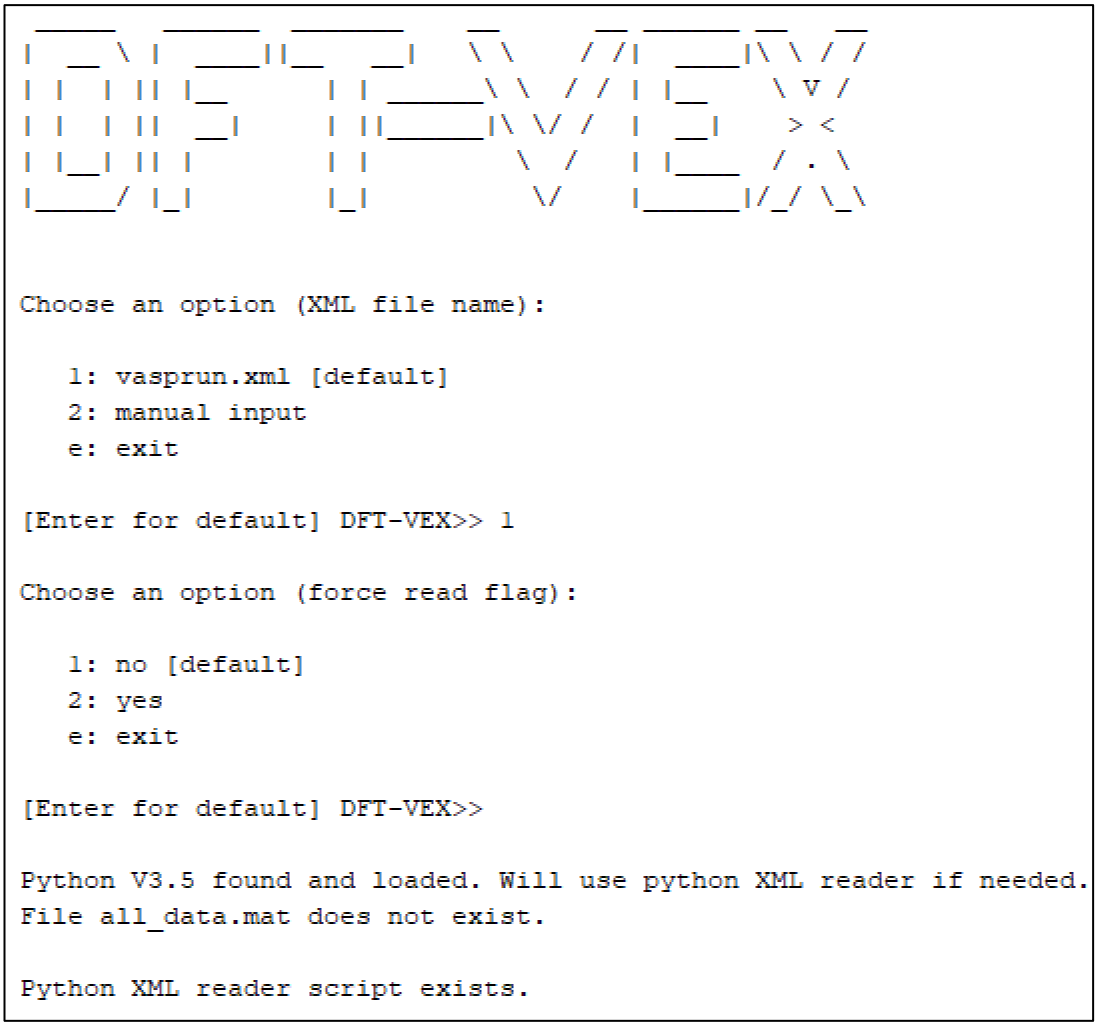
For visualization, the user needs to change the current directory to the directory where the XML file is located and run the DFT_VEX.m script. Running DFT_VEX.m executes the text-based menu as implemented within ADFT-VEX. At the beginning of execution, ADFT-VEX tries to determine whether a Python version is available or not. If a Python version is available, then ADFT-VEX uses Python to read the XML file. When a Python environment is unavailable, ADFT-VEX uses the default XML reader provided by MATLAB. The caveat of using the default XML reader is that it fails for a large atomic structure. This happens because of the memory limitation in MATLAB. In case of such memory limitation, the user needs to install a Python environment that is accessible to MATLAB. After installing Python, MATLAB needs to be restarted. After restarting MATLAB, the command “pyversion” can be used to determine whether the Python environment is available to MATLAB or not.

During the execution of the text-based menu, the user is asked various questions to determine the visualization or parameter extraction. An impatient user can use the ModularVaspXML.m script to manually modify the input parameters for the visualization or parameter extraction. The script contains input parameters that are accepted by ADFT-VEX with detailed documentation of each option.

A.2 Text-based Menu

ADFT-VEX can be executed using a text-based menu and as a stand-alone script. The text-based menu gives the user a way to interact with the program without modifying the script. On the other hand, the stand-alone script can be used to plot the data without providing inputs one by one.

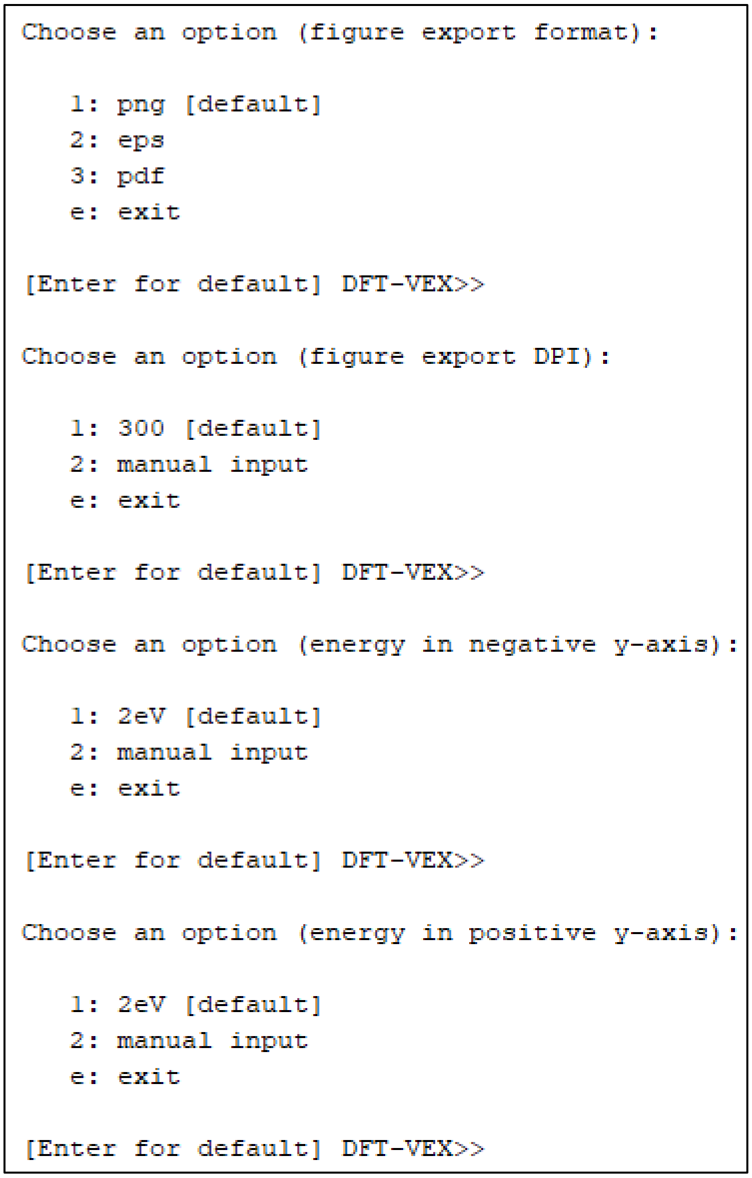
Executing the ADFT-VEX script runs the text-based menu. For each mode within ADFT-VEX, the menu shows the available options. For each option, a default value is shown. If the user does not input a value, then the default value is used. For example, Fig. A-1 shows a screenshot of the main menu. First, the name of the XML file can be specified if the name is different. If no input is provided, the default name “vasprun.xml” is assumed. For the second option, the user specifies whether to force-read the XML file or to use the caching feature of the ADFT-VEX.



```
 _____   ______  _______    __      __ ______ __   __
|  __ \ |  ____||__   __|   \ \    / /|  ____|\ \ / /
| |  | || |__      | | ______\ \  / / | |__    \ V /
| |  | ||  __|     | ||______|\ \/ /  |  __|    > <
| |__| || |        | |         \  /   | |____  / . \
|_____/ |_|        |_|          \/    |______|/_/ \_\


Choose an option (XML file name):

   1: vasprun.xml [default]
   2: manual input
   e: exit

[Enter for default] DFT-VEX>> 1

Choose an option (force read flag):

   1: no [default]
   2: yes
   e: exit

[Enter for default] DFT-VEX>>

Python V3.5 found and loaded. Will use python XML reader if needed.
File all_data.mat does not exist.

Python XML reader script exists.
```

Fig. A-1 Main menu of ADFT-VEX

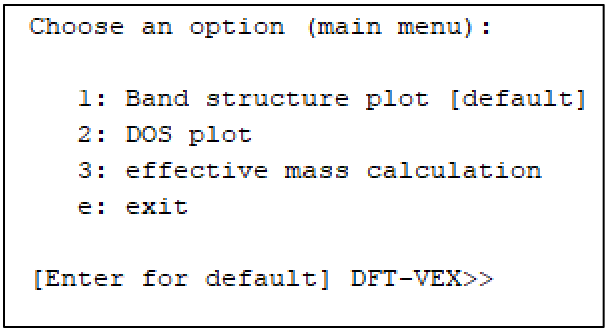
Figure A-2 shows common options within the menu. From this menu, the user can define the aesthetics of the figure, such as the output format of the visualization, the resolution of the visualized plots, and the energy range for the property that is visualized.



```
Choose an option (figure export format):

   1: png [default]
   2: eps
   3: pdf
   e: exit

[Enter for default] DFT-VEX>>

Choose an option (figure export DPI):

   1: 300 [default]
   2: manual input
   e: exit

[Enter for default] DFT-VEX>>

Choose an option (energy in negative y-axis):

   1: 2eV [default]
   2: manual input
   e: exit

[Enter for default] DFT-VEX>>

Choose an option (energy in positive y-axis):

   1: 2eV [default]
   2: manual input
   e: exit

[Enter for default] DFT-VEX>>
```

Fig. A-2 Common menu options within ADFT-VEX

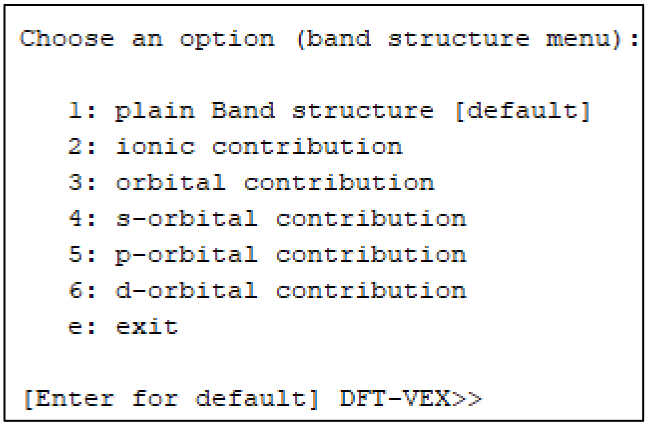
Figure A-3 shows the main menu options.



```
Choose an option (main menu):

   1: Band structure plot [default]
   2: DOS plot
   3: effective mass calculation
   e: exit

[Enter for default] DFT-VEX>>
```

Fig. A-3 Main menu options of ADFT-VEX

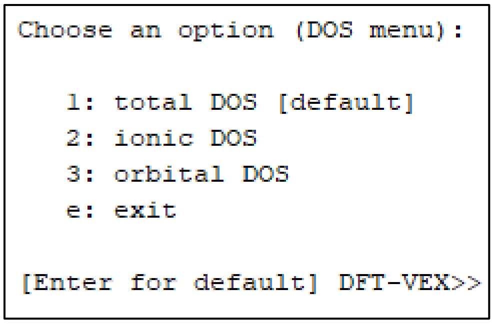
For the band structure mode, Fig. A-4 shows the options provided in the menu.



```
Choose an option (band structure menu):

   1: plain Band structure [default]
   2: ionic contribution
   3: orbital contribution
   4: s-orbital contribution
   5: p-orbital contribution
   6: d-orbital contribution
   e: exit

[Enter for default] DFT-VEX>>
```

Fig. A-4 Band structure plotting menu of ADFT-VEX

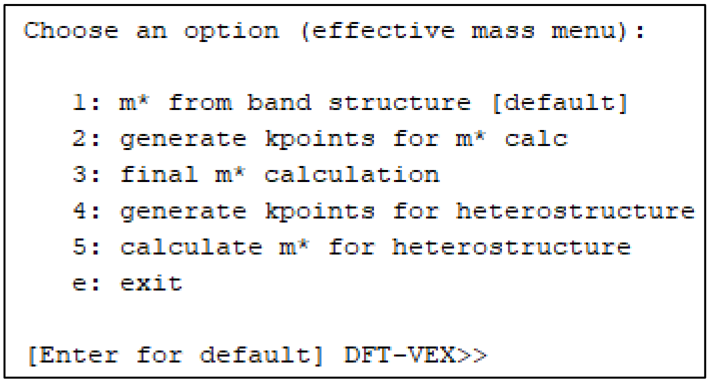
Figure A-5 shows the density of states (DOS) menu as designed in ADFT-VEX.



```
Choose an option (DOS menu):

   1: total DOS [default]
   2: ionic DOS
   3: orbital DOS
   e: exit

[Enter for default] DFT-VEX>>
```

Fig. A-5 DOS menu within ADFT-VEX

The effective mass calculation menu is shown in Fig. A-6.



```
Choose an option (effective mass menu):

   1: m* from band structure [default]
   2: generate kpoints for m* calc
   3: final m* calculation
   4: generate kpoints for heterostructure
   5: calculate m* for heterostructure
   e: exit

[Enter for default] DFT-VEX>>
```

Fig. A-6 Effective mass menu within ADFT-VEX

A.3 The Code

In this section, several important aspects within ADFT-VEX are discussed. For example, Fig. A-7 shows a function that is used to choose between Python or MATLAB to read and extract the data. In this function, Python is used to read the XML data. If it fails, then the MATLAB reader is used.

Figures A-8 and A-9 show the orbital sum calculation done for plotting the orbital-projected band structure. In Fig. A-8, the contribution of s, p, and d orbitals is summed to the orbital_data matrix. In Fig. A-9, the contribution of individual s, p, and d orbital data is stored in individual matrices. Figure A-10 shows the calculation process of effective mass given the degree of the polynomial for the fitting. The dispersion at minima or maxima is fitted to a polynomial whose degree is provided by user.

```
function python_or_matlab(xml_file, mat_file, FORCE_READ)
% PYTHON_OR_MATLAB Determines whether to use python or Matlab to read
% the XML file.
%
% Tries to determine whether python is loaded or not.
% If loaded, tries to use python.
% If fails, uses Matlab to read the XML file.

python_v = 2.7;

[version, ~, ~] = pyversion;

if str2double(version)> python_v %&& isloaded
    fprintf(' Python V%s found and loaded. Will use python XML reader if
needed.\n', version);
    MATLAB_flag=false;
else
    fprintf(' Working python not found.\n Using Matlab''s xml reader. It
might take some time.\n')
    MATLAB_flag=true;
end

if FORCE_READ
    READ_FLAG = true;
else
    READ_FLAG = readOrNOT(xml_file, mat_file);
end

% mat_fullpath = fullfile(cd, mat_file);
xml_fullpath = fullfile(cd, xml_file);

if READ_FLAG

    fprintf('\n')

    if MATLAB_flag
        XMLReadMatlab(xml_fullpath)
    else
        try
            [script_path,~,~]=fileparts(mfilename('fullpath'));
            readFromPython(script_path, xml_file);
        catch
            warning('Reading from python failed. Using Matlab XML reader.');
            XMLReadMatlab(xml_fullpath)
        end

    end
else
    fprintf(' Reading from mat file %s.\n', mat_file);
end

end
```

Fig. A-7 Deciding whether to use Python or MATLAB for data collection

```
orbital_data=zeros(sp_spin, nokpoints, bands, ions_no,3);
for is=1:sp_spin
for ik=1:nokpoints
for ib=1:bands
for io=1:orbital_length
    if spd_flag(io)==1
        orbital_data(is, ik, ib, :, 1) = orbital_data(is, ik,ib,:, 1) +
procar_data(ik,ib,is,:, io);
    elseif spd_flag(io)==2
        orbital_data(is, ik, ib, :, 2) = orbital_data(is, ik,ib,:, 2) +
procar_data(ik,ib,is,:, io);
    elseif spd_flag(io)==3
        orbital_data(is, ik, ib, :, 3) = orbital_data(is, ik,ib,:, 3) +
procar_data(ik,ib,is,:, io);
    else
        error('Something is wrong.');
    end
end
end
end
end
```

Fig. A-8 Orbital data sum for orbital-projected bad structure plot

```
s_contribution=zeros(sp_spin,nokpoints,bands,ions_no);
p_contribution=zeros(sp_spin,nokpoints,bands,ions_no);
d_contribution=zeros(sp_spin,nokpoints,bands,ions_no);
ion_data=zeros(sp_spin,nokpoints,bands,ions_no);
Total_Orbital=zeros(sp_spin,nokpoints,bands,final_orbital_no);
grand_sum=zeros(sp_spin,nokpoints, bands);

for is=1:sp_spin
for ik=1:nokpoints
for ib=1:bands
   ssum=sum(orbital_data(is,ik,ib,:,1));
   psum=sum(orbital_data(is,ik,ib,:,2));
   dsum=sum(orbital_data(is,ik,ib,:,3));

   sum1=ssum+psum+dsum;

    s_contribution(is,ik,ib,:) = orbital_data(is,ik,ib,:,1)/ssum;

    p_contribution(is,ik,ib,:) = orbital_data(is,ik,ib,:,2)/psum;

    d_contribution(is,ik,ib,:) = orbital_data(is,ik,ib,:,3)/dsum;

    for ii=1:ions_no
        sum2(ii)=sum(orbital_data(is,ik,ib,ii,:));

grand_sum(is,ik,ib)=grand_sum(is,ik,ib)+sum(orbital_data(is,ik,ib,ii,:));
    end

    ion_data(is,ik,ib,:) = sum2./sum1;

    Total_Orbital(is,ik,ib,1) = ssum/sum1;
    Total_Orbital(is,ik,ib,2) = psum/sum1;
    Total_Orbital(is,ik,ib,3) = dsum/sum1;
end
end
end
```

Fig. A-9 s, p, and d orbital sum for orbital-projected ADFT-VEX

```
        for id=1:length(degree)

        deg = degree(id);

        poly_terms(is,band_ind, direction_ind, id,1:deg+1) =
polyfit(this_kpath, this_band, deg);

        mstar(is, band_ind, direction_ind, id) = ...
            hbarc * hbarc /2/mcsq/poly_terms(is, band_ind, direction_ind, id,
deg-1);

        fprintf('\tUsing polynomial of order %d: %0.4f\n',...
            deg, mstar(is, band_ind, direction_ind, id));

        if id == length(degree)
            fprintf('\n\n');
        end

        end
```

Fig. A-10 Effective mass calculation using ADFT-VEX

List of Symbols, Abbreviations, and Acronyms

ADFT-VEX	Automated Density Functional Theory–based Parameter Visualization and Extraction
BZ	Brillouin zone
DFT	density functional theory
DOS	density of states
HSE	Heyd–Scuseria–Ernzerhof
IBZ	irreducible Brillouin zone
kT	room temperature thermal energy
m*	effective mass
SOC	spin orbit coupling

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