**Vaspy-vis**

**a Three-dimensional Visualization package for VASP output files**

**Leszek Nowakowski**

*Faculty Of Chemistry, Jagiellonian University,*

*Gronostajowa 2, 30-387, Cracow*

*Jagiellonian University, Doctoral School of Exact and Natural Sciences,*

*Prof. St. Łojasiewicza St 11, PL30348, Cracow, Poland*

Spis treści

[1. LICENSE AGREEMENT 3](#_Toc201058400)

[2. INTRODUCTION AND BACKGROUND 3](#_Toc201058401)

[2.1. Motivation 3](#_Toc201058402)

[2.2. AS **Błąd! Nie zdefiniowano zakładki.**](#_Toc201058403)

[2.3. FGFG **Błąd! Nie zdefiniowano zakładki.**](#_Toc201058404)

[3. OVERVIEW OF THE PROGRAM 3](#_Toc201058405)

[3.1. General features 3](#_Toc201058406)

[3.2. Visualization of structural models 3](#_Toc201058407)

[3.3. Visualization of Volumetric Data 4](#_Toc201058408)

[3.4. DOS plot visualization 4](#_Toc201058409)

[3.5. Calculation convergence monitoring 4](#_Toc201058410)

[3.6. Programming 4](#_Toc201058411)

[4. REQUIRMENTS 5](#_Toc201058412)

[5. MAIN WINDOW 5](#_Toc201058413)

[5.1. Composition 5](#_Toc201058414)

[5.2. Menus 5](#_Toc201058415)

[5.2.1. File Menu 5](#_Toc201058416)

[5.2.2. Edit Menu 6](#_Toc201058417)

[5.2.3. Modify Menu 6](#_Toc201058418)

[5.2.4. View Menu 6](#_Toc201058419)

[5.3. Toolbar 6](#_Toc201058420)

[6. VISUALISING STRUCTURES 7](#_Toc201058421)

[6.1. Interactor 7](#_Toc201058422)

[6.1.1. Composition 7](#_Toc201058423)

[7. GRID DATA 13](#_Toc201058424)

[8. DOS PLOTS 14](#_Toc201058425)

# LICENSE AGREEMENT

# INTRODUCTION AND BACKGROUND

## Motivation

Modeling the electronic properties materials requires, among other tasks, visualizing density-of-states (DOS) plots and directly manipulating crystal structures within VASP output files. It is also necessary to monitor calculation progress with ease. The development of this software is crucial for fast and efficient interpretation of complex simulation data, enabling researchers to make informed decisions during ongoing calculations and to explore electronic structures interactively. Existing tools often require switching between multiple applications or involve steep learning curves, which hinders workflow efficiency. By integrating DOS analysis, structural visualization, and calculation monitoring into a unified, user-friendly interface tailored to the specific needs of catalytic materials research, this software will significantly accelerate data analysis, reduce errors, and support high-throughput computational workflows.

# OVERVIEW OF THE PROGRAM

## General features

Vaspy-vis is a simple visualization program for 3D-periodic structural models, volumetric data and Density of States data produced by a computational package VASP. Primarly aim of this software is to provide fast and easy-to-use tool to visualize 3D atomic structure and monitor various quantity during geometry optimization calculation run by VASP.

## Visualization of structural models

3D-periodic models, as read from VASP files such as CONTCAR and POSCAR, can be read and displayed on the screen, together with a table with atoms cartesian coordinates, magnetic moments and movement constraints. These quantities can be easily changed and saved into VASP formats files, which – in case of movement cosntraints especially – is first seen within VASP visualization software. Atoms can be added, moved and deleted.

## Visualization of Volumetric Data

Vaspy-vis is cabaple of visualizing VASP volumetric data, including CHGCAR, CHG and PARCHG files. Charge density can be easily converted to alpha-, beta- and spin-density within one click and only one file loading, which previously WYMAGAŁO many separate tools.

## DOS plot visualization

Projected Density of states plots of spin-polarized calculations can be visualized and interactively manipulated, plotted and exported into various formats

## Calculation convergence monitoring

Geometric optimization Energy plot, together with each step SCF energy and atom movements can be visualized to verify the correctness of the ongoing calculation.

## Programming

Vaspy-vis GUI part is based on PyQt5 python package and VTK visualization toolkit to render 3D structures. Atomic Simulation Environment is employed also.

# REQUIRMENTS

# MAIN WINDOW

## Composition

Obraz zawierający tekst, zrzut ekranu, numer, oprogramowanie

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 5.1:** Main Window of Vaspy-vis.

Figure 5.1 shows the main window of Vaspy-vis running on Windows 11 right after opening a file. Main window is based on several parts:

1. Title bar: with version and opened file path up to 6 directories up
2. Menu bar: *File*, *Edit*, *Modify* and *View* menus are present here
3. Toolbar: Frequently used tools (see XXXXX)
4. Visualization area: an area in main window where plots and structures are displayed and interactively manipulated. Area can be resized horizontally using splitter between Visualization area and Manipulation area. See XXXXX
5. Manipulation area – an area in main window where most of the buttons, boxes and tables are placed in order to manipulate the data (see XXXXX)

## Menus

### File Menu

* **New** – does nothing right now, soon to be developed
* **Open** – Choose a directory with VASP files to open
* **Save** – does nothing right now, soon to be developed
* **Quit –** does nothing right now, soon to be developed

### Edit Menu

* **Copy** – copies to clipboard the data of the selected atoms: symbol, number, position, constraints and magnetic moments as listed in Structure Table (see XXXX )
* **Cut** – does nothing right now, soon to be developed
* **Paste** – does nothing right now, soon to be developed

### Modify Menu

* **Modify constraints** – this menu will open a window, where user can create an ICONST file with bonds or angles between selected atoms freezed (see VASP ICONST)
* **Move Atoms** -this menu will open a window with a buttons to translate or rotate the selected atoms

### View Menu

#### Actors

* **Clear Bonds** – this menu will clear all bond distances in the view area.

## Toolbar

The Toolbar consist of many useful tools for manipulating the atoms:

Obraz zawierający zrzut ekranu, krąg, Grafika, Wielobarwność

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms to the right

Obraz zawierający zrzut ekranu, krąg, Grafika, Wielobarwność

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms to the left

Obraz zawierający Grafika, krąg, Wielobarwność, zrzut ekranu

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms down

Obraz zawierający Grafika, krąg, Wielobarwność, zrzut ekranu

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms up

Obraz zawierający krąg, Wielobarwność, Grafika

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms out of screen

Obraz zawierający symbol, krąg, Grafika, Wielobarwność

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. move selected atoms into the screen

Obraz zawierający symbol, krąg, kreatywność

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. add atoms

Obraz zawierający krąg, zrzut ekranu, Grafika, Wielobarwność

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. remove selected atoms

Obraz zawierający kula, krąg

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna. add bond length between two selected atoms

# VISUALISING STRUCTURES

## Interactor

### Composition

An interactor is a place where the 3D structure is rendered and its composition is shown on **Figure 6.1**. You can choose the Interactor by clicking on “Structure” tab. On the top of the Interactor there is a tip regarding selection an atoms (see XXXX). In the top-right corner there is an orientation widget.

Obraz zawierający tekst, zrzut ekranu, wzór, design

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 6.1**. Composition of Structure visualizer tab (an interactor)

### Structure tab

Structure tab is a tab where Interactor is rendering the scene. The tab can be deattached both by double clicking or by drag and drop and float around the screen, as shown in the Figure 6.2. Closing the floating window will attach the tab again to the main window.

Obraz zawierający tekst, oprogramowanie, Ikona komputerowa, Oprogramowanie multimedialne

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

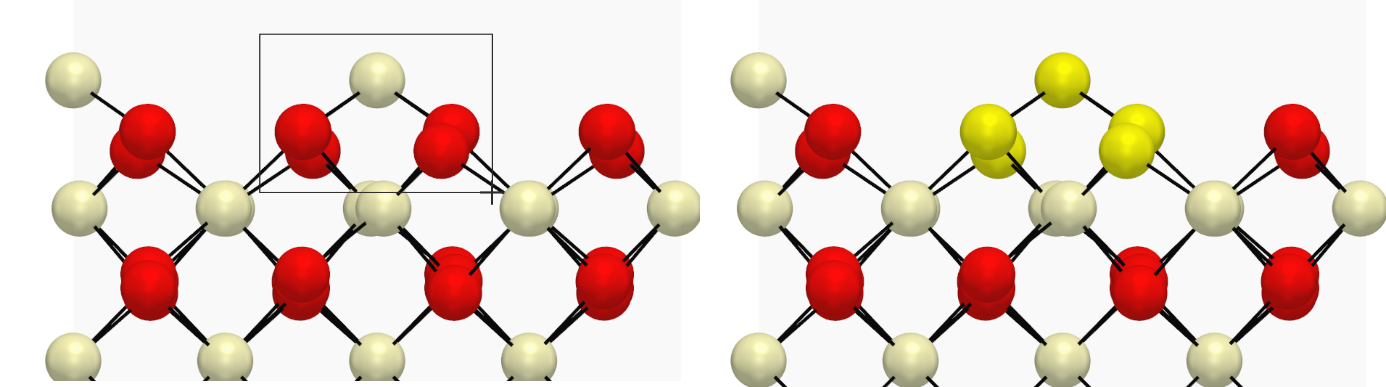
**Figure 6.2**. Deattached Structure tab.

### Selection

The tip on the top of the screen will remind us that the selection tool can be switched on by clicking ‘r’ key on the keybord. The cursor will change its shape to cross-hair: ╋ indicating that the selection tool is switched on. Do perform the selection, one have to move the mouse with left click down. An rectangle will be shown on the screen, as shown in **Figure 6.3**.

Only the atoms which **center** is within the selection rectangle will be selected! When selected, atoms will appear yellow. If You want to select more atoms, just draw another rectangle. To remove atoms from selection, one can click on atom in the Structure Variables Control tab (see XXXX), or just draw again an rectangle on selected atoms that should be deselected. To clear the selection, draw a rectangle with no atom inside.

“R” button should be pressed again to deactivate the selection tool and fall back to interaction style.



**Figure 6.3.** A selection tool at work.

### Orientation widget

Orientation widget is placed at the top-right corner of the Interactor. Its main job is to show the directions of the cartesian coordinates.

**WARNING! It does not work properly with non-orthogonal unit cell basis.**

If mouse is hovered over one of the axis letter on Orientation widget, the letter will change color to white and when clicked, it will position the camera within that axis.

### Rendering area

The main area of Interactor is rendering area. These names can be used interchangeably. The interactor is responsible for rendering and interacting with the scene. The interactions can be triggered by:

* Scroll down – zoom out
* Scroll up – zoom in
* RMB + move up – zoom in
* RMB + move down – zoom out
* LMB – rotate
* “X” key – align camera with x-axis
* “Y” key – align camera with y-axis
* “Z” key – align camera with z-axis
* “R” – toggle selection tool

## Structure Plot Control tab

### Visualization part

Structure Plot Control tab is located in the manipulation area and has several useful features for controlling the visuals.Obraz zawierający tekst, oprogramowanie, zrzut ekranu, Ikona komputerowa

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

Figure 6.4. Composition of visual part of Structure Plot Control tab

In this tab, in the first frame, as written next to checkboxes or sliders, one can:

* Toggle atoms (spheres) on and off
* Toggle bonds on and off
* Toggle unit cell on and off
* Toggle numbers of all atoms (as in the POSCAR file) on and off
* Toggle numbers of atoms between planes on and off (see below)
* Toggle magnetization of atoms (as read from OUTCAR file) on and off
* Show x-axis movement constraint (“T” or “F”, as in the POSCAR) on and off
* Show x-axis movement constraint of atoms between planes on and off
* Change sphere radius with a slider
* Change bond distance rendering threshold

The second frame controls the visualization of specific geometry step during optimization calculation:

* Slider can smoothly change the number of geometric step
* Buttons can move to first, previous, next and last step

If no optimization were calculated, these buttons and slider will have no effect.

Third frame controls the positions and color of the planes. These plane primary job is to “cut-off” atoms out of our interest, mainly these in the bulk part of the slab. Very useful when dealing with slab calculations. These planes can cut-off atoms visually, but also their position affects the numbers, magnetizations and constraints switched on in the first frame.

* Top and bottom plane checkboxes can toggle on and off top and bottom plane
* Range slider can change their position:
  + Click on the left side of the range slider and move to change the bottom plane position
  + Click on the right side of the range slider and move to change the top plane position
  + Click in between (on the green part) of the slider and move to change the position of both planes simultaneously
* Click on a small colorful button to trigger the color picker and change the planes color

### Energy plot part

The last frame on Structure Plot Control tab contains energy plots for geometric optimization. All of the energies up to date collected from OUTCAR file are plotted as a line. Current geometric step (as visualized on Interactor) is shown as little dot on the plot. When we slide through geometries, the position of the dot is moving accordingly. When hovered over a specific point, a green square will appear. When clicked, it will pop up a window with a electronic optimization plot.

Obraz zawierający tekst, zrzut ekranu, diagram, linia

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 6.5** Energy plot frame

The plots are interactive:

* Scroll up and down to zoom in and zoom out with fixed aspect ratio;
* RMB + move to zoom with aspect ratio change
* LMB + move to pan the plot
* Right click for context menu with many useful options, including:
  + Reset view
  + Change x and y axis mode
  + Change mouse mode
  + Many plot options
  + Export plot

## Structure Variables Control tab

### Buttons part

Structure Variables Control tab is responsible for modyfing the structure parameters and selection. It consists several buttons, as shown in **Figure 6.6**. I will describe all of them one by one, from the top-left corner of the tab.

Obraz zawierający tekst, zrzut ekranu, numer, Czcionka

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 6.6**. Structure Variables Control tab

* **“Save Poscar”** button open a window with a file selection to save a POSCAR file. Choose a directory, name and click “save” to save a file in a POSCAR format. A message will be pop up if save was successful, and warning if not.
* **“Delete”** button will delete all selected atoms
* **“T” and “F”** buttons will set X, Y or Z on **all selected atoms** constrain (depending which button You will click) to “T” or “F”
* **“print”** will print all selected atoms numbers to the output
* **“add”** will add to selection all atom number that appear in the input form:

**Obraz zawierający zrzut ekranu, tekst, numer, linia

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.**

**Figure 6.7.** Adding atoms to selection

Please input atom numbers separated by coma as shown in **Figure 6.7**. Otherwise no action will be executed.

* **“print magmoms”** will print **all atoms** magnetic moments (as set in the last column of the table) in the format acceptable by VASP, so You can strictly paste it into INCAR.
* **“set magmom”** will set the magnetization moment for **all selected atoms** with the number provided in the input form. If text in input form is not a number, a warning will be popped up.
* **“sort”**  will sort **all of the atoms** in the alphabetical order, topmost sort is by atom name (first column) and then by atom tag ( third column)
* **“rattle”** will randomly shake the **selected atoms** position
* **“set tags”** will set the tag provided in the input form for **all selected atoms**

### Structural data table widget

Below the buttons structural data table is placed. It contains several columns:

* **Atom** is atom symbol
* **Number** is its current number
* **Tag** can easily diverge the same atoms into different groups and sort them with “sort” button
* **X, Y, Z** are the cartesian coordinates
* **Move X, Move Y, Move Z** are movement constraints
* **MagMom** is the magnetic moment as set in POSCAR or to write to POSCAR.

**!!! It is not the magnetic moment as read from OUTCAR file !!!**

You can easily select/deselect and atom by clicking on the desired row in the table and move mouse up and down.

# GRID DATA

## Overview

VASPy-vis can read and visualize VASP-based volumetric data, such as CHGCAR or PARCHG. The controls are placed in the Crystal Structure -> PARCHG/CHGCAR tab:

Obraz zawierający tekst, Czcionka, linia, numer

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 7.1.** CHGCAR control tab

!! WARNING !! Only spin-polarized data can be processed !!

* **Open CHGCAR** will automatically open a CHGCAR file in the directory where visualized POSCAR is, if CHGCAR exists. When reading a file a progress bar is shown on the screen. If there is no CHGCAR file or when button is pressed again, the file menu will open to choose a volumetric file from.
* **“Total”** will show total charge density isosurfaces
* **“Spin”** will show spin charge density isosurfaces. If no significant spin density is present, a message will be printed to the output.
* **“Alfa”** shows alpha-channel density
* **“Beta”** shows beta-channel density
* **“Clear”** will clear all isosurfaces

The isosurface threshold value can be modified by moving a slider below buttons.

## Flip spin density

A very useful feature was implemented in order to flip the spin density of a CHGCAR file in a particular region. If someone want to change the polarization of a certain region and save it to the CHGCAR file it can be done very easily. In order to do that, click:

* **“Add box”** renders on the screen a parallelopiped box with spheres on a center of each face. The box can be manipulated by:
  + moving white spheres will change the face positions
  + LMB + move on the box can rotate it
  + RMB + move can expand and shrink box (the box edges will appear green)
  + Middle mouse click can move the whole box
* **“remove box”** will remove box from the screen
* **“spin flip”** will change all numbers which corresponds to a volume selected by a box to a opposite value and change the isosurfaces accordingly.
* **“Save CHGCAR”** will open a pop up window with a filename to provide and save the CHGCAR file.

**!!! WARNING !!!**

**Manipulating calculation data can have serious implications. It is not recommended to use such a CHGCAR as a final result of the calculations. ALWAYS use it as an input file to calculations (ICHARG = 1 flag in INCAR).**

Obraz zawierający zrzut ekranu, Wielobarwność, clipart

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

Figure 7.2. Flipping spin density: a box around the adsorbed O2 molecule with the majority of alpha spin (a) and the same box with flipped spin density.

# DOS PLOTS

Originally, VASPy-vis was created in order to plot the density of state data (DOSCAR file). Already existing GUI tools are really stubborn, hence there was need to create easy-to-use tool to deal with DOS plots. This can be done with DOS tab on Visualizer section and DOS parameter tab on Manipulation section.

!!! WARNING !!!

Only spin-polarized, site- and orbital-projected DOS can be analyzed

Obraz zawierający tekst, zrzut ekranu, oprogramowanie, numer

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

Figure 8.1. DOS plot manipulation panels

In the Figure 8.1 You can see a DOS manipulation panels when no atoms are selected. On the left, there are two plots. The underlying logic of these will be described later. On the right side You will find three frames:

* Atoms frame
* Orbitals frame
* Utility frame

## Atoms frame

Atoms frame contain scrollable area with checkboxes. Each of them represents an atom from POSCAR file, before every manipulation in their order (like “sort” button), just like read from file. Atoms are represented as atomic symbol and a number, like in the Structure Data Table. You can click on the checkbox to select atom to see the DOS plot, but at least one orbital checkboxe have to be selected as well to see a plot.

## Orbitals frame

Orbitals frame contain checkboxes with all of the orbitals present in the system. Click on the checkbox to select the orbitals. Atom checkbox have to be selected as well to see the plot.

!!! WARNING !!!

Selecting many atoms and orbitals can have serious consequences in terms of robustness of plotting. For example, selectin 20 atoms to plot all *d*-orbitals will result in plotting 100 lines, which is not only useless in case of interpreting data, but also very demanding computationally

## Utilities frame

Last frame contain useful button for manipulating the selection and plots. The topmost group of button can select/deselect whole set of orbitals. If clicked, all orbitals of current type will be selected or deselected, e.g. all *p* orbitals, all *d* orbitals etc.

Next group will select/deselect a set of similar atoms, based on their name. You can also select/deselect all atoms.

The last group can manipulate the plots in a different way. For example, if You want to look at all oxygen atoms p-orbitals DOS plot, simply selecting all O atoms and all p orbitals will result a way to many plots.

!!! WARNING !!!

Selecting many atoms and orbitals can have serious consequences in terms of robustness of plotting. For example, selectin 20 atoms to plot all *d*-orbitals will result in plotting 100 lines, which is not only useless in case of interpreting data, but also very demanding computationally

That’s why You’ll see a message on the status bar blinking in red that You’ve chosen too many plots to render. A message will be shown at the top of the plotting area as well. In order to plot the data, follow the messages and click the “Plot merged” button.

Explanation of the buttons:

* **Color button** – with colored rectangle – represents the color which will have the merged plot when “Plot merged” button will be clicked. You can click on this button to change the color with color picker. Color will change automatically whenever “Plot merged” button is pressed.
* **“Plot merged”** button will plot all of the selected plots as one plot, with summed data, in the color depicted by the color of the rectangle inside the Color button. If any separated plots are visible, they will vanish and merged into one. If any already merged plots are present, they will still be visible.
* **“total DOS”** will plot the total DOS with blue color. It will vanish every time “Plot merged” is clicked.
* **“Save plots”** will save **last merged plot** to a list. You can view all saved plots with “show saved plots” button
* **“show saved plots”** will show separately all saved plots. It is convenient when comparing the different plots in different regions.
* **“Clear plots”** will clear all of the plots from plotting area.

## Plotting area

Plotting area in full operational mode with all features are showed in **Figure 8.2**.

Obraz zawierający tekst, diagram, linia, Równolegle

Zawartość wygenerowana przez sztuczną inteligencję może być niepoprawna.

**Figure 8.2**. Plotting area in DOS plot widget

On the top of plots there can be a message that data have not been shown due to too many atoms and orbitals selected. It will create a mess in the plotting area if too many plots will be rendered. Also it can heavily affect performance, causing even a crash of the program. To prevent this situation only 10 separate plots can be seen at once. There is no limit of merged plots.

On the left side of plotting area there is a full plot. It shows all the energy scale of the DOS data.