



# VASP Plotter— Electronic Band Structure App

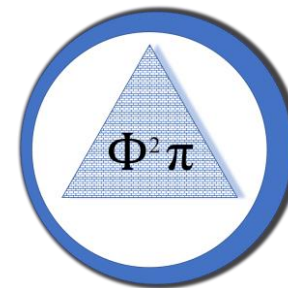
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March 2021

Hamilton ON Canada


$$\Phi^2 \pi$$



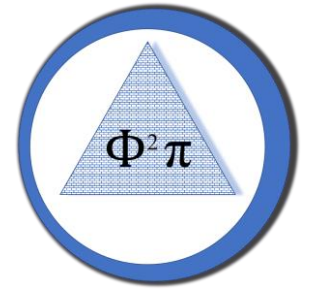
# Introduction

Welcome to the VASP Plotter - Electronic Band Structure App.

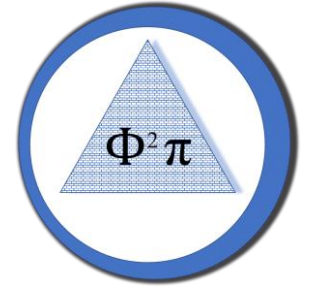
The App is using the electronic band structure calculations from VASP and plot them:

- Electronic band structure including projected density of states (DOS)
- DOS and projected DOS
- Create KPOINTS files for calculations
- Edit your plot and save it with high resolution

# Installation



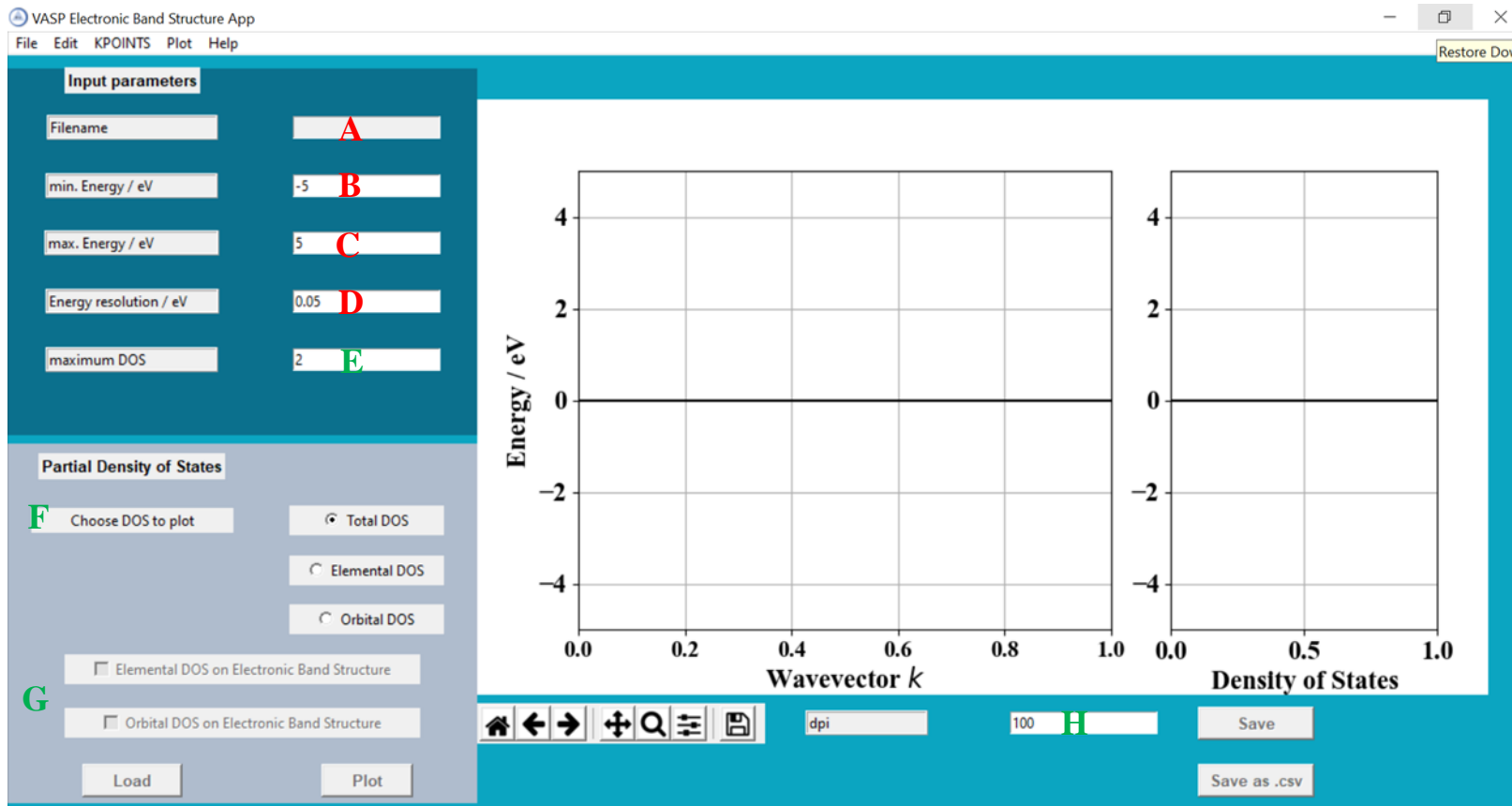
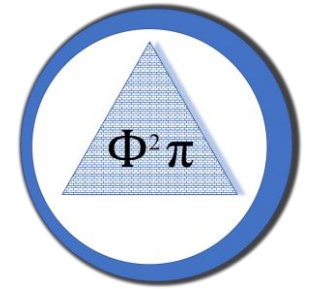
- Download the executable (i.e., VASP\_Plotter.exe), the images (i.e. gb\_line.png, rb\_line.png, rg\_line.png, and rgb\_triangle.png) , and the icon (i.e., icon\_band.ico)
- Create a new folder and move all files in the folder (please note that the default file will be save in the folder as well)
- Please note that the App won't work if all files are not in the same folder than the executable



# Starting the program

- Double-click of the executable and a window will open
- The opening of the App takes some time depending on your processor (no worries if nothing happens for the first minute)

# Start Window – Input Parameters



**A** : Folder name (from File → Open File); disabled

**B** : minimum energy to plot in eV

**C** : maximum energy to plot in eV; maximum must be larger than minimum

**D** : Step size for DOS calculations; Entire Brillouin zone will be summed and place in boxes defined by the step size

**E** : Maximum value of the DOS in Plot

**F** : Choose to plot only the total DOS, or projected DOS (elemental [i.e., for each element] or orbital [i.e., for each orbital])

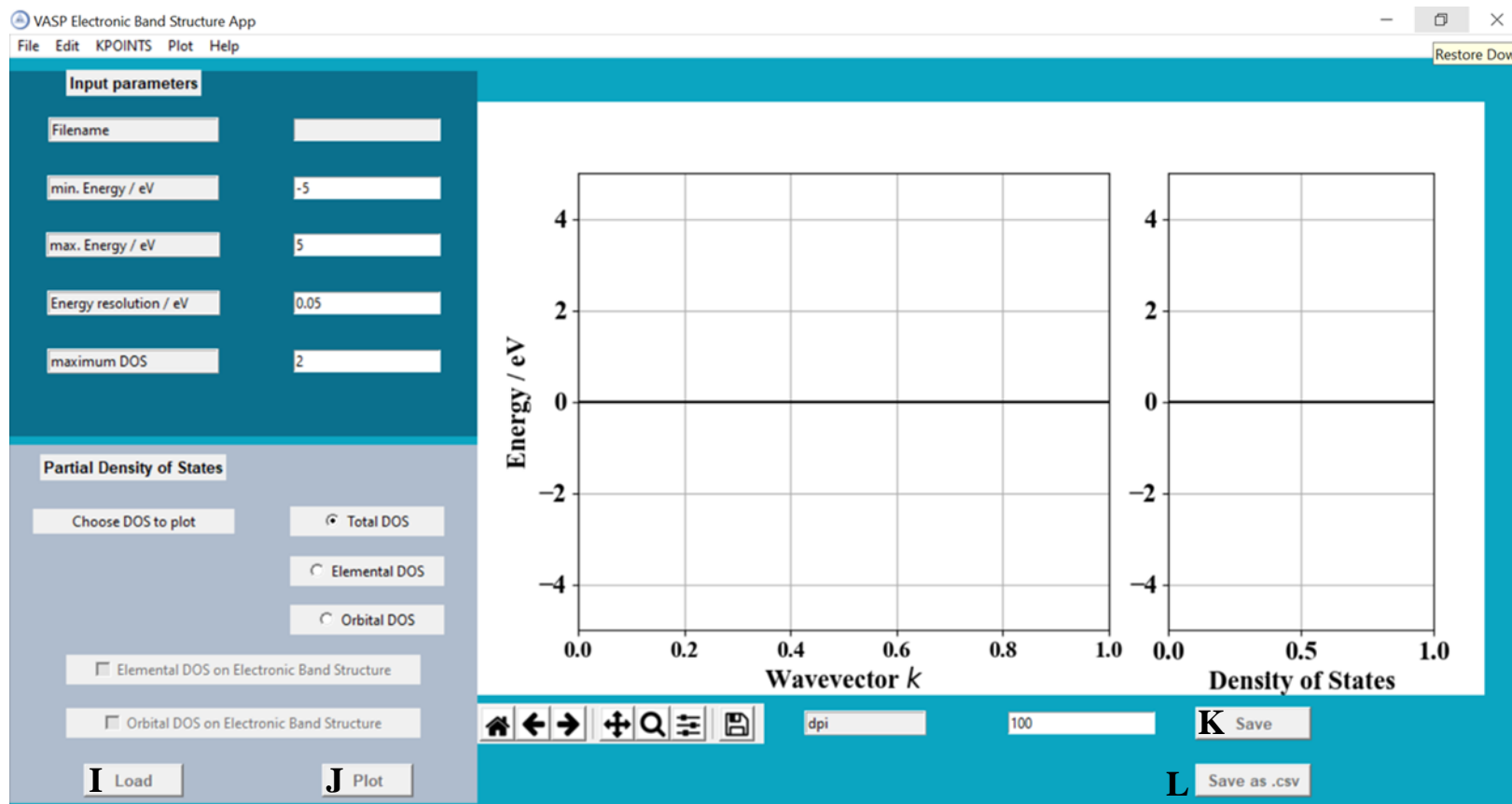
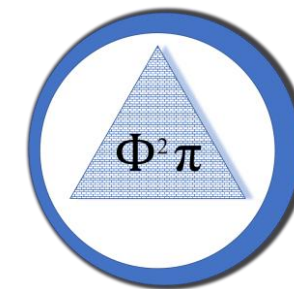
**G** : Include projected DOS (elemental or orbital) to the electronic band structure. This can only be chosen if 2 or 3 elements are in the compound or the compound does not contain *f*-electrons.

**H** : Dots per inch (i.e., resolution) of the figure to save. A good value is between 600-800 dpi. (100 dpi is used for the figures on the plot in the program)

**Red:** if fields in red are changed, you need to reload (Load button at the bottom) the data.

**Green:** You can change these fields without reloading the data; just press Plot.

# Start Window – Buttons



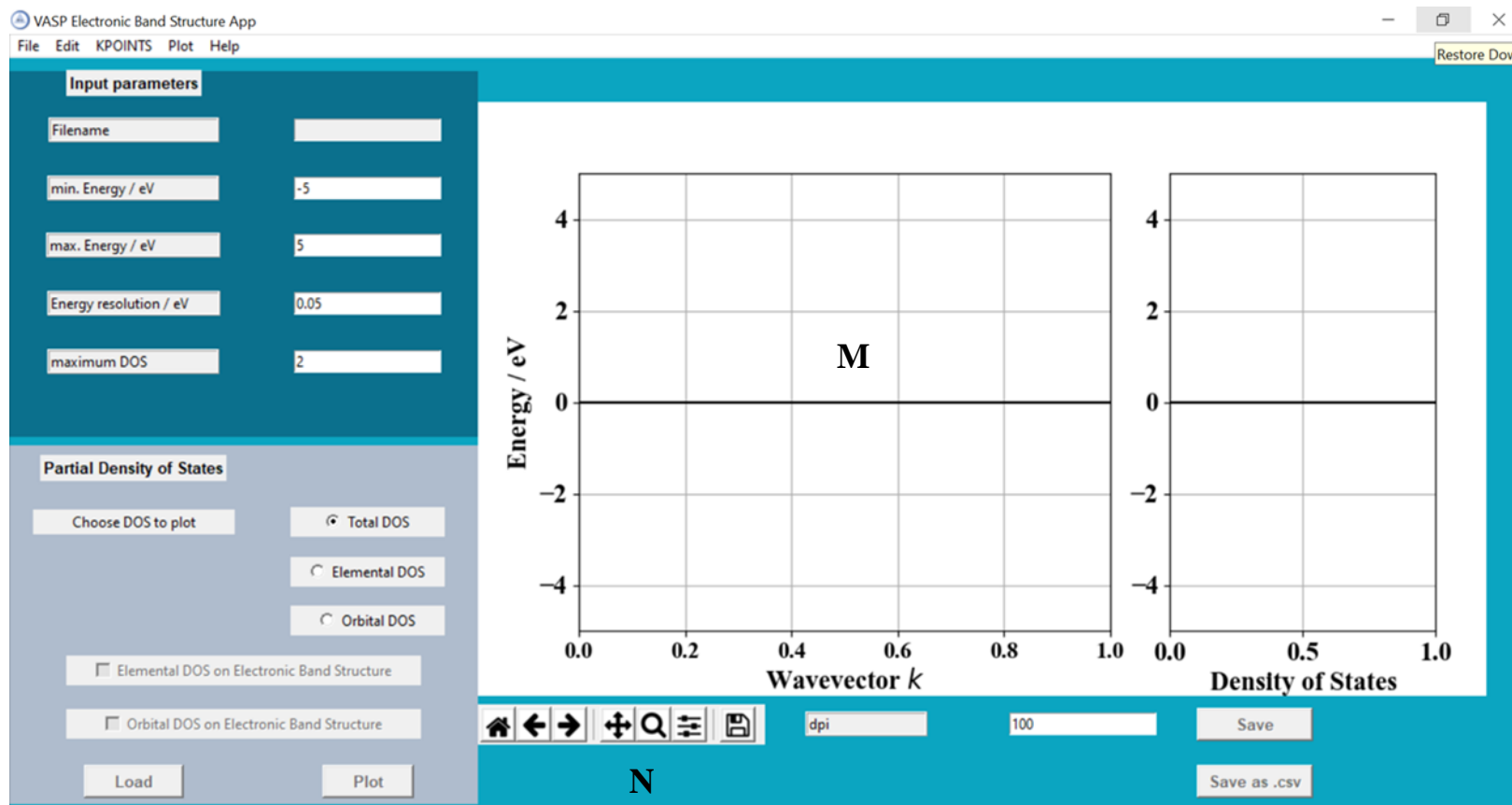
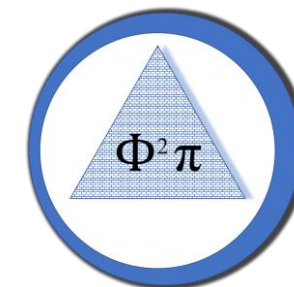
**I** : Load button loads the data and computes the DOS and projected DOS. This process can take several minutes. Button is enabled when a file is opened (File → Open File)

**J** : Plot button plots figure; is enabled when the data is loaded

**K** : Save the figure with the dpi chosen in H; is enabled when a figure was plotted

**L** : Save the data as two files \*\_DOS.csv has the projected and total DOS; \*\_Band.csv has the ticks, k-points (between 0 and 1), energy in eV and bands

# Start Window – Plot



**M : Plot (left: band structure; right: DOS)**

**N : (from left to right)**

**House : Original Plot**

**Arrow left : Go to last step (if you zoomed in)**

**Arrow right : Go one step forward (if you went back)**

**Cross : Left-click → move axes**

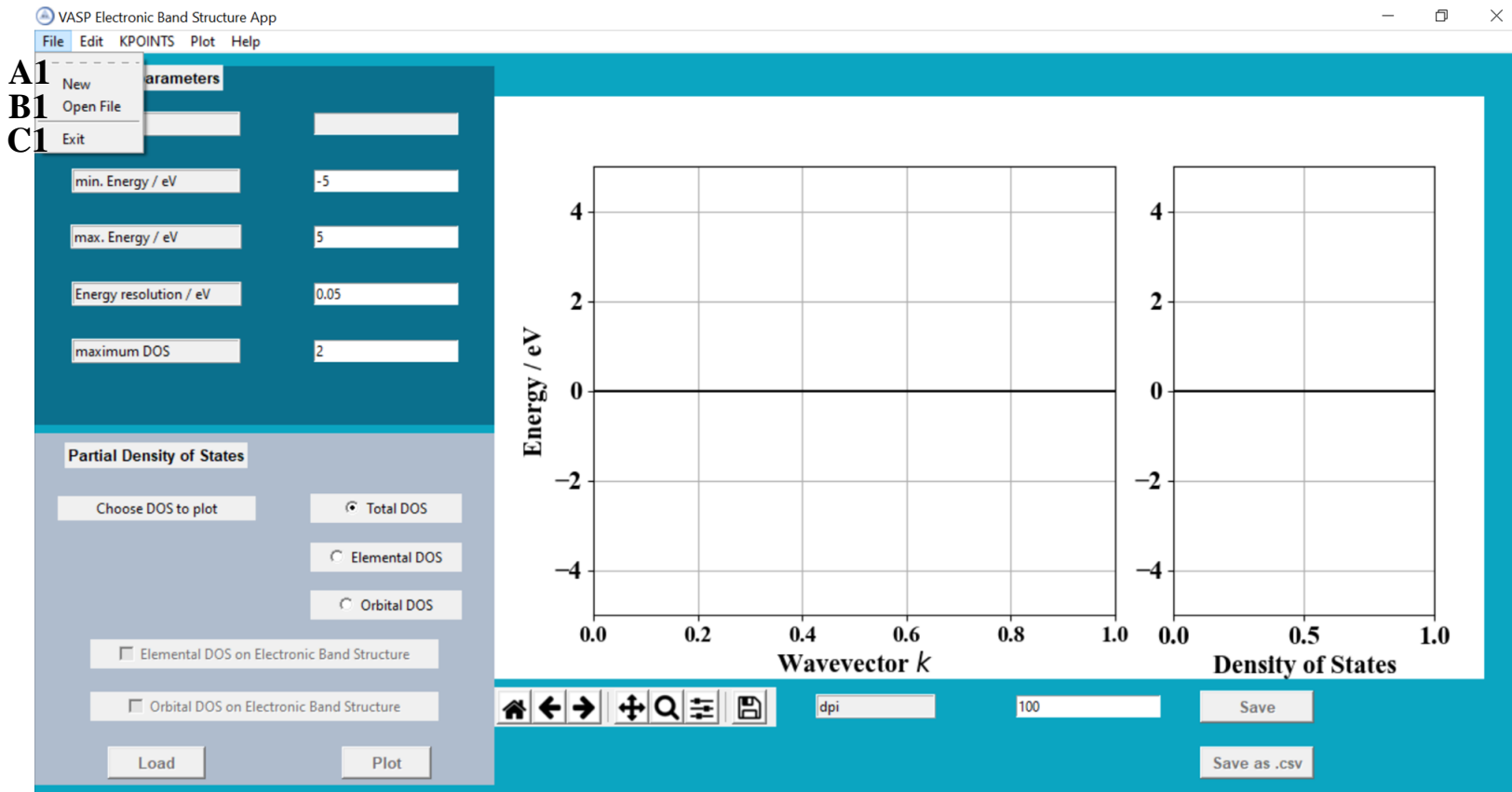
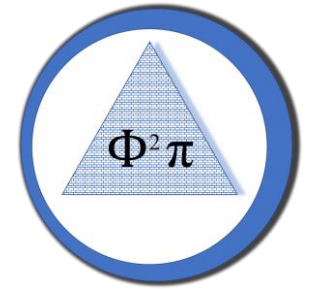
**Right-click → zoom in**

**Magnifying glass : Zoom in**

**Shifters : No effect**

**Disk : Save the plot**

# File Menu



## A1 : New

- Clean Plot
- Remove all data

## B1: Open File

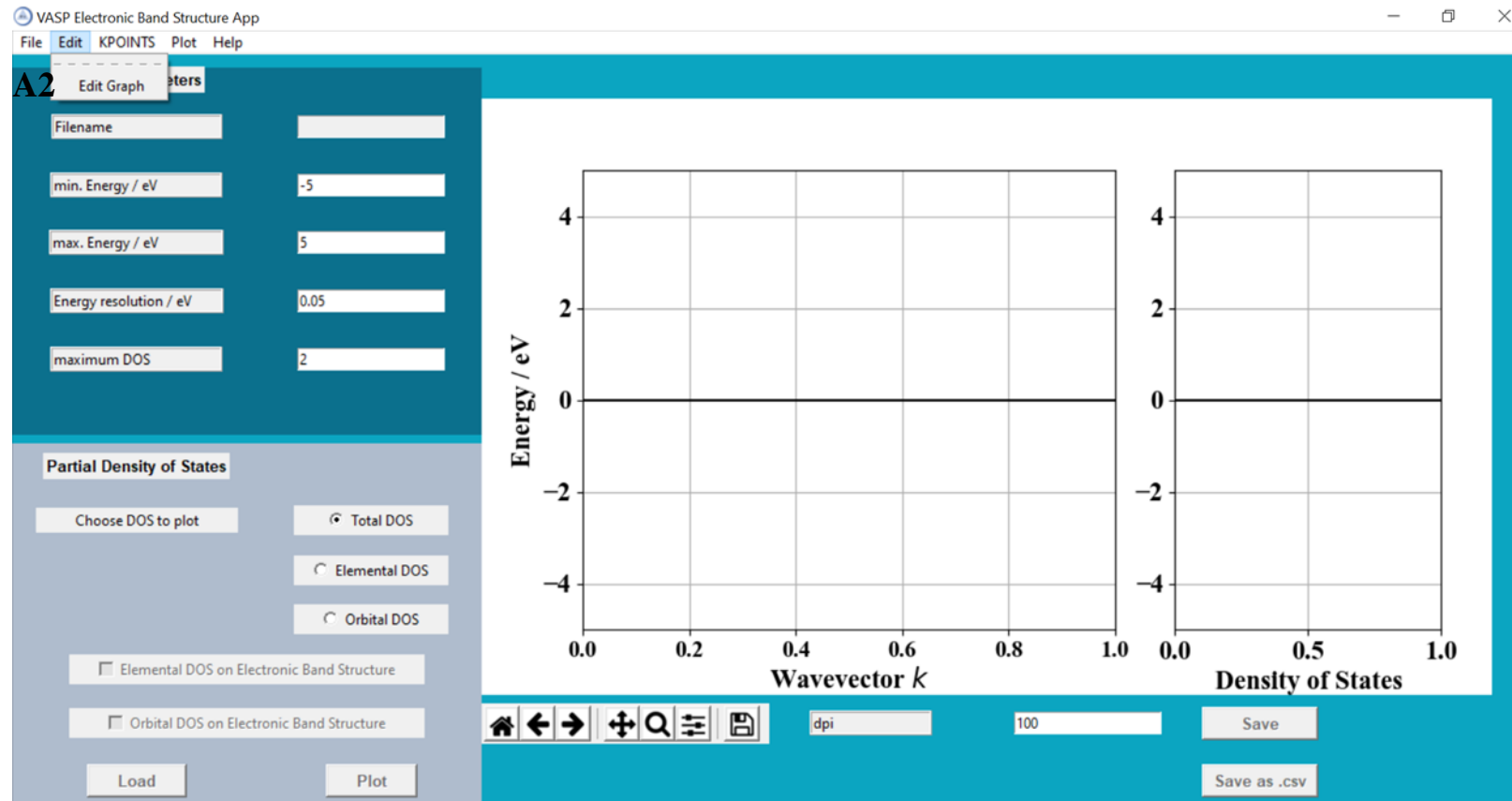
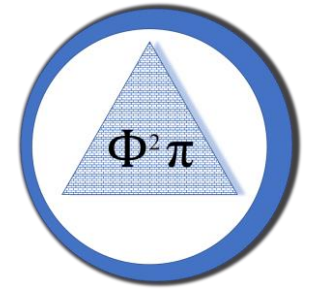
- Open folder
- Folder needs to include **CONTCAR**, **KPOINTS** (from program), **POINTS.json** (from program), **PROCAR\_DOS** (using a grid) and **PROCAR\_band** (computed using KPOINTS from this program)

## C1: Exit

- Close the App



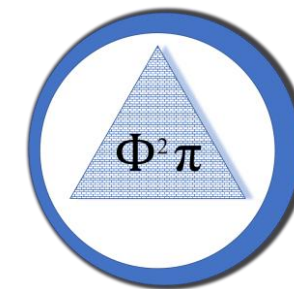
# Edit Menu



## A2 : Edit Graph

- Edit the electronic band structure and DOS graphs
- Change:
  - Font
  - Font size
  - Label
  - Grid
  - Color
  - Figure
  - Position

# Edit Graph



VASP Electronic Band Structure App

Labels/Ticks		Figure	
Font Size Bandstructure x	16 <b>A_graph</b>	Figure Width	8.5
Font Size Bandstructure y	16 <b>B_graph</b>	Figure Height	5.0
Font Size Bandstructure ticks x	14 <b>C_graph</b>	Figure Move Horizontal	0.18
Font Size Bandstructure ticks y	16 <b>D_graph</b>	Figure Move Vertical	0.23
Font Size DOS x	16 <b>E_graph</b>	Figure Length Horizontal	0.78
Font Size DOS y	16 <b>F_graph</b>	Figure Length Vertical	0.68
Font Size DOS ticks	16 <b>G_graph</b>	Color Band Structure	
Font <b>H_graph</b>	Times New Roman	Color for 2 Elements	red-blue
<b>I_graph</b> <input checked="" type="checkbox"/> Energy Label Band Structure	<b>L_graph</b> <input checked="" type="checkbox"/> Wavevector Label	<input checked="" type="checkbox"/> Ticks Energy Band	<b>O_graph</b>
<b>J_graph</b> <input type="checkbox"/> Energy Label DOS	<b>M_graph</b> <input checked="" type="checkbox"/> DOS Label	<input checked="" type="checkbox"/> Ticks Wavevector	<b>P_graph</b>
<b>K_graph</b> <input checked="" type="checkbox"/> Grid Band Structure	<b>N_graph</b> <input checked="" type="checkbox"/> Grid DOS	<input checked="" type="checkbox"/> Ticks Energy DOS	<b>Q_graph</b>
<input type="button" value="Save as Default"/>		<input checked="" type="checkbox"/> Ticks DOS	<b>R_graph</b>
<input type="button" value="Save/Close"/>			

**A\_graph** : Font Size of the  $x$ -axis label for Band Structure  
**B\_graph** : Font Size of the  $y$ -axis label for Band Structure  
**C\_graph** : Font Size of the  $x$ -axis ticks for Band Structure  
**D\_graph** : Font Size of the  $y$ -axis ticks for Band Structure  
**E\_graph** : Font Size of the  $x$ -axis label for DOS  
**F\_graph** : Font Size of the  $y$ -axis label for DOS  
**G\_graph** : Font Size of the  $x$ -axis ticks for DOS  
 (y-axis is the same as y-axis of the Band Structure)

**H\_graph** : Font \*

**I\_graph** : Check to show  $y$ -axis label of Band Structure

**J\_graph** : Check to show  $y$ -axis label of DOS

**K\_graph** : Check to show grid of Band Structure

**L\_graph** : Check to show  $x$ -axis label of Band Structure

**M\_graph** : Check to show  $x$ -axis label of DOS

**N\_graph** : Check to show grid of DOS

**O\_graph** : Check to show  $y$ -axis ticks for Band Structure

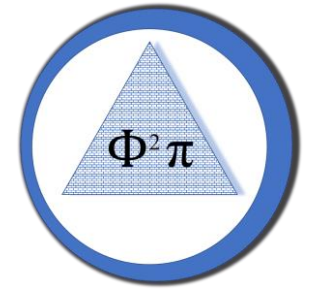
**P\_graph** : Check to show  $x$ -axis ticks for Band Structure

**Q\_graph** : Check to show  $y$ -axis ticks for DOS

**R\_graph** : Check to show  $x$ -axis ticks for DOS

\* For more fonts, please send me an email

# Edit Graph



VASP Electronic Band Structure App

Labels/Ticks		Figure		
Font Size Bandstructure x	16	Figure Width	8.5	<b>S_graph</b>
Font Size Bandstructure y	16	Figure Height	5.0	<b>T_graph</b>
Font Size Bandstructure ticks x	14	Figure Move Horizontal	0.18	<b>U_graph</b>
Font Size Bandstructure ticks y	16	Figure Move Vertical	0.23	<b>V_graph</b>
Font Size DOS x	16	Figure Length Horizontal	0.78	<b>W_graph</b>
Font Size DOS y	16	Figure Length Vertical	0.68	<b>X_graph</b>
Font Size DOS ticks	16	Color Band Structure		<b>Y_graph</b>
Font	Times New Roman	Color for 2 Elements	red-blue	<b>Z_graph</b>
<input checked="" type="checkbox"/> Energy Label Band Structure		<input checked="" type="checkbox"/> Wavevector Label		
<input type="checkbox"/> Energy Label DOS		<input checked="" type="checkbox"/> DOS Label		
<input checked="" type="checkbox"/> Grid Band Structure		<input checked="" type="checkbox"/> Grid DOS		
		<input checked="" type="checkbox"/> Ticks Energy Band		
		<input checked="" type="checkbox"/> Ticks Wavevector		
		<input checked="" type="checkbox"/> Ticks Energy DOS		
		<input checked="" type="checkbox"/> Ticks DOS		
Save as Default		Save/Close		

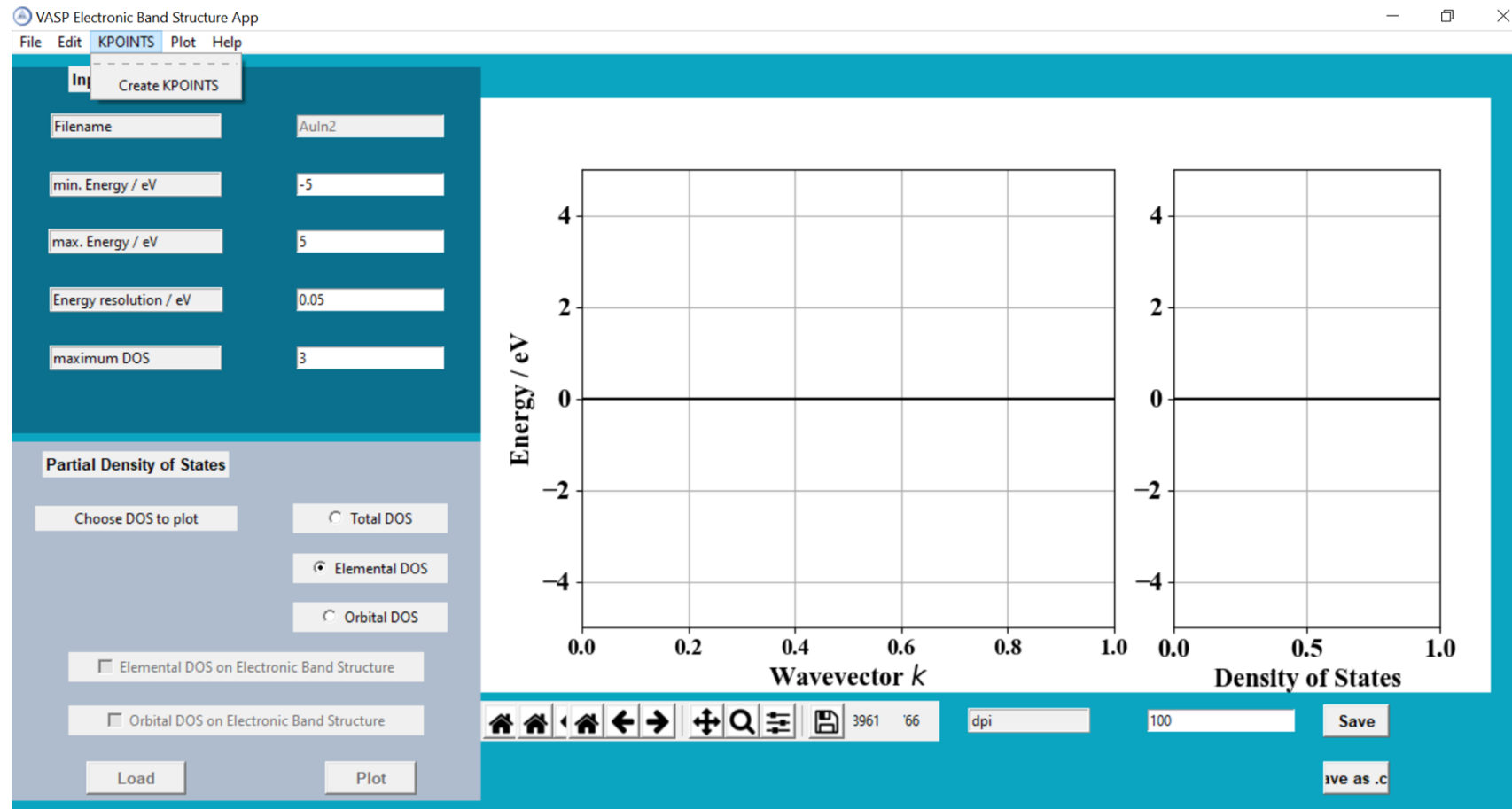
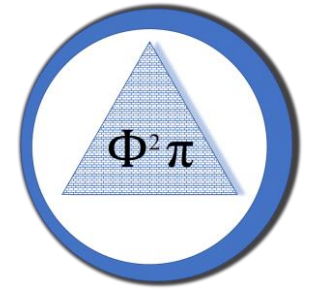
**Button1** **Button2**

**S\_graph** : Width of the figure  
**T\_graph** : Height of the figure  
**U\_graph** : Move the figure horizontal  
**V\_graph** : Move the figure vertical  
**W\_graph** : Increase the width of the plot  
**X\_graph** : Increase the height of the plot  
**Y\_graph** : Color for single color plots  
**Z\_graph** : Color for two-color plots

**Button 1** : Save values as default; a default file is produced and will be saved in the same folder as the .exe file. The program will start with the default values

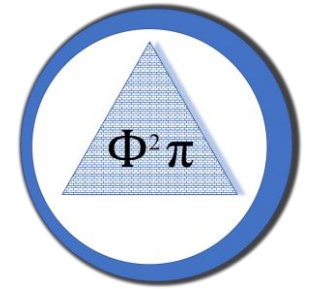
**Button 2** : Close the Edit window and update the figure

# KPOINTS Menu



**Create KPOINTS file for Band Structure calculations in VASP along a certain path**

# KPOINTS window



A\_kpoints

B\_kpoints

C\_kpoints

D\_kpoints

E\_kpoints

F\_kpoints

G\_kpoints

H\_kpoints

VASP Electronic Band Structure App

Crystal System	Triclinic, primitive, aP
Lattice parameter a / Ang	1
Lattice parameter b / Ang	1
Lattice parameter c / Ang	1
Alpha / deg	90
Beta / deg	90
Gamma / deg	90
Minimum # of points	10

Create List of High-Symmetry Points

Create KPOINTS file

Close

A\_kpoints : Choose crystal system

B\_kpoints : Lattice parameter  $a$  in Angstrom

C\_kpoints : Lattice parameter  $b$  in Angstrom

D\_kpoints : Lattice parameter  $c$  in Angstrom

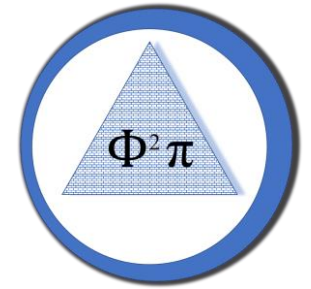
E\_kpoints : Angle  $\alpha$  in degrees

F\_kpoints : Angle  $\beta$  in degrees

G\_kpoints : Angle  $\gamma$  in degrees

H\_kpoints : Choose the minimum number of  
k-points between the shortest distance  
of high-symmetry points

# KPOINTS window



VASP Electronic Band Structure App

Crystal System: Cubic, primitive, cP

KPoint\_Path

L\_kpoints

☒ Gamma --> X

☒ X --> M

☒ M --> Gamma

☒ Gamma --> R

☒ R --> X

☒ M --> R

M\_kpoints

Number of Kpts: 75

I\_kpoints: Create List of High-Symmetry Points

J\_kpoints: Create KPOINTS file

K\_kpoints: Close

Lattice parameter a / Ang: 1

Lattice parameter b / Ang: 1

Lattice parameter c / Ang: 1

Alpha / deg: 90

Beta / deg: 90

Gamma / deg: 90

Minimum # of points: 10

**I\_kpoints** : Create a specific of path between high-symmetry points for a certain crystal system

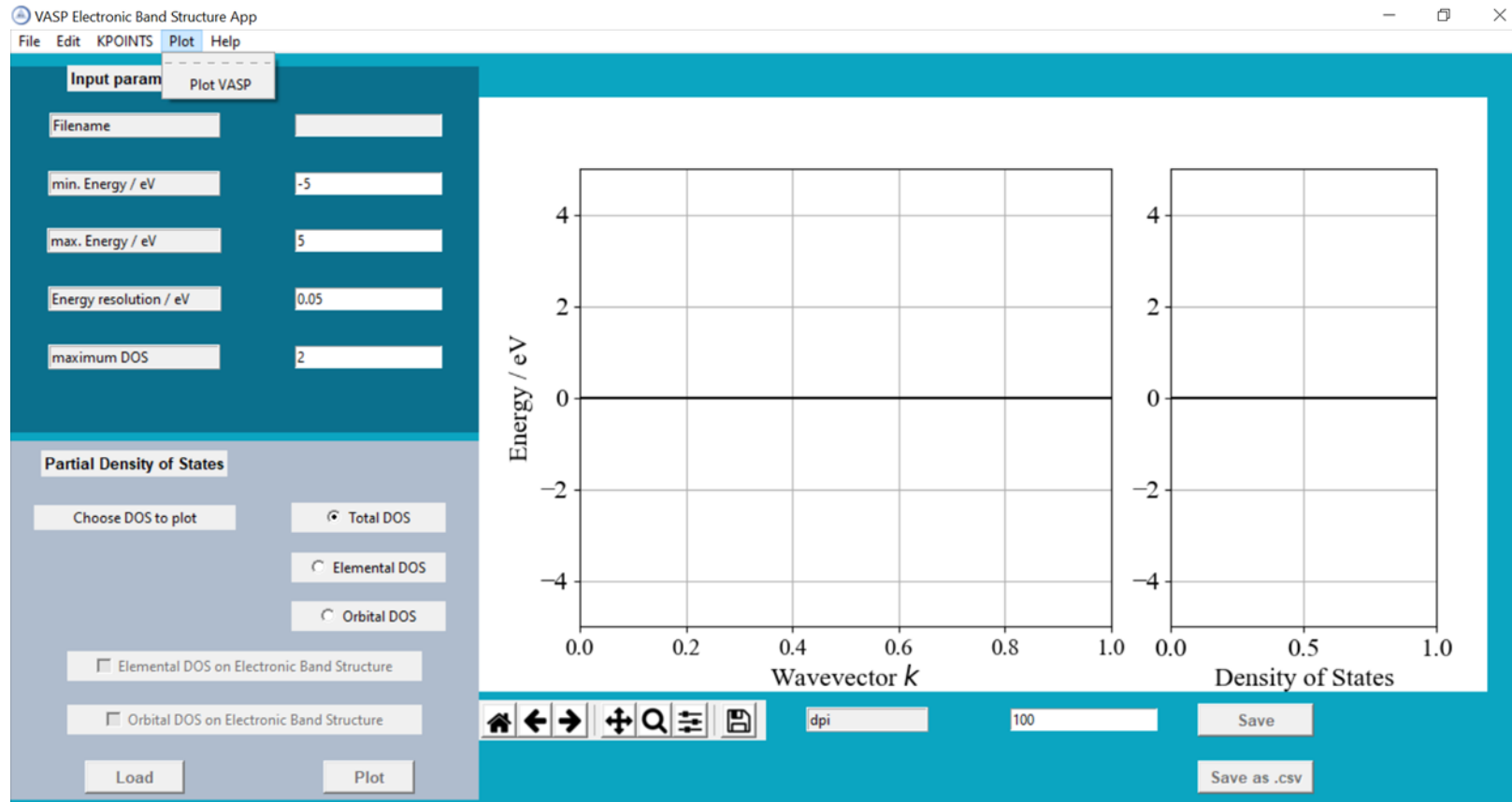
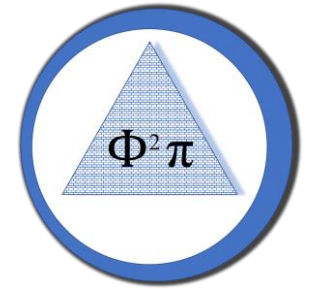
**J\_kpoints** : Save the chosen path as a KPOINTS file (an addition file [POINTS.json] will be produced which is needed for plotting); enabled when a list of high-symmetry paths is created

**K\_kpoints** : Close the KPOINTS window

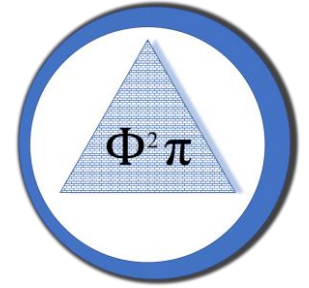
**L\_kpoints** : List of high-symmetry paths. Only checked path will be written in the KPOINTS file

**M\_kpoints** : Number of k-points which will be written in the KPOINTS file. A larger number of k-points leads to longer calculation time

# KPOINTS Menu



**Plot the electronic band structure  
(similar to the Plot button)**



# Questions?

- If you have questions or concerns or find some errors, please send me an email: [Jan.Poehls@Dal.ca](mailto:Jan.Poehls@Dal.ca)
- Thank you for choosing the VASP Plotter– Electronic Band Structure App