Description of the Graphical User Interface for the calculation of band-structures from fcc-crystals using the Plane-Wave-Method

What does the matlab function fcc\_plane\_wave\_gui()?

The matlab function fcc\_plane\_wave\_gui() generates a graphical user interface where you are able to choose from predefined fcc crystals or set your own atomic number $Z$ and lattice constant $a$. As well you have to set the number of nearest neighbours $n$ for the calculation. After pressing the calculation button a new figure, that plots the band-structure of your chosen atom at 1 atm and room temperature (in case of inert gases at 4 K), will be generated.

How to use the fcc\_plane\_wave\_gui()?

• First of all you should check if all of the necessary content (fcc\_plane\_wave\_gui.m, fcc\_plane\_wave.m and my_xticklabels.m) is in your current matlab path.

• Now you are able to run the function fcc\_plane\_wave\_gui() (press F5) and the following GUI will be generated.

![Figure 1: Generated Graphical User Interface of the fcc\_plane\_wave\_gui() function](image_url)

Figure 1: Generated Graphical User Interface of the fcc\_plane\_wave\_gui() function
Step by step:

1. choose a predefined atom e.g. ‘Copper’ or for self-defined values ‘Other’

Figure 2: List of predefined atoms
2. check/set the atomic number $Z$ and lattice constant $a$ (a in angstrom)

![Figure 3: Copper as chosen predefined atom](image)

3. set the number of nearest neighbours $n$ e.g. '2' for second nearest neighbours (high numbers leads to high usage of memory)

![Figure 4: Setting the number of nearest neighbours $n$](image)
4. press the calculation button

Figure 5: Pressing the calculation button

5. if the input was correct and no error message appears you will see the band-structure of your chosen atom

Figure 6: Generated band-structure of the chosen atom copper
More information and hints

For more informations about the used functions use their matlab help functions e.g. 'help fcc_plane_wave_gui'. Also the comments in the source code of the functions should be helpful by understanding the implementation.