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.
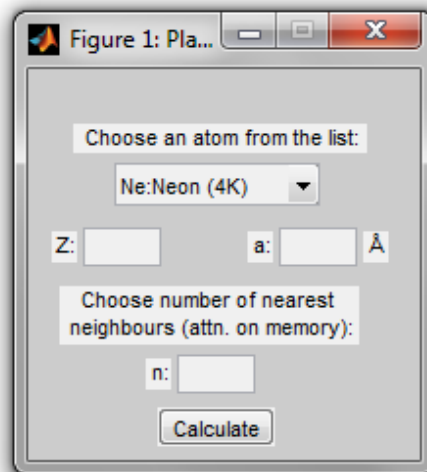

Figure 1: Generated Graphical User Interface of the fcc_plane_wave_gui() function

Step by step:

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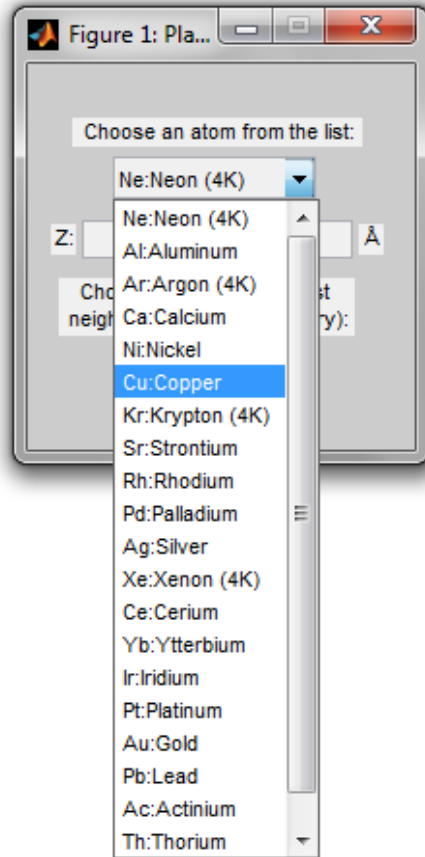

Figure 2: List of predefined atoms

2. check/set the atomic number Z and lattice constant a (a in angstrom)
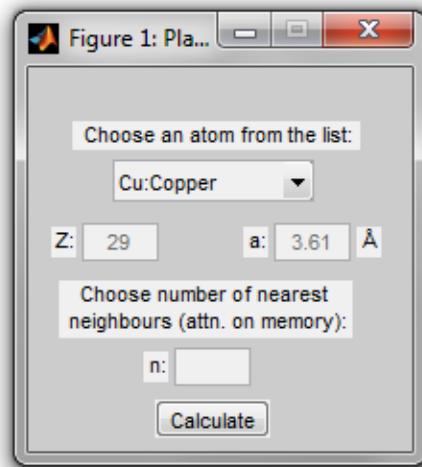

Figure 3: Copper as chosen predefined atom

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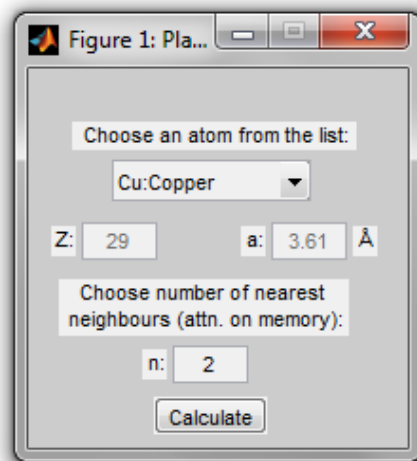   (high numbers leads to high usage of memory)

Figure 4: Setting the number of nearest neighbours n
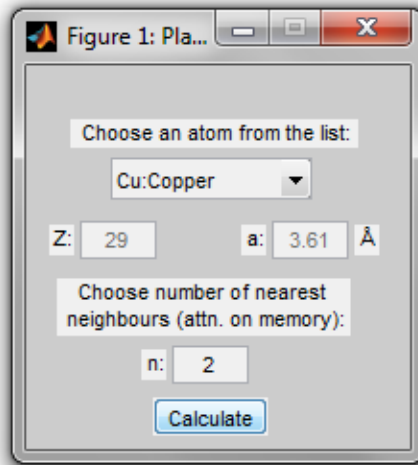
4. press the calculation button

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
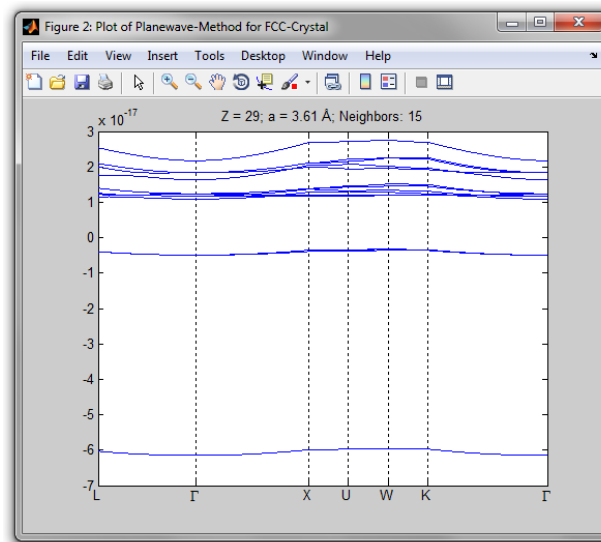
Figure 6: Generated band-structure of the chosen atom copper

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.