Example: comparison with experiments

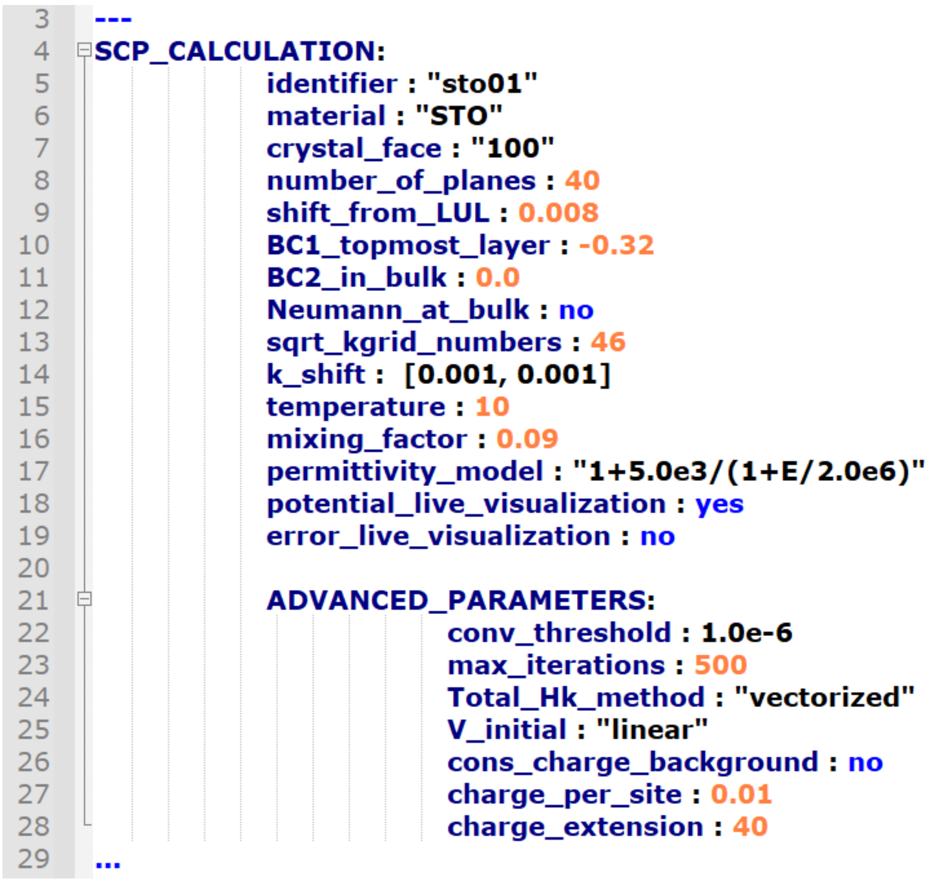
This file is intended to detail the calculation presented in Sections 4.4 of our *BinPo* manuscript. Importantly, we remind you that any *BinPo* component looks for the input parameters at command-line at first, whereas the omitted and more advanced parameters are set by default from the configuration file. Keeping this in mind, we will show how the configuration files are set for each case and what to type from command-line. For a description of all the parameters in the configuration files, see *~/config_files/help_config.md*. Parameters modifiable through the command-line can be checked by means of help command as:

$ python BP-component.py -h

where *BP-component.py* is any *BinPo* component.

Self-consistent potential energy calculation

We will assume that the pre-processing step for STO(100) is already done. So, here it is how the *scp.yaml* configuration file looks like:

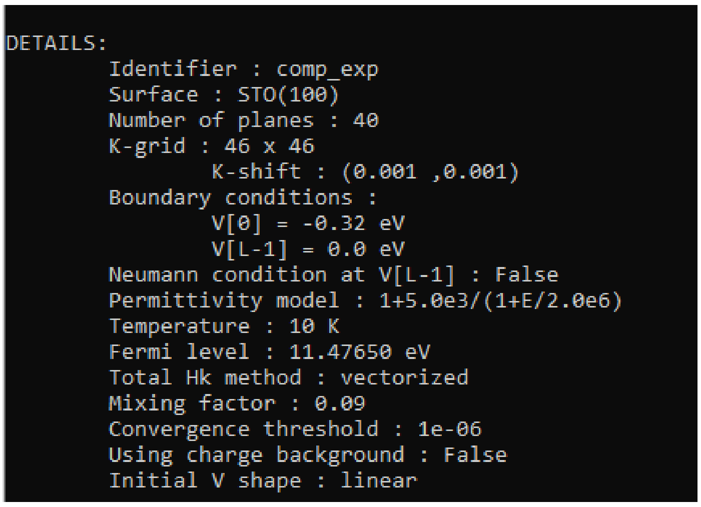


```
---
SCP_CALCULATION:
        identifier : "sto01"
        material : "STO"
        crystal_face : "100"
        number_of_planes : 40
        shift_from_LUL : 0.008
        BC1_topmost_layer : -0.32
        BC2_in_bulk : 0.0
        Neumann_at_bulk : no
        sqrt_kgrid_numbers : 46
        k_shift :  [0.001, 0.001]
        temperature : 10
        mixing_factor : 0.09
        permittivity_model : "1+5.0e3/(1+E/2.0e6)"
        potential_live_visualization : yes
        error_live_visualization : no

        ADVANCED_PARAMETERS:
                conv_threshold : 1.0e-6
                max_iterations : 500
                Total_Hk_method : "vectorized"
                V_initial : "linear"
                cons_charge_background : no
                charge_per_site : 0.01
                charge_extension : 40
...
```

Now, we will compute a SC-calculation under the “comp_exp” job identifier (*id*), so:

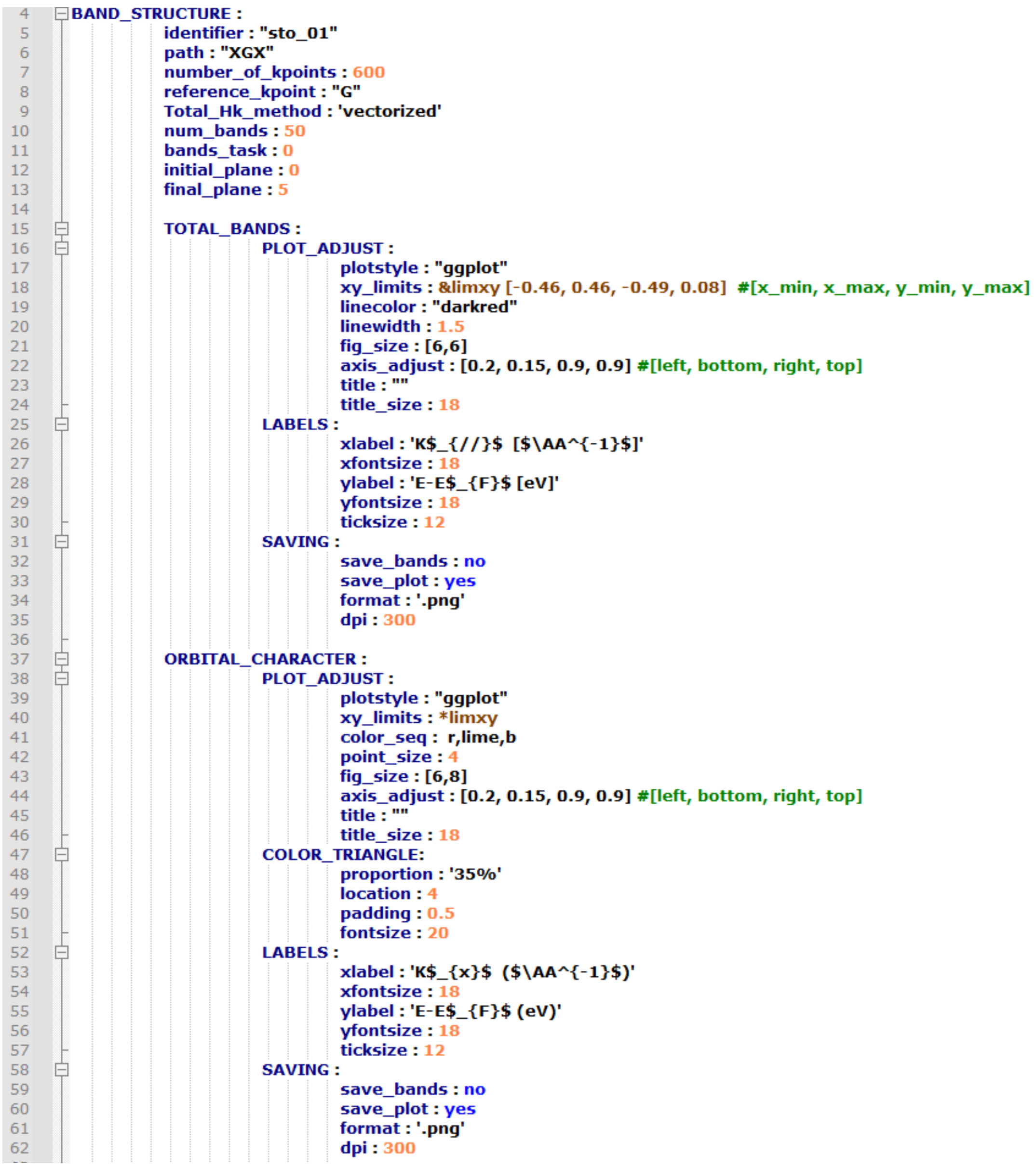
$ python BP-scp.py -id comp_exp

In the output text at command-line we will see printed the following details:



```
DETAILS:
        Identifier : comp_exp
        Surface : STO(100)
        Number of planes : 40
        K-grid : 46 x 46
                K-shift : (0.001 ,0.001)
        Boundary conditions :
                V[0] = -0.32 eV
                V[L-1] = 0.0 eV
        Neumann condition at V[L-1] : False
        Permittivity model : 1+5.0e3/(1+E/2.0e6)
        Temperature : 10 K
        Fermi level : 11.47650 eV
        Total Hk method : vectorized
        Mixing factor : 0.09
        Convergence threshold : 1e-06
        Using charge background : False
        Initial V shape : linear
```

Note that, in this particular case, we are using a model for relative permittivity as input. Now, we will see the *bands.yaml* file for the calculation of bandstructure projected onto the atomic orbitals:

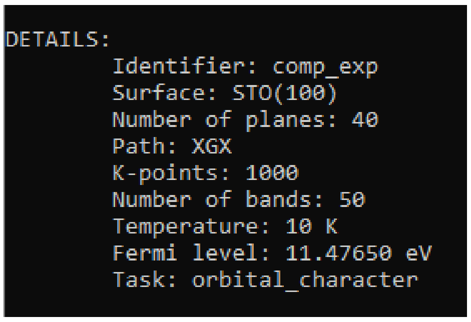


```
BAND_STRUCTURE :
        identifier : "sto_01"
        path : "XGX"
        number_of_kpoints : 600
        reference_kpoint : "G"
        Total_Hk_method : 'vectorized'
        num_bands : 50
        bands_task : 0
        initial_plane : 0
        final_plane : 5

        TOTAL_BANDS :
                PLOT_ADJUST :
                        plotstyle : "ggplot"
                        xy_limits : &limxy [-0.46, 0.46, -0.49, 0.08]  #[x_min, x_max, y_min, y_max]
                        linecolor : "darkred"
                        linewidth : 1.5
                        fig_size : [6,6]
                        axis_adjust : [0.2, 0.15, 0.9, 0.9] #[left, bottom, right, top]
                        title : ""
                        title_size : 18
                LABELS :
                        xlabel : 'K$_{//}$ [$\AA^{-1}$]'
                        xfontsize : 18
                        ylabel : 'E-E$_{F}$ [eV]'
                        yfontsize : 18
                        ticksize : 12
                SAVING :
                        save_bands : no
                        save_plot : yes
                        format : '.png'
                        dpi : 300

        ORBITAL_CHARACTER :
                PLOT_ADJUST :
                        plotstyle : "ggplot"
                        xy_limits : *limxy
                        color_seq :  r,lime,b
                        point_size : 4
                        fig_size : [6,8]
                        axis_adjust : [0.2, 0.15, 0.9, 0.9] #[left, bottom, right, top]
                        title : ""
                        title_size : 18
                COLOR_TRIANGLE:
                        proportion : '35%'
                        location : 4
                        padding : 0.5
                        fontsize : 20
                LABELS :
                        xlabel : 'K$_{x}$  ($\AA^{-1}$)'
                        xfontsize : 18
                        ylabel : 'E-E$_{F}$ (eV)'
                        yfontsize : 18
                        ticksize : 12
                SAVING :
                        save_bands : no
                        save_plot : yes
                        format : '.png'
                        dpi : 300
```

We compute the desired bandstructure as:

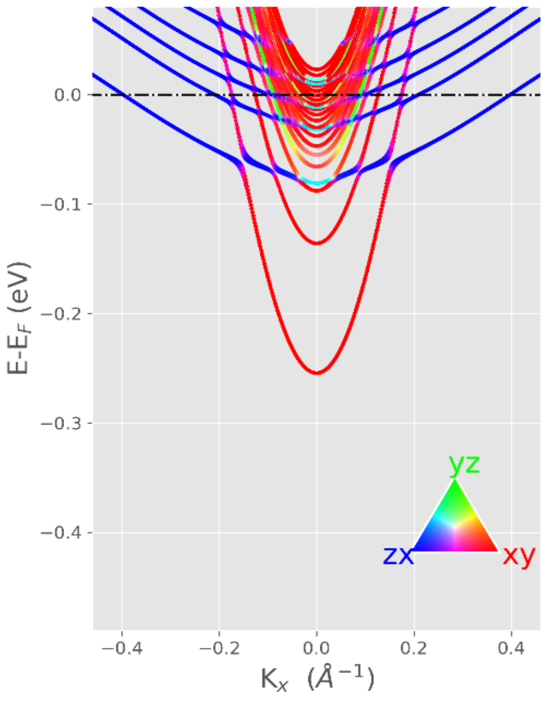
$ python BP-bands.py -id comp_exp -kp 1000 -tk 1

The details in the output text will be:



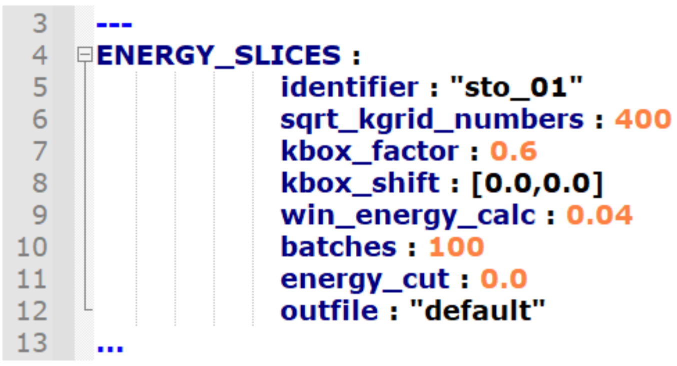
```
DETAILS:
        Identifier: comp_exp
        Surface: STO(100)
        Number of planes: 40
        Path: XGX
        K-points: 1000
        Number of bands: 50
        Temperature: 10 K
        Fermi level: 11.47650 eV
        Task: orbital_character
```

The output plot we get is:



Fermi surface calculation

The *energy_slices.yaml* configuration file looks:

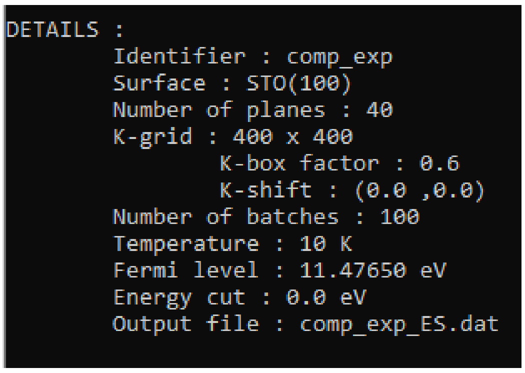


```
---
ENERGY_SLICES :
                identifier : "sto_01"
                sqrt_kgrid_numbers : 400
                kbox_factor : 0.6
                kbox_shift : [0.0,0.0]
                win_energy_calc : 0.04
                batches : 100
                energy_cut : 0.0
                outfile : "default"
...
```

We will run the component *energy_slices.py* to get the Fermi surface as follows:

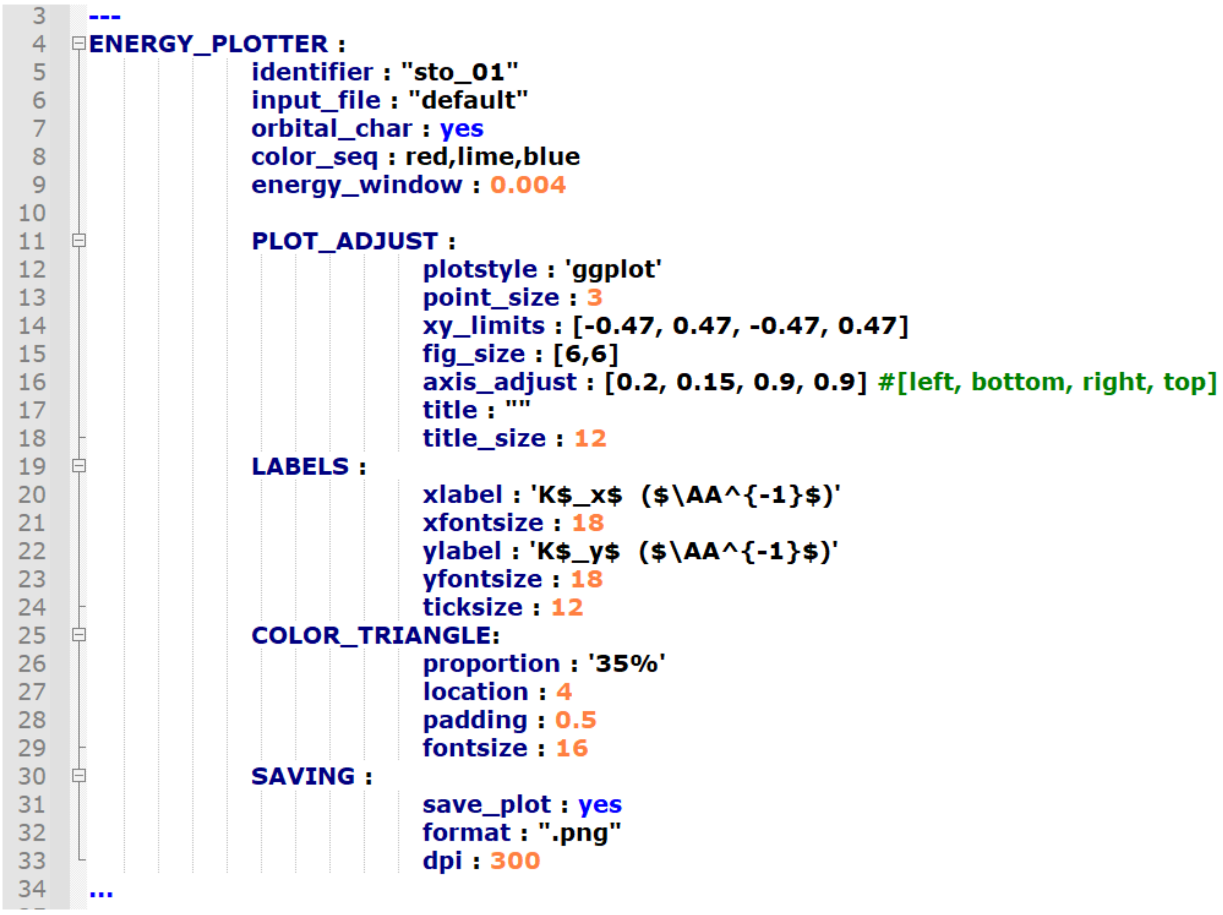
$ python BP-energy_slices.py -id comp_exp

The following details will be printed:



```
DETAILS :
        Identifier : comp_exp
        Surface : STO(100)
        Number of planes : 40
        K-grid : 400 x 400
                K-box factor : 0.6
                K-shift : (0.0 ,0.0)
        Number of batches : 100
        Temperature : 10 K
        Fermi level : 11.47650 eV
        Energy cut : 0.0 eV
        Output file : comp_exp_ES.dat
```

After *BP-energy_slices.py* finishes the output file with the Fermi surface to plot will be automatically saved to the *comp_exp* folder. To plot the output, we will use the *BP-energy_plot.py*, whose configuration file *energy_plot.yaml* looks:

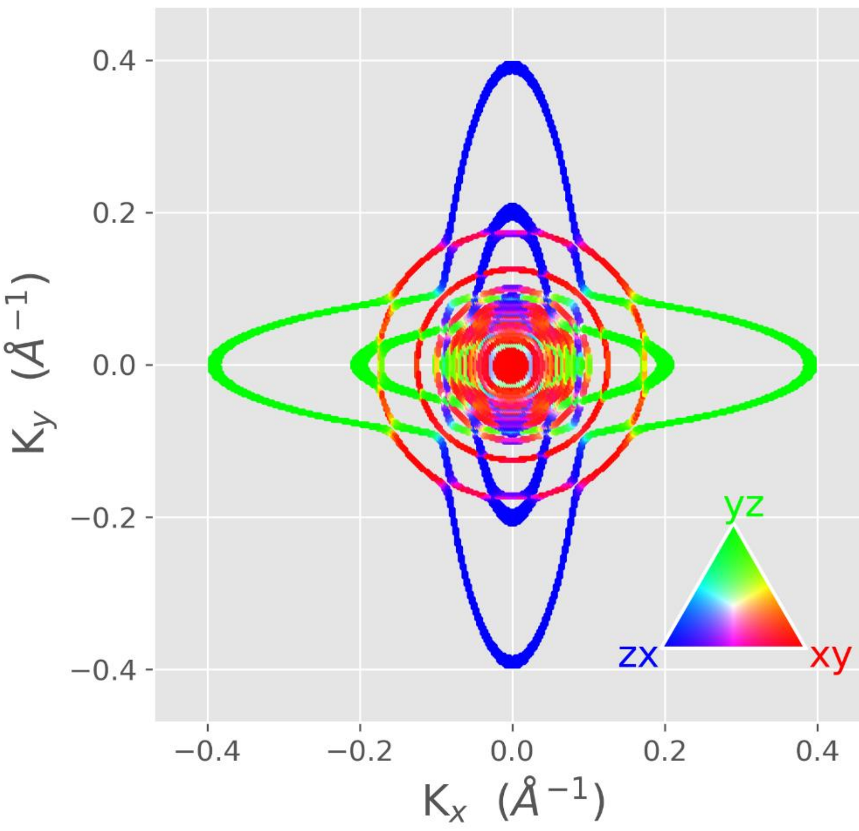


```
---
ENERGY_PLOTTER :
            identifier : "sto_01"
            input_file : "default"
            orbital_char : yes
            color_seq : red,lime,blue
            energy_window : 0.004

            PLOT_ADJUST :
                        plotstyle : 'ggplot'
                        point_size : 3
                        xy_limits : [-0.47, 0.47, -0.47, 0.47]
                        fig_size : [6,6]
                        axis_adjust : [0.2, 0.15, 0.9, 0.9] #[left, bottom, right, top]
                        title : ""
                        title_size : 12
            LABELS :
                        xlabel : 'K$_x$  ($\AA^{-1}$)'
                        xfontsize : 18
                        ylabel : 'K$_y$  ($\AA^{-1}$)'
                        yfontsize : 18
                        ticksize : 12
            COLOR_TRIANGLE:
                        proportion : '35%'
                        location : 4
                        padding : 0.5
                        fontsize : 16
            SAVING :
                        save_plot : yes
                        format : ".png"
                        dpi : 300
...
```

Thus, by typing the following line:

$ python BP-energy_plot.py -id comp_exp

the output plot that we get is:


K_y $(\AA^{-1})$
K_x $(\AA^{-1})$
yz
zx
xy