Example: fixed background density approach

This file is intended to detail the calculation presented in the Appendix D of our *BinPo* manuscript. Importantly, we remind you that any *BinPo* component looks for the input parameters at the 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*. Those parameters updatable by command-line in any *BinPo* components (*BP-component.py*) can be checked by means of help command as:

$ python BP-component.py -h

Firstly, we will show how the *scp.yaml* is configured for the case of not considering the background charge.

```yaml
---
SCP_CALCULATION:
        identifier : "sto01"
        material : "STO"
        crystal_face : "100"
        number_of_planes : 40
        shift_from_LUL : 0.008
        BC1_topmost_layer : -0.36
        BC2_in_bulk : 0.0
        Neumann_at_bulk : no
        sqrt_kgrid_numbers : 36
        k_shift :  [0.001, 0.001]
        temperature : 10
        mixing_factor : 0.09
        permittivity_model : "Cop"
        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 : 0.06
                charge_extension : 40
...
```

We run the BP-scp.py component as:

$ python BP-scp.py -id sto_nofixQ

The immediate details in the output text reads:

```
DETAILS:
        Identifier : sto_nofixQ
        Surface : STO(100)
        Number of planes : 40
        K-grid : 36 x 36
                K-shift : (0.001 ,0.001)
        Boundary conditions :
                V[0] = -0.36 eV
                V[L-1] = 0.0 eV
        Neumann condition at V[L-1] : False
        Permittivity model : Cop
        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, as specified in the *scp.yaml* file, the use of a constant background of charge is set to "no". After a successful calculation, a folder under the name "*sto_nofixQ*" with the SC-solution will appear.

In order to generate the bandstructure, we will run the *BP-bands.py* component. The corresponding *bands.yaml* configuration file looks:

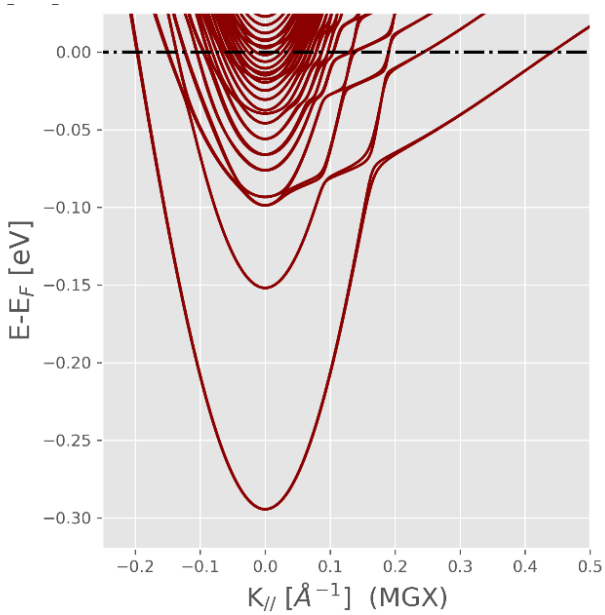
```yaml
---
BAND_STRUCTURE :
        identifier : "sto_01"
        path : "XGX"
        number_of_kpoints : 600
        reference_kpoint : "G"
        Total_Hk_method : 'vectorized'
        num_bands : 50
        bands_task : 0
        initial_plane : 0
        final_plane : 5

        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
```

Note that, for this example, we are just interested in the total bandstructure block. With these configurations and typing:

$ python BP-bands.py -id sto_nofixQ -ph MGX -xy -0.3 0.5 -0.32 0.03

where we use the identifier (id) defined above, the path (*ph*) M-Γ-X in reciprocal space and we set the x and y scales by the *xy* parameter. We get the following output plot:



In order to perform the calculation with the addition of a constant background, we must set the "cons_charge_background" keyword to "yes" in the *scp.yaml* file and set the corresponding values for "charge_per_site" and "charge_extension" keywords. Now, this file looks:

```
3  ---
4  SCP_CALCULATION:
5              identifier : "sto01"
6              material : "STO"
7              crystal_face : "100"
8              number_of_planes : 40
9              shift_from_LUL : 0.008
10             BC1_topmost_layer : -0.36
11             BC2_in_bulk : 0.0
12             Neumann_at_bulk : no
13             sqrt_kgrid_numbers : 36
14             k_shift :  [0.001, 0.001]
15             temperature : 10
16             mixing_factor : 0.09
17             permittivity_model : "Cop"
18             potential_live_visualization : yes
19             error_live_visualization : no
20
21             ADVANCED_PARAMETERS:
22                         conv_threshold : 1.0e-6
23                         max_iterations : 500
24                         Total_Hk_method : "vectorized"
25                         V_initial : "linear"
26                         cons_charge_background : yes
27                         charge_per_site : 0.01
28                         charge_extension : 40
29 ...
```

We run the BP-scp.py component with a different identifier, as:

$ python BP-scp.py -id sto_fixQ

The immediate details in the output text reads:

```
DETAILS:
        Identifier : sto_fixQ
        Surface : STO(100)
        Number of planes : 40
        K-grid : 36 x 36
                K-shift : (0.001 ,0.001)
        Boundary conditions :
                V[0] = -0.36 eV
                V[L-1] = 0.0 eV
        Neumann condition at V[L-1] : False
        Permittivity model : Cop
        Temperature : 10 K
        Fermi level : 11.47650 eV
        Total Hk method : vectorized
        Mixing factor : 0.09
        Convergence threshold : 1e-06
        Using charge background : True
                Charge per site : 0.01
                Charge extent : 40
        Initial V shape : linear
```

Given that the fixed background is used now, the details about the charge per site and the charge extent are printed out.

We can compute the bandstructure in the same way as before:

$ python BP-bands.py -id sto_fixQ -ph MGX -xy -0.3 0.5 -0.32 0.03

and we get the following output plot: