

Example: energy slices calculation

This file is intended to detail the calculation presented in Sections 4.3.2 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`. 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 *energy_slices.yaml* is configured.

```
3 ---
4 ENERGY_SLICES :
5     identifier : "sto_01"
6     sqrt_kgrid_numbers : 400
7     kbox_factor : 0.6
8     kbox_shift : [0.0,0.0]
9     win_energy_calc : 0.04
10    batches : 100
11    energy_cut : 0.0
12    outfile : "default"
13 ...
```

Now, we will compute an energy slice on a previous SC calculation under the “run2” identifier, so:

```
$ python BP-energy_slices.py -id run2 -ec 0.0 -nk 300 -ba 60 -bf 0.7
```

The energy cut (*ec*) is set to 0.0, indicating that we are computing just the Fermi surface. A k-grid (*nk*) of 300 x 300 points will be used and it will be split in 60 batches (*ba*). The k-box factor parameter (*bf*) is to enlarge or reduce the mapped first Brillouin zone (BZ1). When running this component, we will see the following details:

```
DETAILS :
  Identifier : run2
  Surface : STO(100)
  Number of planes : 40
  K-grid : 300 x 300
    K-box factor : 0.7
    K-shift : (0.0 ,0.0)
  Number of batches : 60
  Temperature : 10 K
  Fermi level : 11.47650 eV
  Energy cut : 0.0 eV
  Output file : run2_ES.dat
```

After the calculation is done, the output file is automatically saved to the *run2* folder. We must plot the energy slice by means of *BP-energy_plot.py* component, whose configuration file (*energy_plot.yaml*) looks like:

```

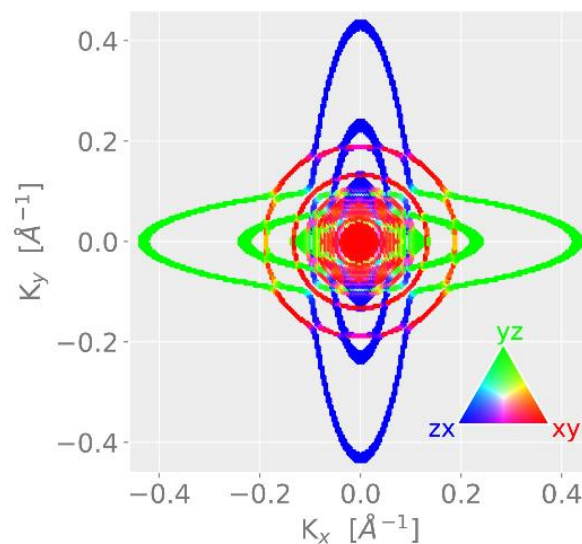
3  ---
4  ENERGY_PLOTTER :
5      identifier : "sto_01"
6      input_file : "default"
7      orbital_char : yes
8      color_seq : red,lime,blue
9      energy_window : 0.005
10
11  PLOT_ADJUST :
12      plotstyle : 'ggplot'
13      point_size : 7
14      xy_limits : [-0.46, 0.46, -0.46, 0.46] #[x_min, x_max, y_min, y_max]
15      fig_size : [6,6]
16      axis_adjust : [0.2, 0.15, 0.9, 0.9] #[left, bottom, right, top]
17      title : ""
18      title_size : 12
19
20  LABELS :
21      xlabel : 'K$_x$ [$\text{\AA}^{-1}$]'
22      xfontsize : 18
23      ylabel : 'K$_y$ [$\text{\AA}^{-1}$]'
24      yfontsize : 18
25      ticksize : 17
26
27  COLOR_TRIANGLE:
28      proportion : '35%'
29      location : 4
30      padding : 0.5
31      fontsize : 16
32
33  SAVING :
34      save_plot : yes
35      format : ".png"
36      dpi : 300

```

So that, we generate the interactive plot by typing:

```
$ python BP-energy_plot.py -id run2
```

This is how the output plot looks like:



Now we will compute another energy slice, this time at 50 meV below the Fermi level. This could be done by typing:

```
$ python BP-energy_slices.py -id run2 -ec -0.05 -nk 300 -ba 60 -bf 0.7
```

Here, we can see that just the energy cut (*ec*) has been modified. In consequence, the details for this calculation will be now:

```

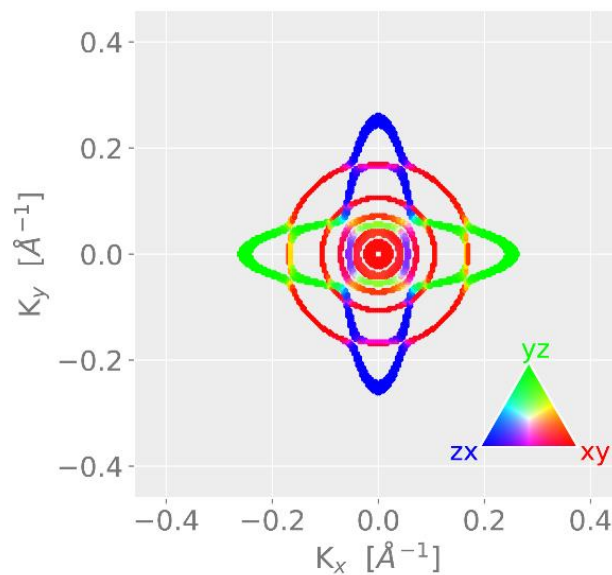
DETAILS :
  Identifier : run2
  Surface : STO(100)
  Number of planes : 40
  K-grid : 300 x 300
           K-box factor : 0.7
           K-shift : (0.0 ,0.0)
  Number of batches : 60
  Temperature : 10 K
  Fermi level : 11.47650 eV
  Energy cut : -0.05 eV
  Output file : run2_ES.dat

```

Note that, because we did not change the name of the output file, it will be overwritten. We will get the interactive plot by using the *BP-energy_plot.py* component just as before:

```
$ python BP-energy_plot.py -id run2
```

This is how the output plot looks like:



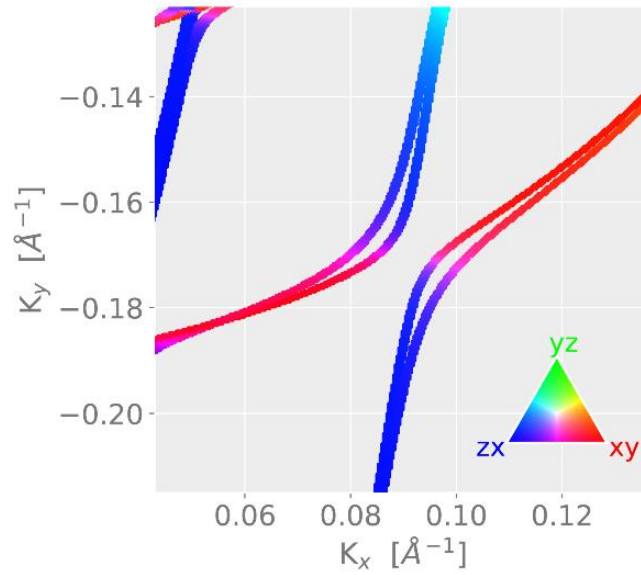
Now, we will take a closer look at one of the avoided crossing regions at the Fermi surface. There, we will find the unconventional Rashba spin splitting of this system. By typing:

```
$ python BP-energy_slices.py -id run2 -ec 0.0 -nk 300 -ba 60 -bf 0.06 -dk 0.09 -0.17
```

We are reducing significantly the area sampled in the BZ1 and, due to keep constant the total k-points (*kp*), the resolution is increased at the same computational cost. The additional parameter *dk* is for centering the k-grid. After the calculation is done, we can easily plot the output by the following line:

```
$ python BP-energy_plot.py -id run2 -ew 0.002 -ps 5 -xy 0.043 0.137 -0.215 -0.123
```

Note that, we are modifying the plot without modifying the *energy_plot.yaml* file. In doing that, now we set the energy window for the plot (*ew*), the point size (*ps*) and the limits for the plot (*xy*). The outplot plot is:



NOTE: To avoid overwriting when performing several energy slices calculations, we could use the “outfile” parameter in *energy_slices.yaml* file.