

Individualized band weights/local axes

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In this first fatband task we learn to use `xfplo -bw` to reduce the size of the `+bweights` file and to setup individual local axes. The axes decide in which coordinate system the spherical harmonics are expressed. The solution will be found in the `solution` directory. You will work in the `task` directory.

We already setup and converged a simple CaCuO_2 calculation. The structure is shown in Fig. 1.

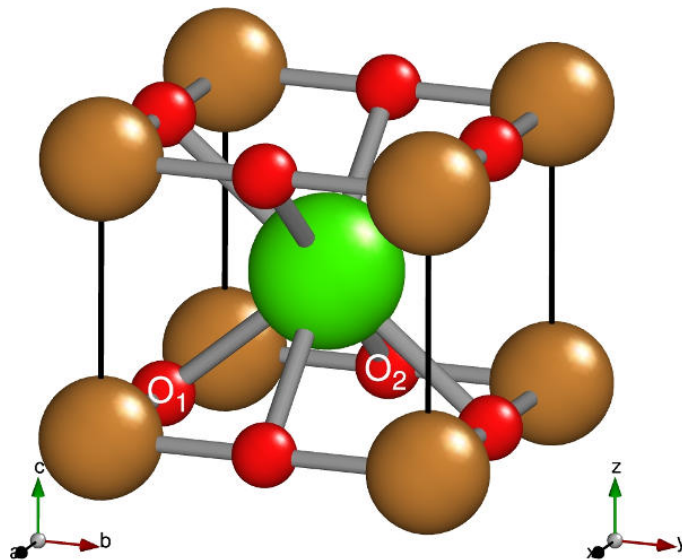


Figure 1: CaCuO_2 unit cell

Please follow the instructions below:

- Please execute

```
xfplo -bw &
```

You get the Band weight editor (BWE), Fig. 2

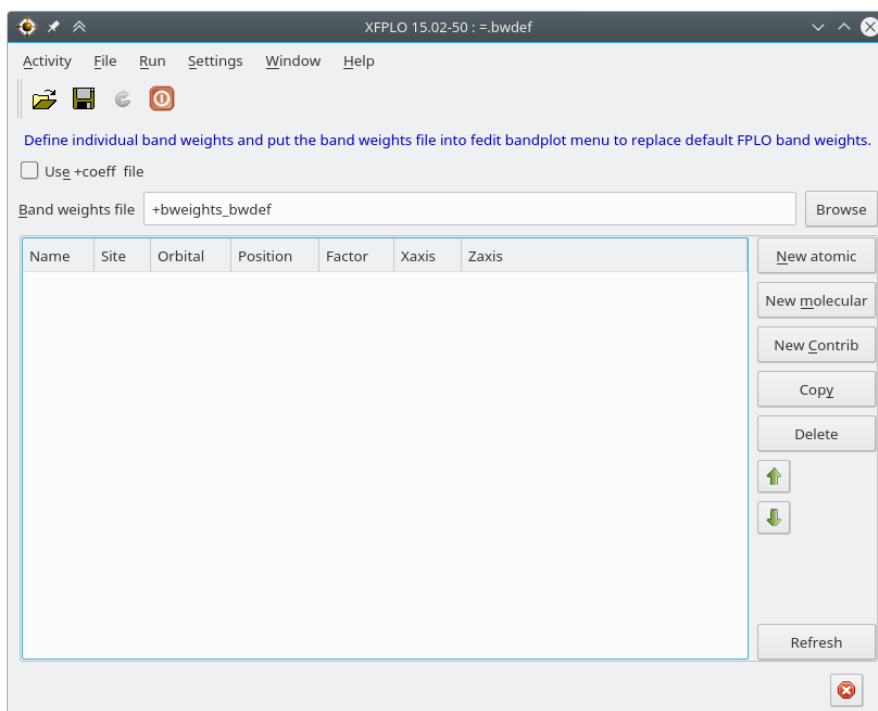


Figure 2: The empty band weight editor

- From the menu select **Activity** \triangleright **Structure =.in** to open the structure view (SV).
- Now, click on the SV to make it the current window and press **a a** (two times the a-key). This will show the cartesian coordinate frame in the lower right corner (Fig 3).

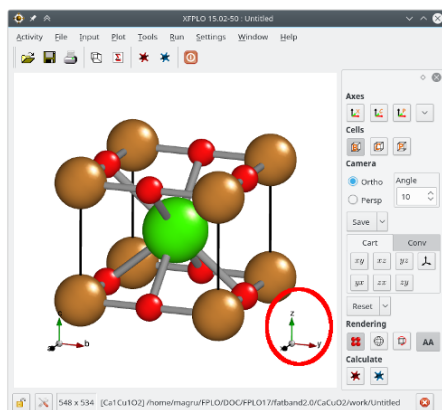


Figure 3: The structure view (SV).

- In the BWE click the **New atomic** button to open the atomic orbital dialog (AOD), Fig. 4



Figure 4: Atomic orbital dialog

- Click on the **Get Atom** button in the AOD and then click on a brown (Cu) atom in the SV. Now, the site in the AOD is 2. Go to the **orbital** line edit and start typing “3d”. Select exactly “3d” (which means all 3d orbitals). Next, press the **OK** button to close the AOD → a new line appears in the BWE.
- For practicing, click onto the line in the BWE and either press **space**, **enter** or **double click** to re-open the AOD. This way you can edit the settings later on. You also can click the **Get Atom** button again and select another atom in the SV. What ever is needed. OK, now close the AOD.
- Let’s proceed by clicking the **New atomic** button in the BWE again. Use **Get Atom** in the AOD to select oxygen 1 (see Fig. 1), which results in site 3 in the AOD. Set the **orbital** to 2p and click **OK**.
- Finally, add a **New atomic** weight by selecting oxygen 2, which is site 4 (see Fig. 1). In the AOD select **orbital** 2p and set the **x-axis** to (010) such that the local axis of oxygen 2 points into the y-direction.

Your BWE now looks like Fig. 5

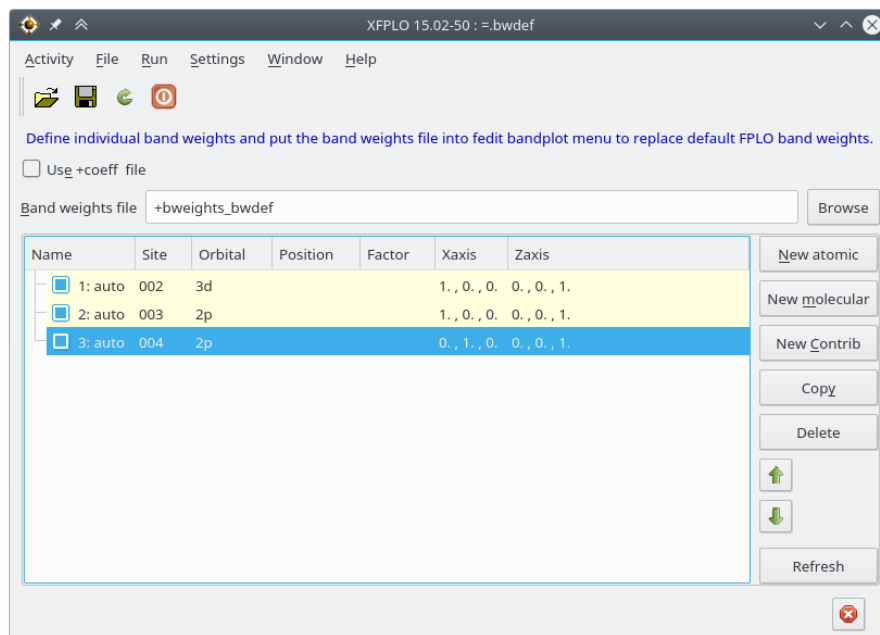


Figure 5: band weight editor with content

- In the BWE select the menu **File** > **Save** and accept the default file name `=.bwdef`.
- Hit **Ctrl-Q** (**Activity** > **Quit all**) and ignore the warning message boxes.
- Have a look at `=.bwdef`:

```
coefficients +coeff
bweights +bweights_bwdef

bwdef simple on
  contrib
    site 2
    orbital 3d
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
bwdef simple on
  contrib
    site 3
    orbital 2p
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
bwdef simple on
  contrib
    site 4
    orbital 2p
    xaxis 0. 1. 0.
    zaxis 0. 0. 1.
```

The only non-trivial setting is the x-axis of site 4. You will notice that the band weights will be written to `+bweights_bwdef` (second line). This can be changed in the BWE.

- Now, open `fedit22.00-62-x86_64`, go to the `bandplot-submenu` and switch on `bandstructure-plot` and `weights`.
- Go to the `fedit main menu` and switch on `use data directories`.
- `Quit/Save fedit` and execute `fplo`:

```
fplo22.00-62-x86_64 | tee out
```

You should now have the sub directory `+dos` and `+band/+bweight`. The file size of `+bweights` is about 28M (execute: `ls -lh`).

- Now, we will make use of the `=.bwdef` file. Open `fedit` and go to the `bandplot-submenu`. Edit `weights def file` (hotkey `f`) and enter `=.bwdef`. Go to the `main menu` and `Quit/Save`.
- Execute `fplo` again.

Additionally, now you have subdir `+bdos` and a file `+bweights_bwdef`. Use `ls -lh` to see that the new file is only 5M big. Furthermore, its oxygen site 4 has a rotated x-axis.

- Open

```
xfbp +bweights_bwdef
```

- go to `Edit > Sets` and select the `weights tab`. You only see Cu 3d and O 2p weights. The rest was not written, as demanded by our `=.bwdef` setup. Eventually, the band weights are not usefull to show the rotated axis, since the two oxygen sit at different sites, which makes the two O 2p_x weights being distributed along different *k*-directions, even though they have the same axis orientation. So, let's look at the `bwdef-dos` files residing in `+bdos`. Execute

```
xfbp bdos.xpy
```

to obtain Fig. 6. If you get error messages, you might have selected the wrong oxygen atoms. In such a case look at the file names in `+bdos` and edit `bdos.xpy` by using `Edit > Script/transformations`.

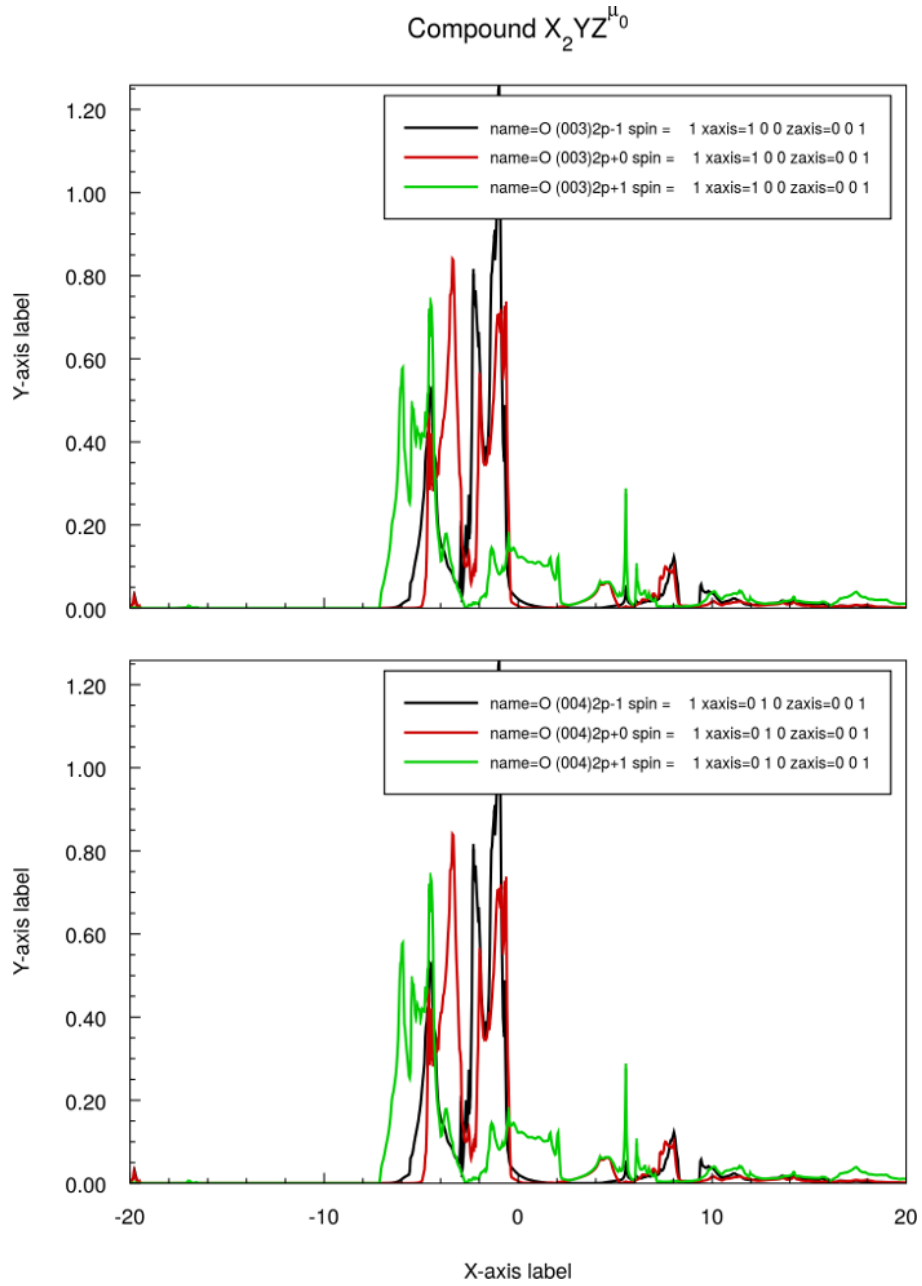


Figure 6: The bdos of the two oxygen. They are identical due to the axis rotation.