

Molecular band weight projectors

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This fatband task teaches you how to construct molecular band weight projectors. The solution will be found in the `solution` directory. You will work in the `task` directory.

We already setup and converged a simple SrRh_2P_2 calculation. The structure is shown in Fig. 1.

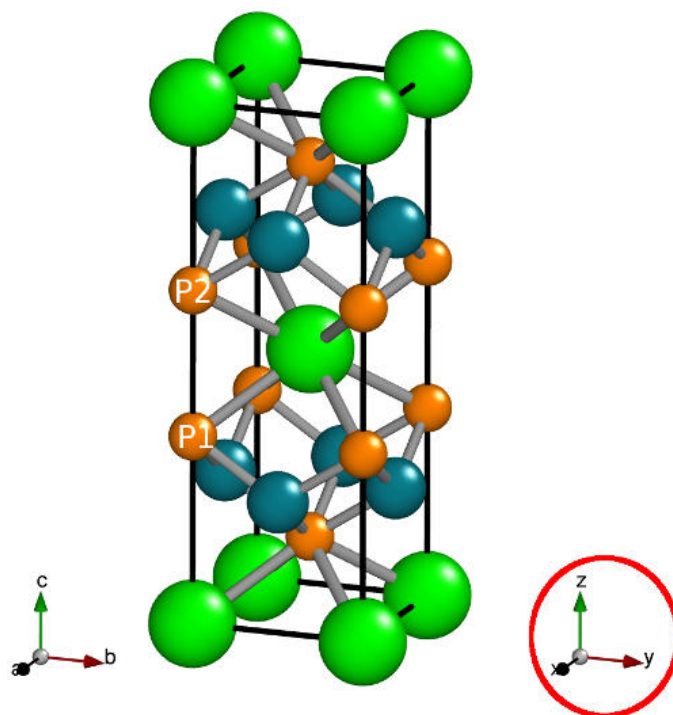


Figure 1: SrRh_2P_2 unit cell.

We also already switched on the `bandplot/weight` options and entered `=.bwdef` into `Weights def file` in the `bandplot` submenu of `fedit`.

The objective is to find out how many electrons take part in the bonding between P_1 and P_2 (see Fig. 1).

Please follow the instructions below:

- Please execute

```
xfplo -bw &
```

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

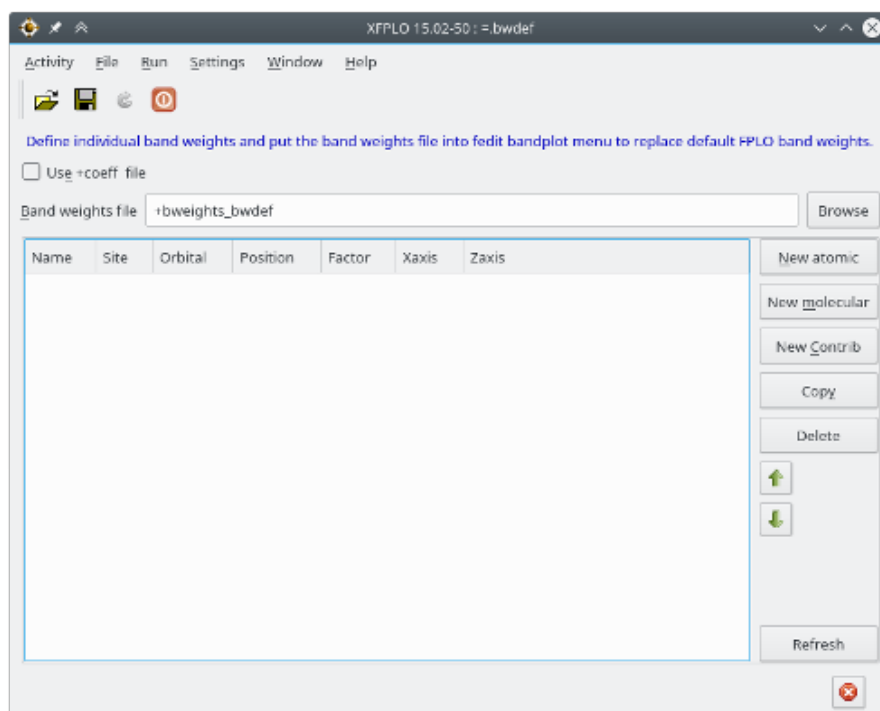


Figure 2: The empty band weight editor

- From the menu select **Activity** > **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 1).
- In the BWE click the **New molecular** button to open the molecular orbital dialog (MOD), Fig. 3

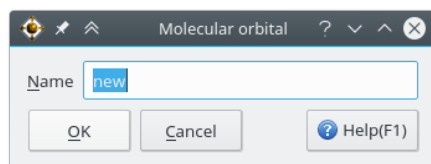


Figure 3: Molecular orbital dialog

- Enter the name: **P p\$_z\$.** **\$~s** (The number of characters is limited. But the name can be changed later while plotting fatbands.)
Now, a new line appeared in the BWE and it should be selected (highlighted). Hit **space**, **enter** or **double click** on it to edit it again.

- Now, we add a contribution to the molecular projector: Hit the **New Contrib** button, which brings up the molecular orbital contribution dialog MOCD Fig. 4. It differs from the Atomic-Orbital-Dialog (AOD) by having an additional **position** and a **factor**.

Figure 4: Molecular orbital contribution dialog

The reason for this is easy to understand. A molecular orbital projector consists of a linear combination of atomic orbitals at particular sites (position), each with a certain coefficient (factor). A molecular projector for a (periodic) system can be defined in any unit cell. It's geometry is then translated into each unit cell to obtain corresponding Bloch sums. In order to define such a projector, we have to specify the positions of the individual orbital contributions in absolute coordinates in order to obtain their relative mutual positioning. (The site vector defined by the site number is not sufficient here.) This is what position is needed for. We will now setup a molecular orbital projector consisting of two p_z orbitals at P_1 and P_2 , such that they form a bonding (Fig. 5) and anti-bonding combination. The MOs are

$$\begin{aligned}\Phi_{\text{bonding}} &= \frac{1}{\sqrt{2}}(p_{z1} - p_{z2}) \\ \Phi_{\text{anti-bonding}} &= \frac{1}{\sqrt{2}}(p_{z1} + p_{z2})\end{aligned}$$

- Hit the **Get atom** button and click on the atom P_1 . Select $3p+0$ in the **orbital** line edit. Set **factor** to 0.707 ($\approx \frac{1}{\sqrt{2}}$) and leave the axes unchanged. Hit **enter**.

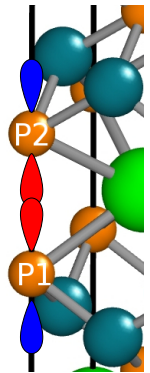


Figure 5: The MO projector.

Note, that the factors matter for the normalization of the resulting fatbands and DOS.

- Hit the **New Contrib** button again followed by the **Get atom** button. Click on the P₂ atom and chose 3p+0 for **orbital** and -0.707 for **factor**. Hit **enter**. Please notice that you can use the **Get Position** button to only correct the position.
- Now, Select the first line by using cursor keys or single clicking on it.
- Hit the **copy** button. Hit **enter** and change the end from \$~s to \$~s*.
- In the BWE select the last line and hit **enter**. Set the **factor** to 0.707 and hit **enter**.
- In general you can move stuff around with the **up/down arrow** buttons or by using **Ctrl-Up/Ctrl-Down**. If the current line is the title line of a molecular projector, the whole projector is moved. If is a contribution only the contrib will be moved.

This is what you should have right now:

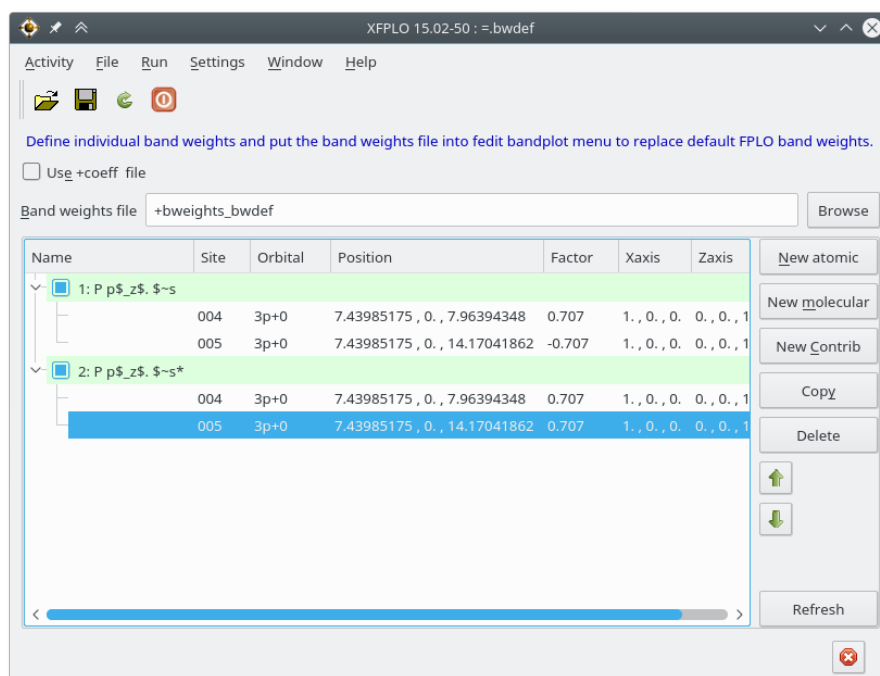


Figure 6: The band weigh editor with content

- In the BWE hit **Ctrl-S** or use **File > Save**.
- Leave the BWE (**Ctrl-Q** or **Activity > Quit all**) and ignore warnings.
- Have a look at **=.bwdef**:

```

coefficients +coeff
bweights +bweights_bwdef

bwdef molecular on
  name P p$_z$. $~s
  contrib
    site 4
    position 7.439851754099762 0. 7.96394348431756
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
    orbital 3p+0
    fac 0.707 0.
  contrib
    site 5
    position 7.439851754099762 0. 14.170418617732352
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
    orbital 3p+0
    fac -0.707 0.
bwdef molecular on
  name P p$_z$. $~s*
  contrib
    site 4
    position 7.439851754099762 0. 7.96394348431756
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
    orbital 3p+0
    fac 0.707 0.
  contrib
    site 5
    position 7.439851754099762 0. 14.170418617732352
    xaxis 1. 0. 0.
    zaxis 0. 0. 1.
    orbital 3p+0
    fac 0.707 0.

```

- Now, open `fedit22.00-62-x86_64`, and convince yourself that in `bandplot-submenu` both `bandstructure-plot` and `weights` are switched on as well as that `weights def` file contains `=.bwdef`. Check that in the `fedit` `main menu` the flag `use data directories` is switched on .

- Execute `fplo`:

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

You should now have the sub directories `+dos`, `+bdos` and the files `+band/+bweights_bwdef`.

- Execute

```
xfbp bond.xpy
```

to obtain Fig. 7. Also, have a look at `bond.xpy` by using `Edit > Script/transformations` to get a flavour of the possibilities.

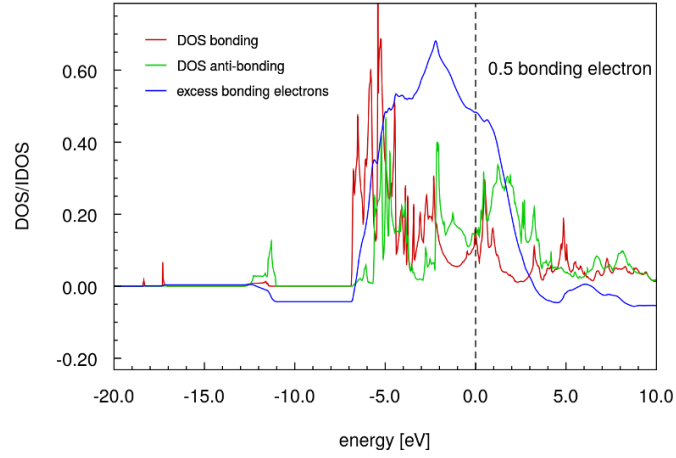


Figure 7: The bonding analysis. The red curve is the spin sum of the bonding MO DOS and the blue the anti-bonding MO DOS. The blue curve is the difference of the two corresponding IDOS and shows how many more bonding electrons there are than anti-bonding electrons. In our case the bond has a net 0.5 bonding electrons. If you use the wrong **factors** this value changes!

- Finally:

`xfbp bwei.xpy`

will show the fatbands (Fig. 8), which are not of much use here.

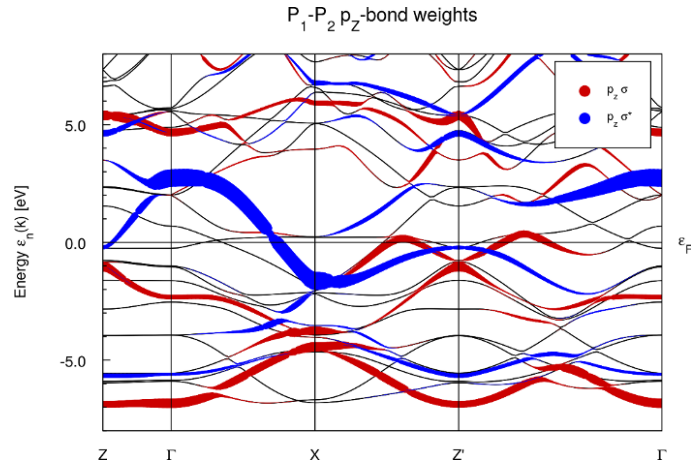


Figure 8: The MO fatbands.