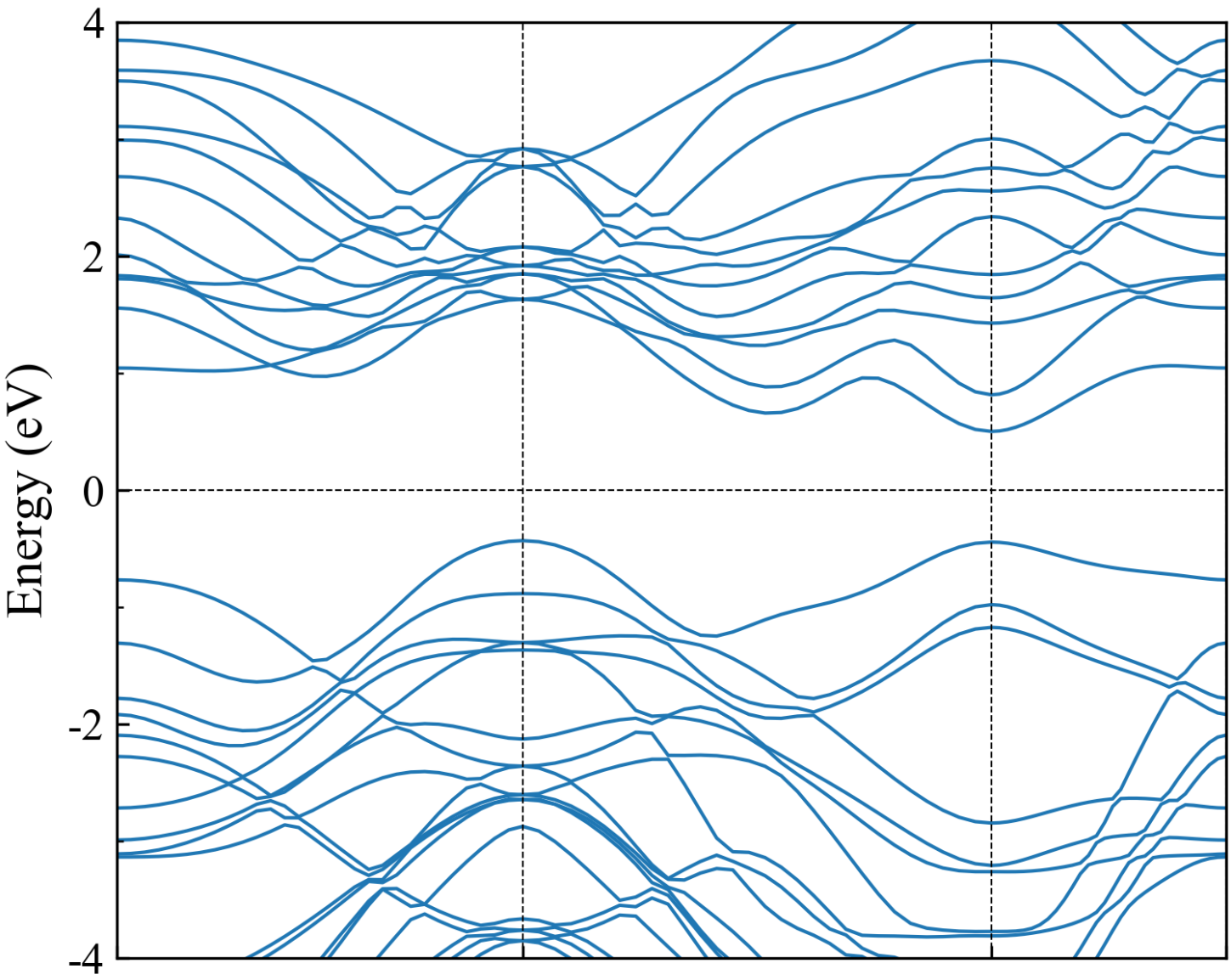
pyband

When no argument is given, pyband reads in OUTCAR (optionally KPOINTS) and find the band information within. It then plots the resulting band structure and save it as band.png.

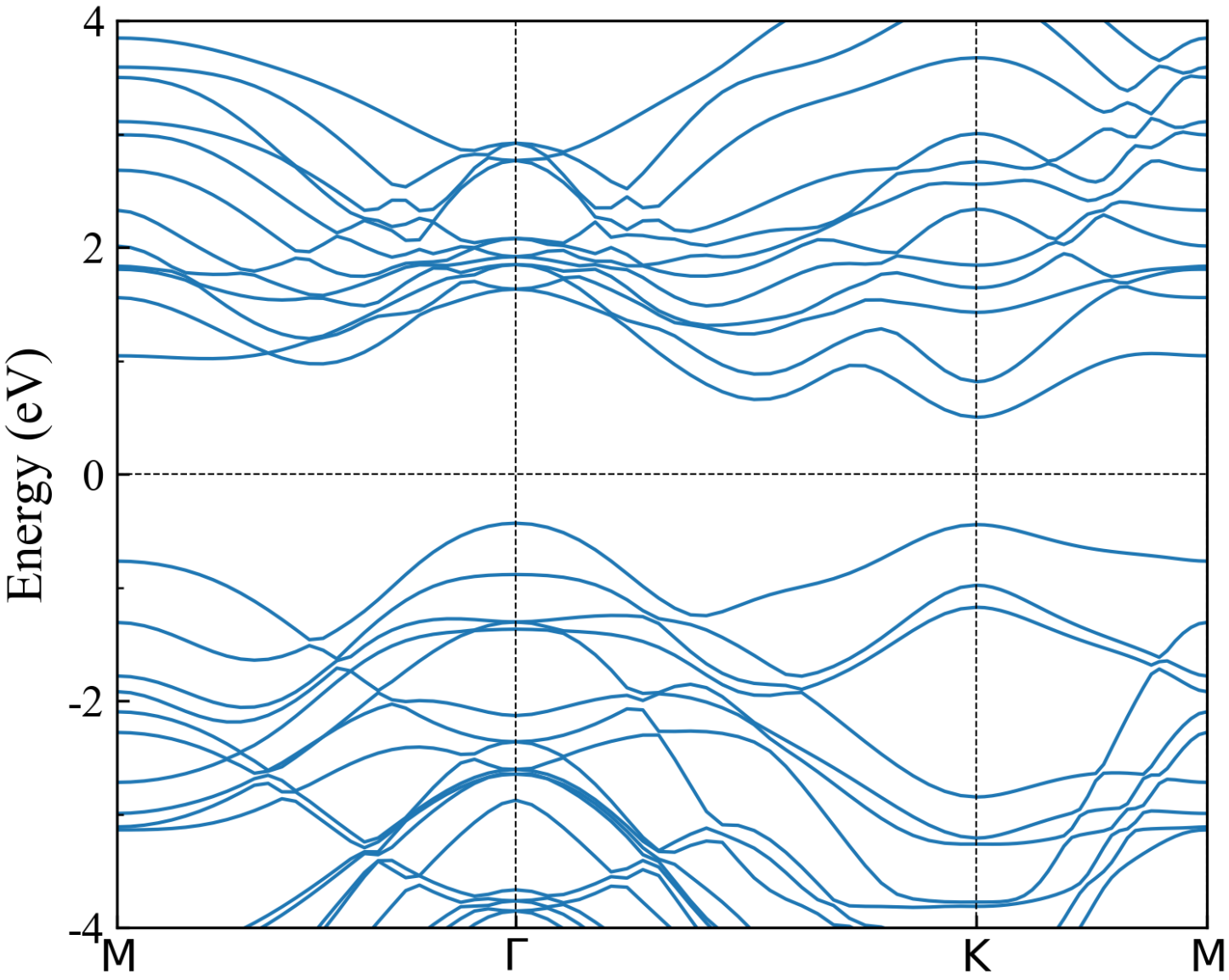
$ pyband



The default output image name can be changed by adding -o YourImageName.suffix to the above command line. Note that the image format is automatically recognized by the script, which can be any format that is supported by matplotlib. The size of the image can also be speified by -s width height command line arguments.

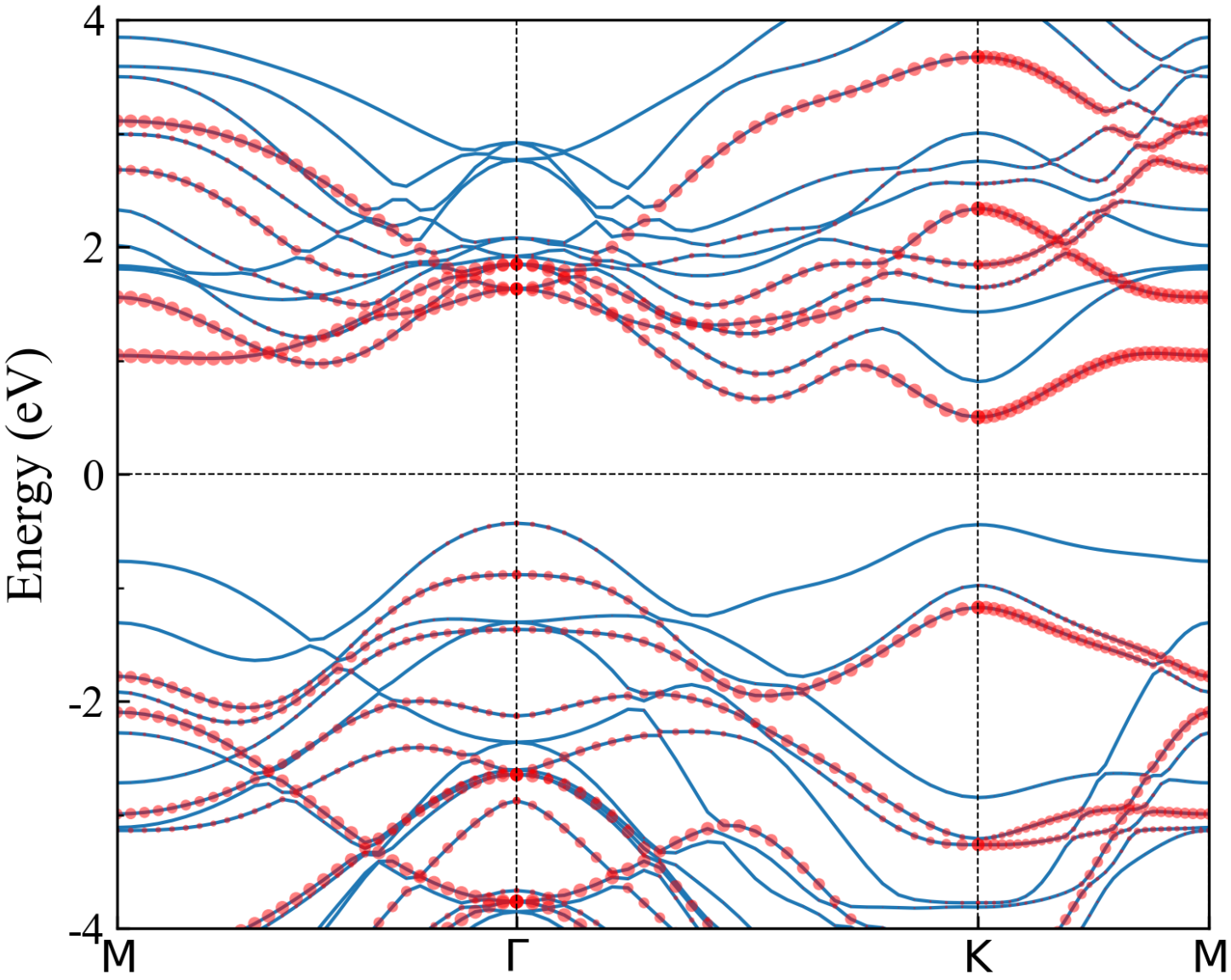
The labels of the high-symmetry K-points, which are not shown in the figure, can be designate by -k flag.

$ pyband -k mgkm



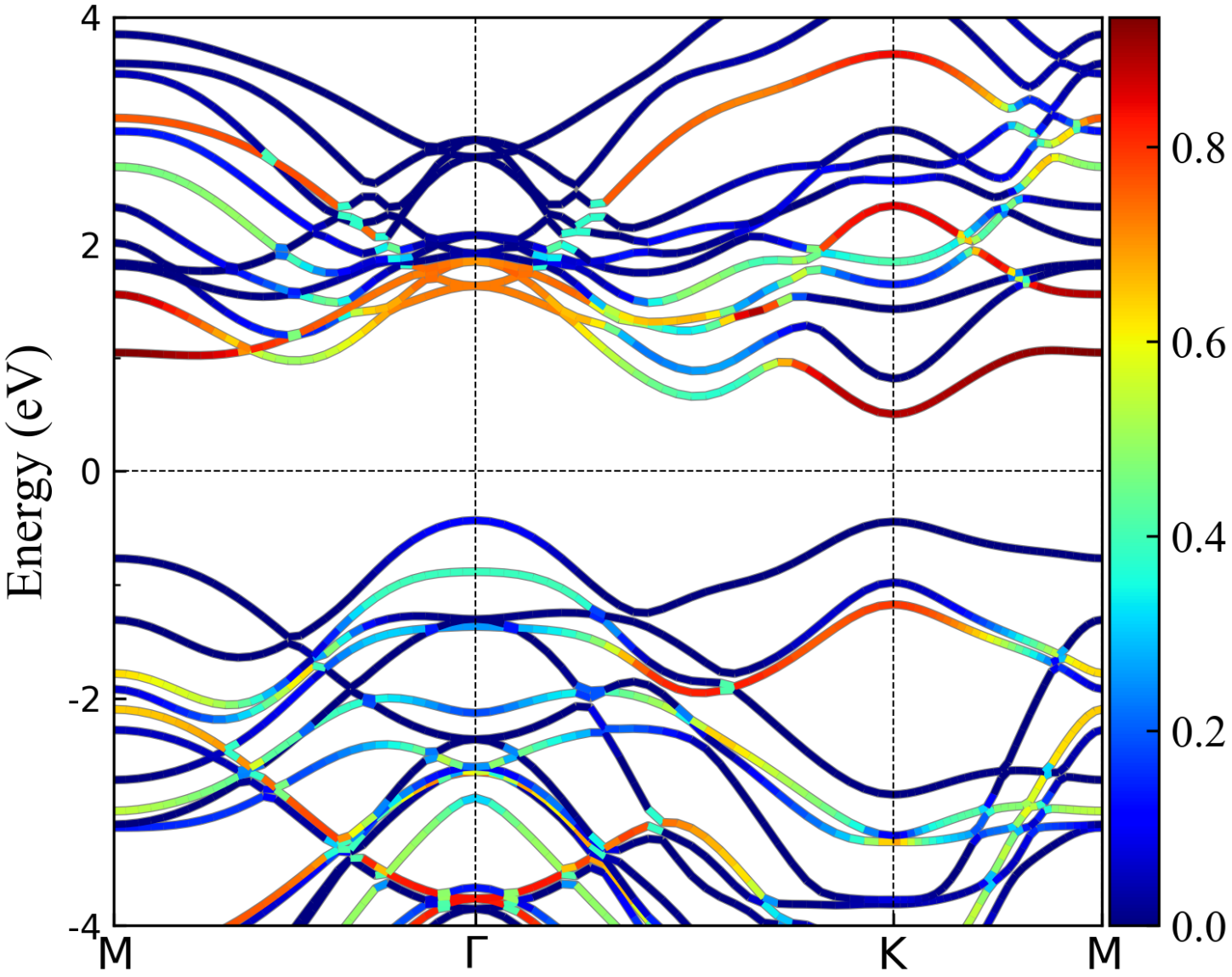
In some cases, if you are interested in finding out the characters of each KS states, e.g. the contribution of some atom to each KS state, the flag --occ atoms comes to help.

$ pyband --occ '1 3 4'



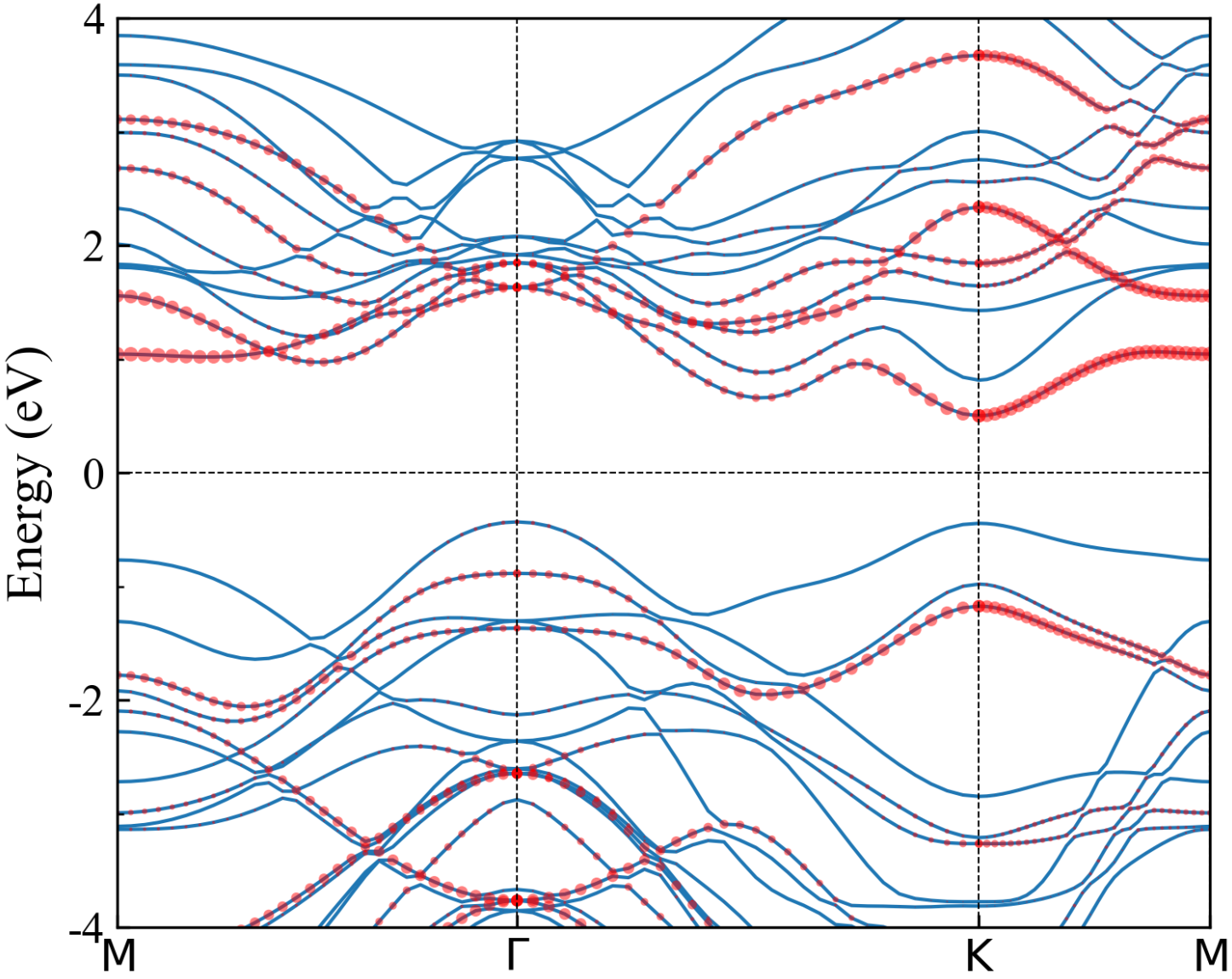
where 1 3 4 are the atom index starting from 1 to #atoms in the above image. The size of red dots in the figure indicates the weight of the specified atoms to the KS states. This can also be represented using a colormap:

```
$ pyband --occ '1 3 4' --occL
```



The spd-projected weight can also be specefied:

```
$ pyband --occ '1 3 4' --spd '4 5 6 7 8'
```



where in the arguments of --spd:

> s orbital: 0

> py, pz, px orbital: 1 2 3

> dxy, dyz, dz2, dxz, dx2 orbital: 4 5 6 7 8

More command line arguments can be found by pyband -h.