

position	$k_x$	$k_y$	$k_z$	name
0.00000	0.0	0.0	0.0	$\Gamma$
0.70711	1/2	1/2	0.0	X
0.83430	1/2	1/2	1/2	P
0.96947	0.457695	0.457695	1	$\Gamma_3$
1.63082	0.0	0.0	1	Z
1.88520	0.0	0.0	0.0	$\Gamma$
2.41756	0.0	0.532355	0.0	$\Gamma_1$
2.88520	0.467644	0.532355	0.0	$\Gamma_2$

Table 1: Default  $k$  path chosen by FPLO.  $\mathbf{k} = (k_x, k_y, k_z)$  is given in units of the reciprocal lattice vectors.

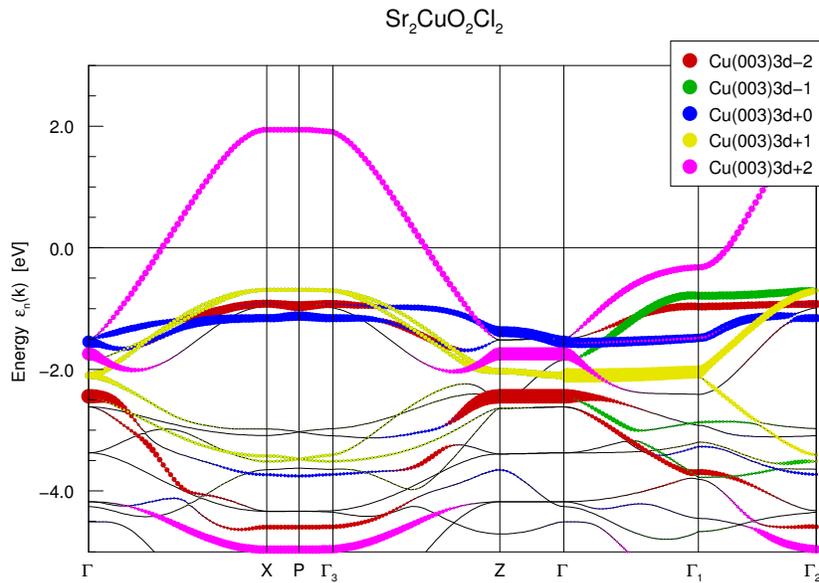


Figure 1: Default FPLO band structure of  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ . Correspondence between magnetic quantum number and orbital are:  $m = -2$  is  $d_{xy}$ ,  $m = -1$  is  $d_{yz}$ ,  $m = 0$  is  $d_{z^2}$ ,  $m = 1$  is  $d_{xz}$ ,  $m = 2$  is  $d_{x^2-y^2}$ .