SrPtAs
SrPtAs.bands.agr

SrPtAs atom 0   size 0.20
SrPtAs.spaghetti_ps

Energy(eV)

E_F

Γ   M   K   Γ   A

Energy (eV)

8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
-6.0
-7.0
-8.0
-9.0
-10.0
-11.0
-12.0
-13.0
-14.0

E_F

Γ   Σ   M   K   Λ   Γ Δ A

WIEN2k 17.1 using https://raw.githubusercontent.com/gsabo/WIEN2k-Patches/master/17.1/bz_lin.patch

SrPtAs.bands.agr (~/wiendata/SrPtAs) - gedit

Open Save Undo Q Q

SrPtAs.bands.agr ✕

```
#     k       ene        character
@ autoscale onread none
@ target g0.s1
@ type xysize

# bandindex:   1
  0.00000 -66.53963   0.07000
  0.02233 -66.53962   0.07000
  0.04467 -66.53956   0.07000
  0.06700 -66.53964   0.07000
  0.08934 -66.53958   0.07000
  0.11167 -66.53810   0.07000
  0.13400 -66.53847   0.07000
  0.15634 -66.53811   0.07000
  0.17867 -66.53851   0.07000
  0.20100 -66.53866   0.07000
  0.22334 -66.53804   0.07000
  0.24567 -66.53842   0.07000
  0.26801 -66.53853   0.07000
  0.29034 -66.53837   0.07000
  0.31267 -66.53831   0.07000
  0.33501 -66.53807   0.07000
  0.35734 -66.53809   0.07000
  0.37968 -66.53845   0.07000
```

SrPtAs.klist_band (~/wiendata/SrPtAs) - gedit

Open Save Undo Q

SrPtAs.klist_band ✕

```
GAMMA    0    0    0   40   2.0-0.5  1.5    Template for hcp
         1    0    0   40   2.0
         2    0    0   40   2.0
         3    0    0   40   2.0
         4    0    0   40   2.0
         5    0    0   40   2.0
         6    0    0   40   2.0
         7    0    0   40   2.0
         8    0    0   40   2.0
         9    0    0   40   2.0
SIGMA   10    0    0   40   2.0
        11    0    0   40   2.0
        12    0    0   40   2.0
        13    0    0   40   2.0
        14    0    0   40   2.0
        15    0    0   40   2.0
        16    0    0   40   2.0
        17    0    0   40   2.0
```

Plain Text ▾   Tab Width: 8 ▾   Ln 9, Col 36

1. SIGMA found as k point number 10 in case.klist_band. Finding case.bands.agr 10 k point number 10 in case.bands.agr gives the k value of 0.22334 for SIGMA.

Grace: SrPtAs.bands.agr

File Edit Data Plot View Window   Help

G0: X, Y = [0.473788, -1.67412]

Draw

Energy(eV)

0

-5

-10

Γ   Σ   M

AutoT
AutoO
ZX ZY
AX AY
PZ Pu
Po Cy
SD:1
CW:0
Exit

2. With case.bands.agr opened in xmgrace, Plot →Axis properties

Grace: Axes

Edit: X axis   ■ Active

Start: 0   Stop: 1.40326

Scale: Linear   ⊐ Invert axis

Main | Axis label & bar | Tick labels | Tick marks | Special

Special ticks: Tick marks and labels ▾

Number of user ticks to use: 6 ▼ ▲

Tick location - Label:

0	0	ΓxG
1	0.22334	ΓxS
2	0.44668	M
3	0.70456	K
4	1.22034	ΓxG
5	1.40326	A

Apply to: Current axis ▾

Apply   Accept   Close

3. Adjust "Number of user ticks to use" and "Tick location - Label" for SIGMA, then click Apply to add Σ to the plot.