

BoltzTraP_Tools Tutorials

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1 Tutorials

For all tutorials only the plot of seebeck coefficient and power factor will be done.

1.1 CoSb₃ System:

1.1.1 Tutorial 1 : Plot at Define Temperature:

For this tutorial CoSb3.trace file is needed, as well as the Fermi level which is about $\epsilon_{Fermi} = 0.55475 \text{ Ry}$ (see *intrans file*).

- *Plotting as a function of Energy :*

```
In [1]: from BoltzTraP_Tools import *
        %pylab inline
        labels=Labels_Init()
        Scaling_DATA(labels)
        Analyse=raw_input("File Extension (Trace, Condens, N-Trace, or N-Condens) ? > ") # or
        File_DATA,Ef=File_Read(Analyse)
        DATA_Process(Analyse,File_DATA,Ef,labels)
```

Populating the interactive namespace from numpy and matplotlib

Setting of Units and Scale Factors (y/n) ? > n

File Extension (Trace, Condens, N-Trace, or N-Condens) ? > Trace

Trace File name ? > ../tests/CoSb3/CoSb3.trace

Fermi Level Value in Ry ? > 0.55475

=====

Parse at fixed Temperature or Energy ? (T/E) > T

Log Scale for Carrier Concentration ? (y/n) > n

Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, c or chi) ? > E

Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, c or chi) ? > S

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 250
250

Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

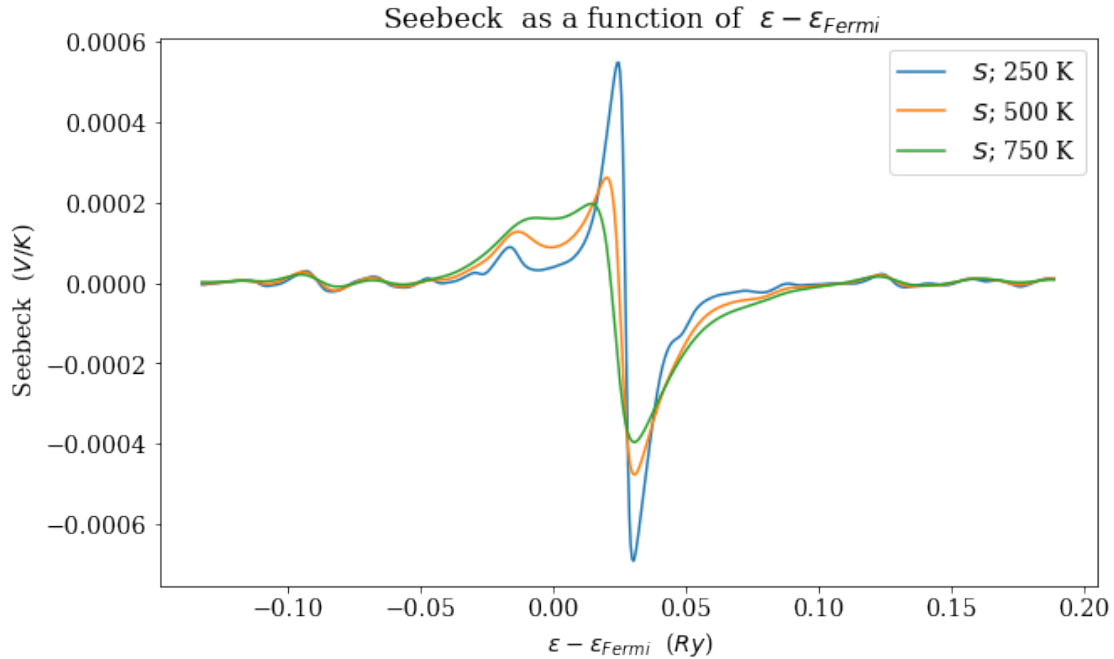
MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 500
500

Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750
750

Plot Other Quantities ? (yes/no)? > no



```

To restart write 'restart' , else no > restart
Parse at fixed Temperature or Energy ? (T/E) > T
Log Scale for Carrier Concentration ? (y/n) > n
Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, c or chi ) ? > E
Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, c or chi ) ? > PF

```

```

Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 250
250
Plot Other Quantities ? (yes/no)? > yes

```

```

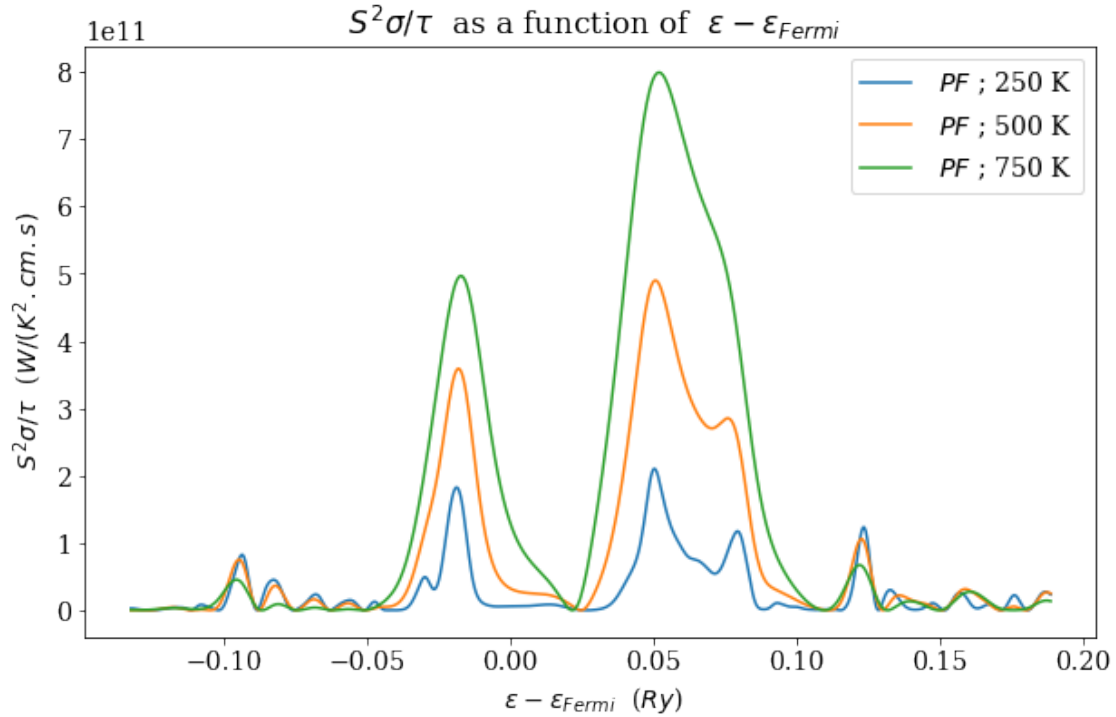
Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 500
500
Plot Other Quantities ? (yes/no)? > yes

```

```

Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 750
750
Plot Other Quantities ? (yes/no)? > no

```



To restart write 'restart' , else no > no

Exit!..

=====

- **Plotting as a function of Carriers :**

To get plot of *n*-Type (electron) or *p*-Type (hole) carriers, the Log Scale of carrier must be selected.

```
In [1]: from BoltzTraP_Tools import *
        %pylab inline
        labels=Labels_Init()
        Scaling_DATA(labels)
        Analyse="Trace"
        File_DATA,Ef=File_Read(Analyse)
        DATA_Process(Analyse,File_DATA,Ef,labels)
```

Populating the interactive namespace from numpy and matplotlib

Setting of Units and Scale Factors (y/n) ? > n

Trace File name ? > ../tests/CoSb3/CoSb3.trace

Fermi Level Value in Ry ? > 0.55475

=====

```

Parse at fixed Temperature or Energy ? (T/E) > T
Log Scale for Carrier Concentration ? (y/n) > y
Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > N
Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > S

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 250
250
Plot electron or hole ? > electron
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 250
250
Plot electron or hole ? > hole
Plot Other Quantities ? (yes/no)? > yes

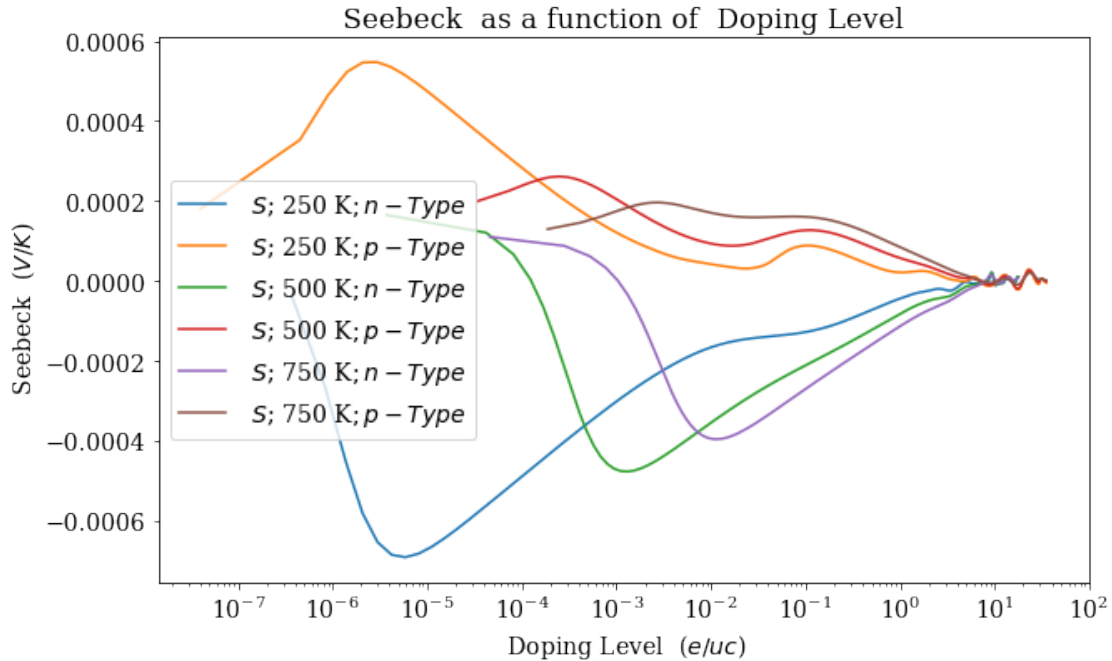
Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 500
500
Plot electron or hole ? > electron
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 500
500
Plot electron or hole ? > hole
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750
750
Plot electron or hole ? > electron
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750
750
Plot electron or hole ? > hole
Plot Other Quantities ? (yes/no)? > no

```



```
To restart write 'restart' , else no > restart
Parse at fixed Temperature or Energy ? (T/E) > T
Log Scale for Carrier Concentration ? (y/n) > y
Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > N
Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > PF
```

```
Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 300
300
Plot electron or hole ? > electron
Plot Other Quantities ? (yes/no)? > yes
```

```
Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 300
300
Plot electron or hole ? > hole
Plot Other Quantities ? (yes/no)? > yes
```

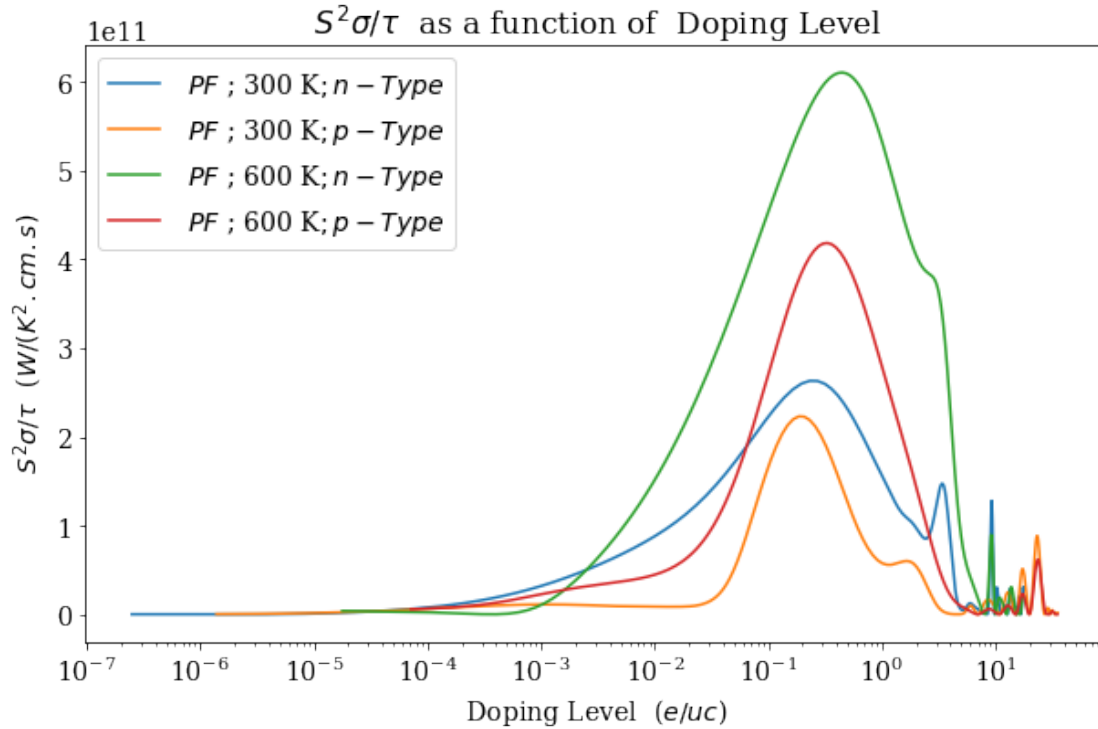
```
Give a Temperature Value :
  MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 600
600
Plot electron or hole ? > electron
Plot Other Quantities ? (yes/no)? > yes
```

```
Give a Temperature Value :
```

```

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 600
600
Plot electron or hole ? > hole
Plot Other Quantities ? (yes/no)? > no

```



To restart write 'restart' , else no > no

Exit!..

=====

1.1.2 Tutorial 2 : Plot at Define Energy Level:

It is also possible to plot Data at fixed energy value. However, the energy value must be in the output file. A trick to give the value :

$$Value = E_{min} + n \times dE \quad ; \quad where, \quad n = 0, 1, 2, \dots, \frac{E_{max} - E_{min}}{dE}$$

```
In [1]: from BoltzTraP_Tools import *
```

```
In [2]: %pylab inline
        labels=Labels_Init()
```

```

Scaling_DATA(labels)
Analyse="Trace"
File_DATA,Ef=File_Read(Analyse)
DATA_Process(Analyse,File_DATA,Ef,labels)

```

Populating the interactive namespace from numpy and matplotlib

Setting of Units and Scale Factors (y/n) ? > n

Trace File name ? > ../tests/CoSb3/CoSb3.trace

Fermi Level Value in Ry ? > 0.55475

=====

Parse at fixed Temperature or Energy ? (T/E) > E

Log Scale for Carrier Concentration ? (y/n) > n

Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi) ? > T

Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi) ? > S

Give a Energy Value :

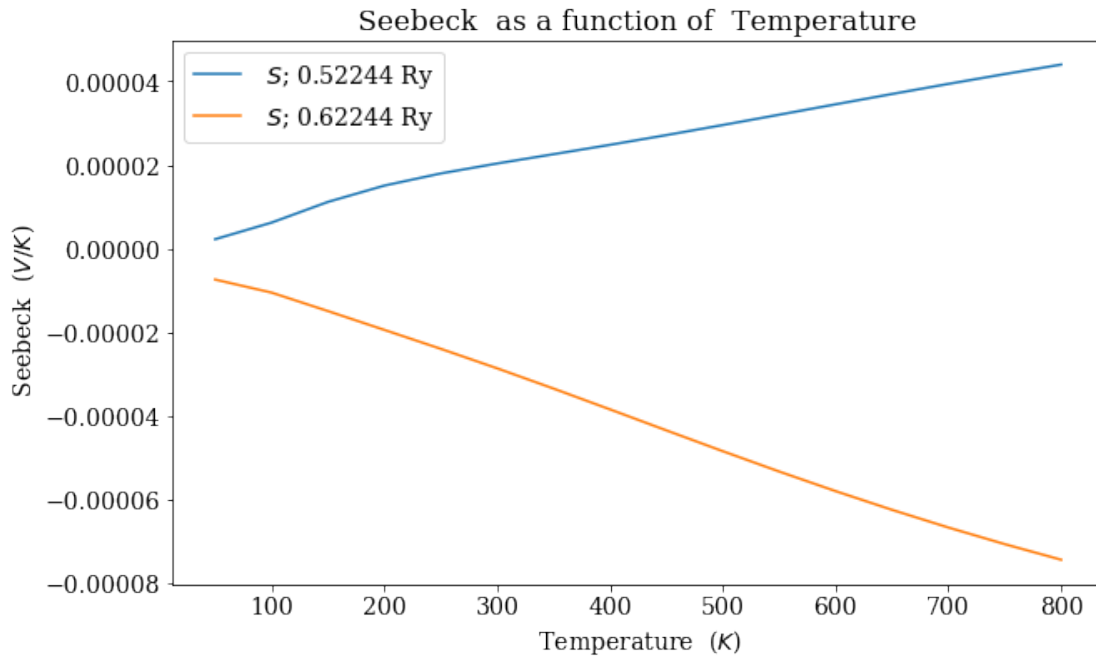
MIN=0.422440 ; MAX=0.743440 ; Delta=0.000500 (unit: Ry) > 0.42244+200*0.0005
0.52244

Plot Other Quantities ? (yes/no)? > yes

Give a Energy Value :

MIN=0.422440 ; MAX=0.743440 ; Delta=0.000500 (unit: Ry) > 0.42244+400*0.0005
0.62244

Plot Other Quantities ? (yes/no)? > no



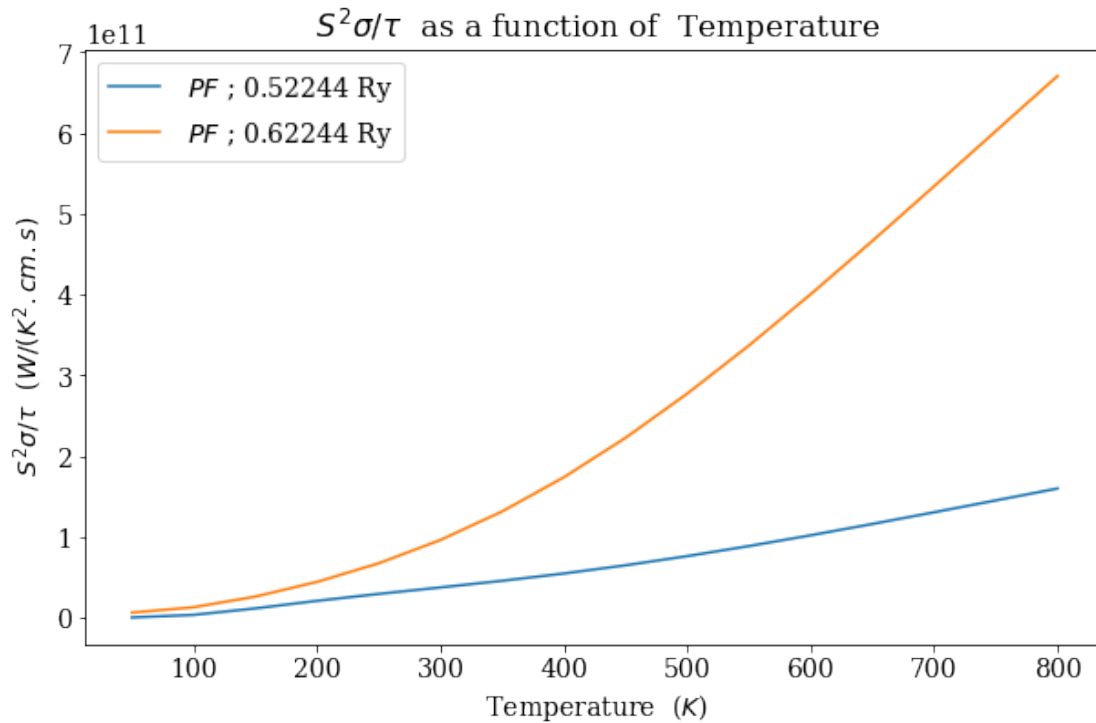

```

To restart write 'restart' , else no > restart
Parse at fixed Temperature or Energy ? (T/E) > E
Log Scale for Carrier Concentration ? (y/n) > n
Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > T
Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > PF

Give a Energy Value :
    MIN=0.422440 ; MAX=0.743440 ; Delta=0.000500 (unit: Ry) > 0.42244+200*0.0005
0.52244
Plot Other Quantities ? (yes/no)? > yes

Give a Energy Value :
    MIN=0.422440 ; MAX=0.743440 ; Delta=0.000500 (unit: Ry) > 0.42244+400*0.0005
0.62244
Plot Other Quantities ? (yes/no)? > no

```



```

To restart write 'restart' , else no > no

```

```

Exit!..

```

```

=====

```

1.1.3 Tutorial 3 : Plot at Define Doping Level:

For this tutorial CoSb3.trace_fixdoping file is needed, as well as the Fermi level which is about $\epsilon_{Fermi} = 0.55475 \text{ Ry}$ (see *intrans* file).

```
In [1]: from BoltzTraP_Tools import *
        %pylab inline
        labels=Labels_Init()
        Scaling_DATA(labels)
        File_DATA,Ef=File_Read("N-Trace")
        DATA_Process("N-Trace",File_DATA,Ef,labels)
```

Populating the interactive namespace from numpy and matplotlib

Setting of Units and Scale Factors (y/n) ? > n

N-Trace File name ? > ../tests/CoSb3/CoSb3.trace_fixdoping

Fermi Level Value in Ry ? > 0.55475

=====

Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi) ? > T

Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi) ? > S

Doping Carrier Concentrations (/uc) : [-0.03691982 0.03691982]

Give a Doping Value from above > -0.03691982

-0.03691982

Give the Cell Volume in cm³ to convert N ; else give 1.0) > 1

Plot Other Quantities ? (yes/no)? > yes

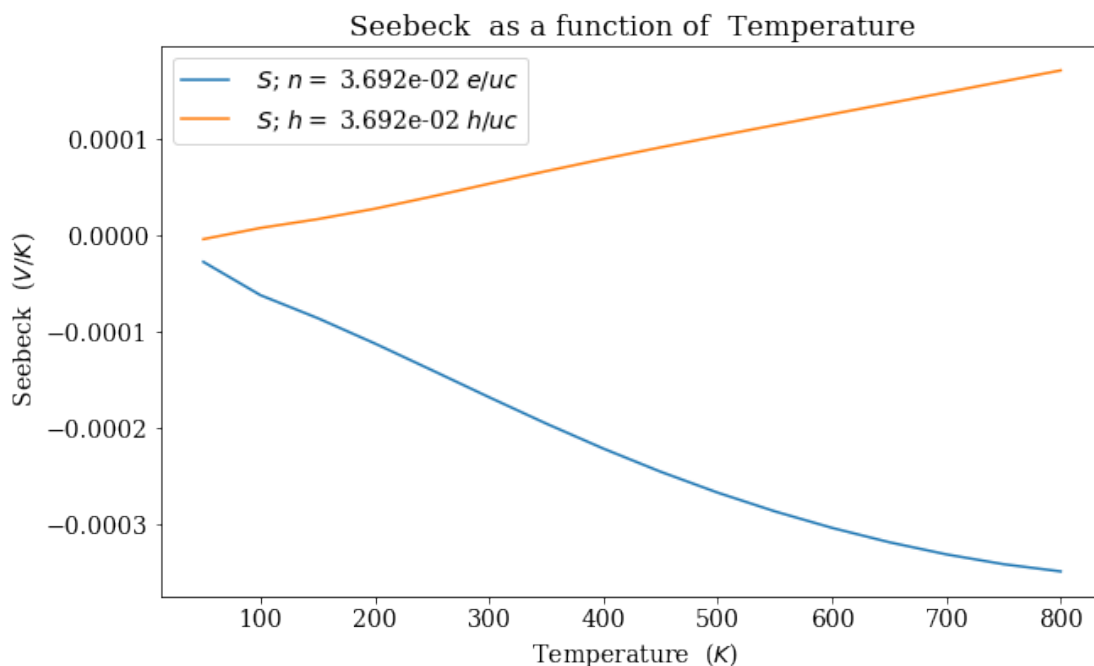
Doping Carrier Concentrations (/uc) : [-0.03691982 0.03691982]

Give a Doping Value from above > 0.03691982

0.03691982

Give the Cell Volume in cm³ to convert N ; else give 1.0) > 1

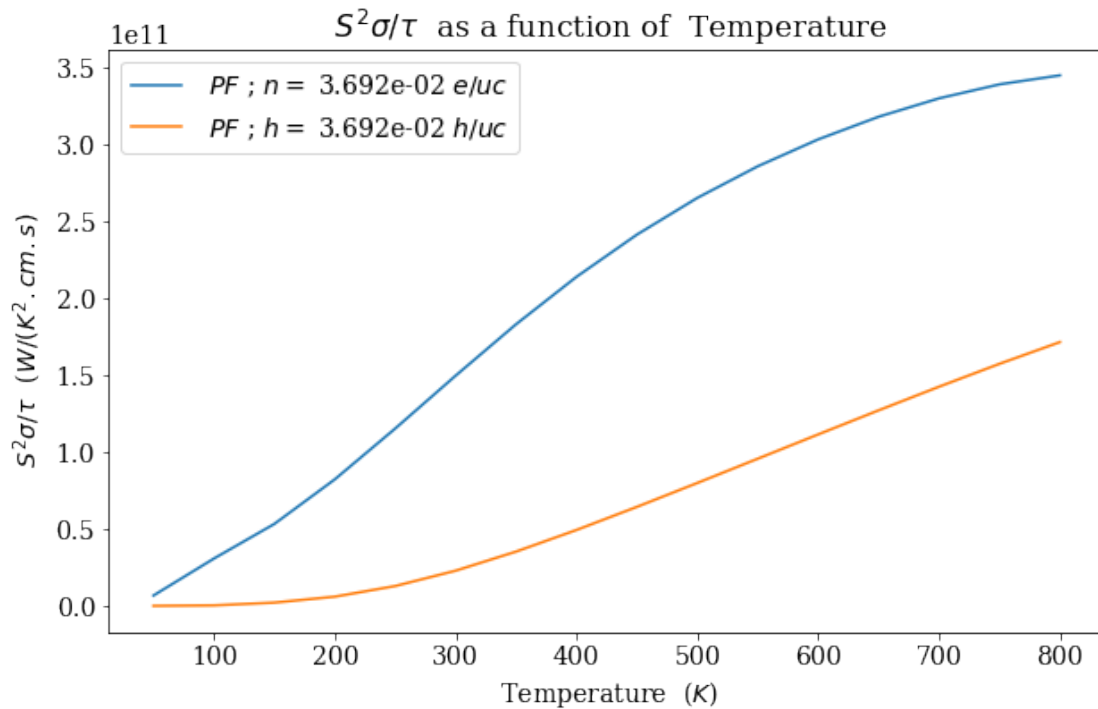
Plot Other Quantities ? (yes/no)? > no



```

To restart write 'restart' , else no > restart
Xplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > T
Yplot (E, T, N, DOS, S, Sigma, PF, R_H, Kappa, C or Chi ) ? > PF
Doping Carrier Concentrations (/uc) : [-0.03691982  0.03691982]
Give a Doping Value from above > -0.03691982
-0.03691982
Give the Cell Volume in cm^3 to convert N ; else give 1.0) > 1
Plot Other Quantities ? (yes/no)? > yes
Doping Carrier Concentrations (/uc) : [-0.03691982  0.03691982]
Give a Doping Value from above > 0.03691982
0.03691982
Give the Cell Volume in cm^3 to convert N ; else give 1.0) > 1
Plot Other Quantities ? (yes/no)? > no

```



```

To restart write 'restart' , else no > no

```

Exit!..

=====

1.2 LiZnSb System:

1.2.1 Tutorial 4 : Plot Tensor (xx and zz):

For this tutorial LiZnSb.condtens file is needed, as well as the Fermi level which is about $\epsilon_{Fermi} = 0.37654$ Ry (see *intrans* file).

```
In [3]: from BoltzTraP_Tools import *
        %pylab inline
        labels=Labels_Init()
        Scaling_DATA(labels)
        Analyse="Condtens"
        File_DATA,Ef=File_Read(Analyse)
        DATA_Process(Analyse,File_DATA,Ef,labels)

Populating the interactive namespace from numpy and matplotlib
Setting of Units and Scale Factors (y/n) ? > n
        Condtens File name ? > ../tests/LiZnSb/LiZnSb.condtens
        Fermi Level Value in Ry ? > 0.37654
=====
Parse at fixed Temperature or Energy ? (T/E) > T
Log Scale for Carrier Concentration ? (y/n) > n
Xplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy,Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 250
250
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy,Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 250
250
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy,Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 500
500
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy,Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
    MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit:  K)  > 500
500
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy,Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :
```

```

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750
750
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

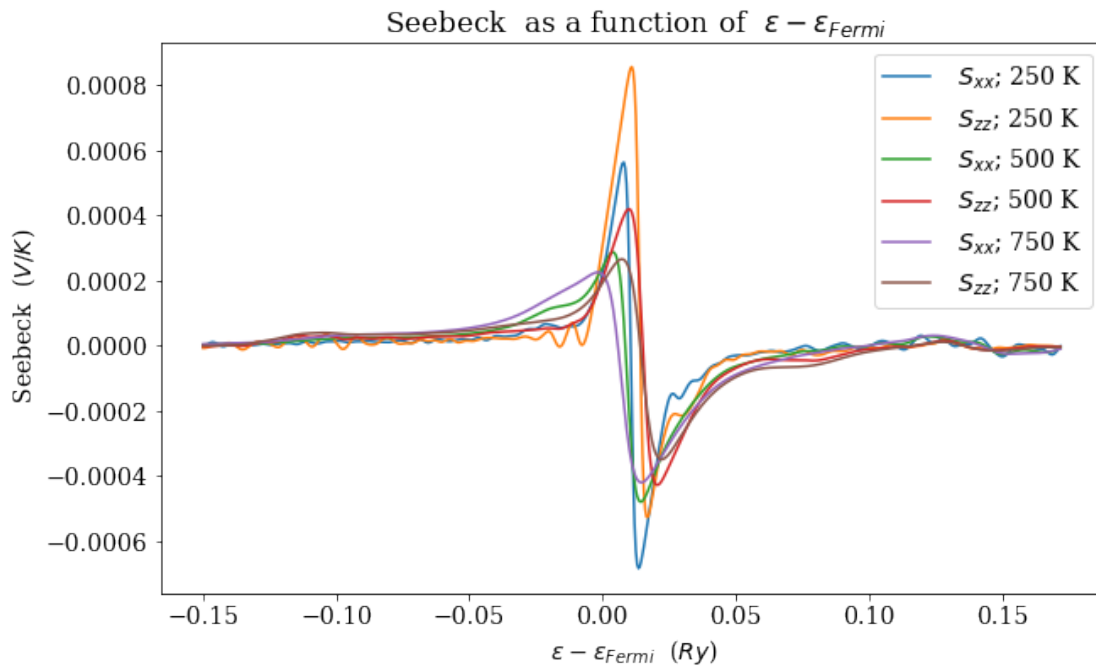
```

Give a Temperature Value :

```

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750
750
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > no

```



```

To restart write 'restart' , else no > restart
Parse at fixed Temperature or Energy ? (T/E) > T
Log Scale for Carrier Concentration ? (y/n) > n
Xplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,

```

Give a Temperature Value :

```

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 250
250
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

```

Give a Temperature Value :

```

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 250

```

250

Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 500

500

Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 500

500

Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750

750

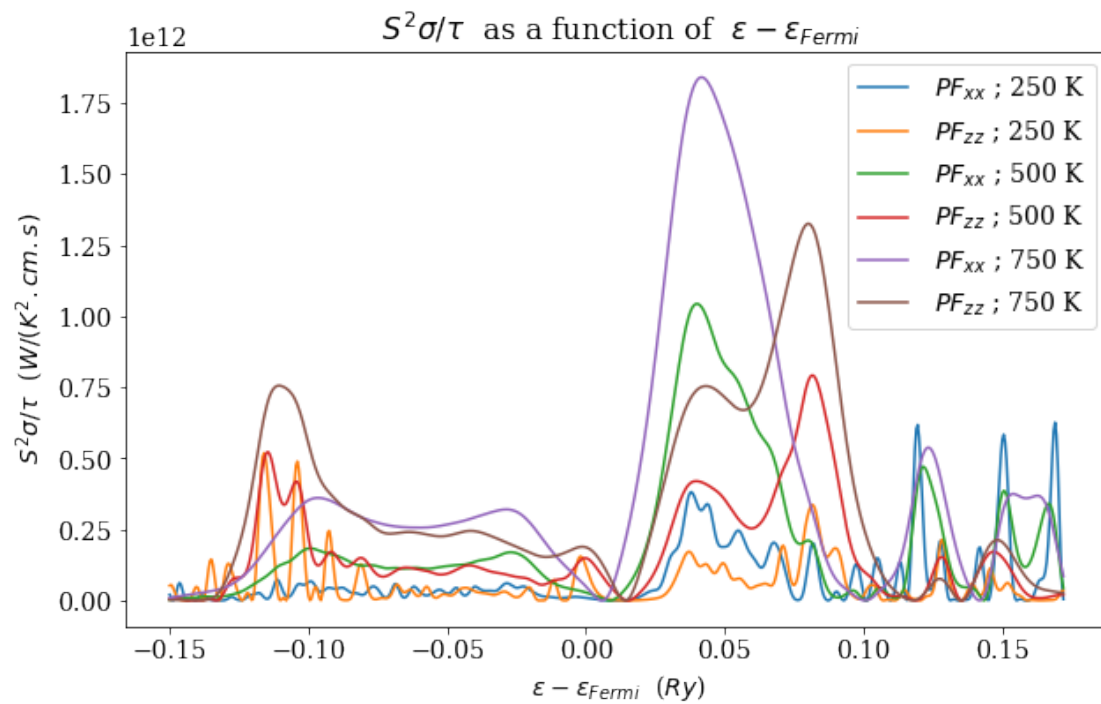
Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > yes

Give a Temperature Value :

MIN=50.000000 ; MAX=800.000000 ; Delta=50.000000 (unit: K) > 750

750

Yplot (E, T, N, S, Sxx, Syy, Szz, Sigma, Sigmaxx, Sigmayy, Sigmazz, PF, PFxx, PFyy, PFzz, Kappa,
Plot Other Quantities ? (yes/no)? > no



To restart write 'restart' , else no > no

Exit!..

=====