Scaling Quantities

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1 Units and Scale Factors

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

```
In [2]: #intializing all quantities
        l=Labels_Init()
        Scaling_DATA(l)
```

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

```
In [3]: for i in sorted(l):
            print "Unit of %10s is : %-25s"%(i,l[i][3])
```

```
Unit of        DOS is :  ($e/uc$)
Unit of          E is :  ($Ry$)
Unit of      Kappa is :  ($W/(m. K . s)$)
Unit of    Kappaxx is :  ($W/(m. K . s)$)
Unit of    Kappayy is :  ($W/(m. K . s)$)
Unit of    Kappazz is :  ($W/(m. K . s)$)
Unit of          N is :  ($e/uc$)
Unit of         PF is :  ($W/(K^2 . cm . s)$
Unit of       PFxx is :  ($W/(K^2 . cm . s)$
Unit of       PFyy is :  ($W/(K^2 . cm . s)$
Unit of       PFzz is :  ($W/(K^2 . cm . s)$
Unit of        R_H is :  ($m^3/C$)
Unit of          S is :  ($V/K$)
Unit of      Sigma is :  ($1/(\Omega . cm . s)$)
Unit of    Sigmaxx is :  ($1/(\Omega . cm . s)$)
Unit of    Sigmayy is :  ($1/(\Omega . cm . s)$)
Unit of    Sigmazz is :  ($1/(\Omega . cm . s)$)
Unit of        Sxx is :  ($V/K$)
Unit of        Syy is :  ($V/K$)
Unit of        Szz is :  ($V/K$)
Unit of          T is :  ($K$)
Unit of          c is :  ($J/(mol . K)$)
Unit of        chi is :  ($m^3/mol$)
```

In [4]:
```
# Scaling of Seebeeck Coefficiens
l["S"][3]= ' ($\mu V/K$) '
for i in ["Sxx","Syy","Szz"]:
    l[i][3]=l["S"][3]
# Check the new units
for i in ["S","Sxx","Syy","Szz"]:
    print "%-5s in %-s"%(i,l[i][3])
```

```
S     in  ($\mu V/K$)
Sxx   in  ($\mu V/K$)
Syy   in  ($\mu V/K$)
Szz   in  ($\mu V/K$)
```

In [5]:
```
#Scaling of Energy
print "Before : Energy unit : %s ; and Scaled by : %s"%(l["E"][3],l["E"][4])
l["E"][3]=' ($eV$) '
l["E"][4]=13.60569
print "After  : Energy unit : %s ; and Scaled by : %s"%(l["E"][3],l["E"][4])
```

```
Before : Energy unit :  ($Ry$)  ; and Scaled by : 1.0
After  : Energy unit :  ($eV$)  ; and Scaled by : 13.60569
```

In [6]:
```
#Scaling of Carriers number to cm^3
print "Before : Carriers unit : %s ; and Scaled by : %s"%(l["N"][3],l["N"][4])
l["N"][3]=' ($e/cm^3$) '
l["N"][4]= 1./6.3e-22  # here 6.3e-22 is an example which corresponds to unit cell volum
print "After  : Carriers unit : %s ; and Scaled by : %s"%(l["N"][3],l["N"][4])
```

```
Before : Carriers unit :  ($e/uc$)  ; and Scaled by : 1.0
After  : Carriers unit :  ($e/cm^3$)  ; and Scaled by : 1.5873015873e+21
```