# Density Functional Theory (DFT) Tutorial # 3

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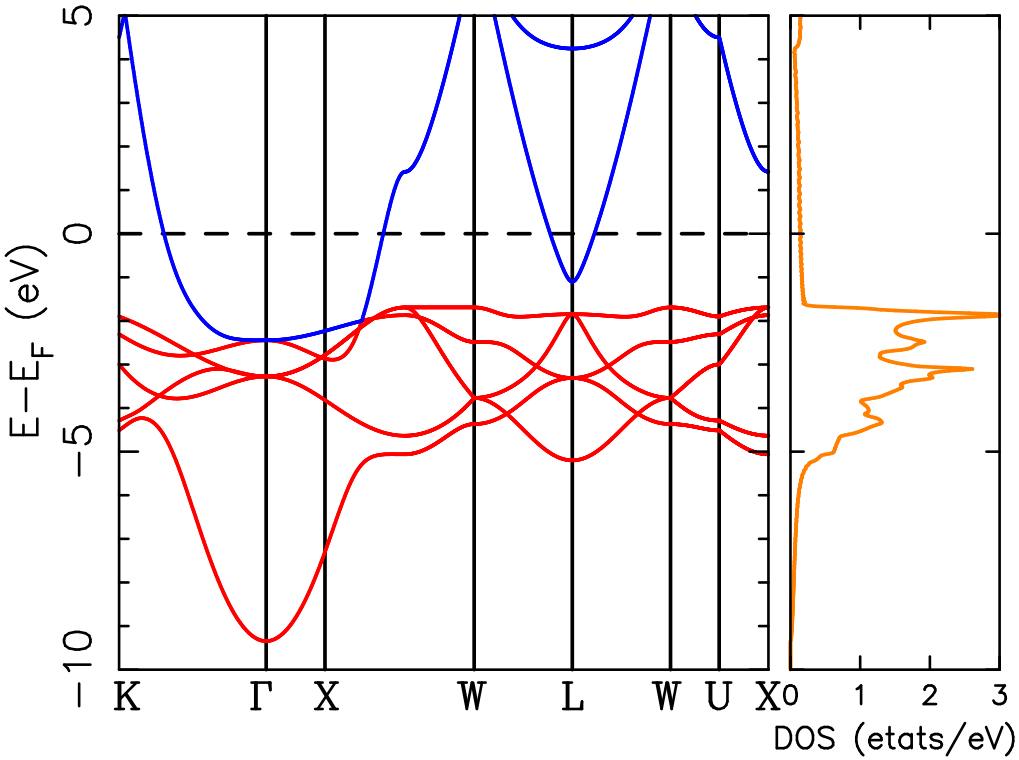
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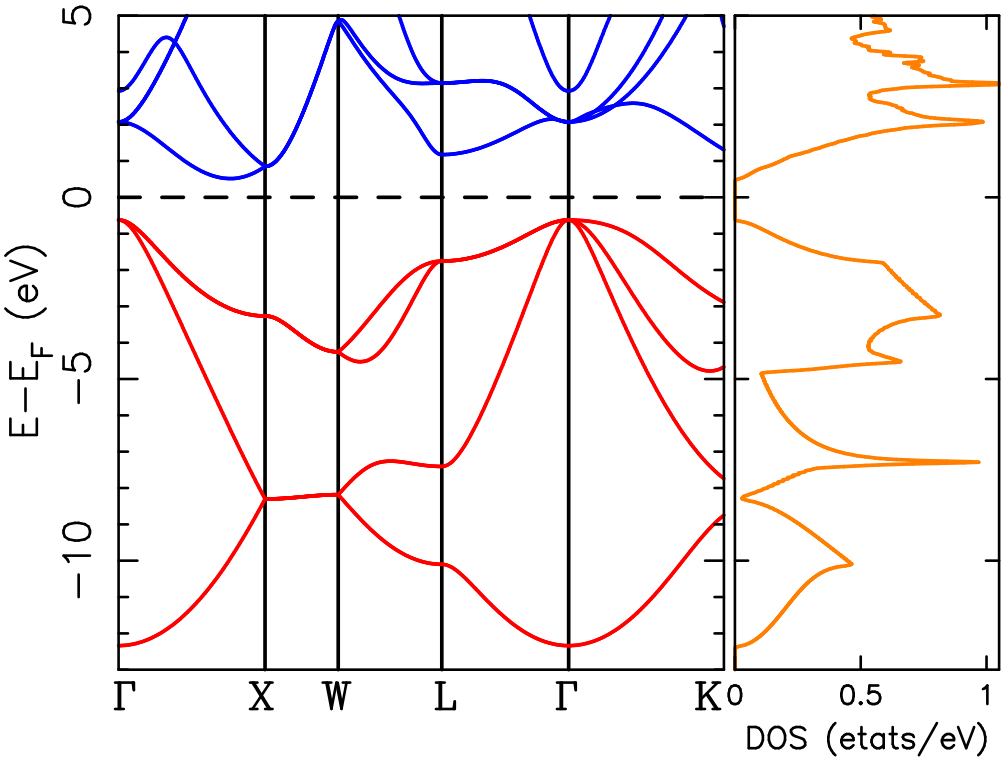
# Band Structure of Metals vs semiconductors

## Copper




- Copper has an even number of valence electrons (11)
- 5 bands are fully filled
- 1 bands is half filled

## Sillicon




- Sillicon has an even number of valence electrons (8)
- 4 bands are fully filled
- There is a gap between the fully filled bands (valence bands) and the empty ones (conduction bands)

# Occupations and Smearing issues

## Aluminum

```
 &control
    prefix='al'
    outdir='./OUT/'
    pseudo_dir = '../pseudo/',
 /
 &system
    ibrav=  2
    celldm(1) =7.50
    nat=  1, ntyp= 1
    ecutwfc =12.0
    occupations='smearing'
    smearing='marzari-vanderbilt'
    degauss=0.05
 /
ATOMIC_SPECIES
 Al  26.98 Al.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Al 0.00 0.00 0.00
K_POINTS automatic
  12 12 12 1 1 1
```

## Sillicon

```
 &control
    prefix='silicon',
    outdir='./OUT/',
    pseudo_dir='../pseudo/'
 /
 &system
    ibrav=  2
    celldm(1) =10.2
    nat=  2, ntyp= 1,
    ecutwfc = 12.0
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
   4 4 4 1 1 1
```

# Density of States Calculation

DOS calculation is a $3$ steps process (as band structure calculation)

$$\boxed{\text{SCF}} \Rightarrow \boxed{\text{NON SCF}} \Rightarrow \boxed{\text{DOS}}$$

- For non SCF calculation, set `calculation='nscf'`
- It reads from the output directory the electronic density and solves the Khon-Sham equation for specific k points
- The DOS calculation requires a very large number of k-points (conversely to the scf calculation)
- The last stet is to compute the DOS from the results of the non scf calculation

# Non SCF calculation

```
 &control
    calculation = 'nscf',
    prefix='al'
    pseudo_dir = '../pseudo/',
    outdir='./OUT/',
 /
 &system
    ibrav=  2
    celldm(1) =7.50
    nat=  1, ntyp= 1
    ecutwfc =12.0
    occupations='smearing'
    smearing='marzari-vanderbilt'
    degauss=0.05
 /
ATOMIC_SPECIES
 Al  26.98 Al.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Al 0.00 0.00 0.00
K_POINTS {automatic}
30 30 30 1 1 1
```

# DOS calculation

```
&dos
    prefix='al'
    degauss=0.01
    Emin=-5.0,Emax=15.0,DeltaE=0.01
    outdir='./OUT/'
    fildos='al.dos.dat'
/
```

Computing the DOS:

```
dos.x -in dos.in
```

Remark: The degauss parameter defines a width associated to the eigenvalues

Computing the Projected DOS:

```
projwfc.x -in pdos.in
```

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- Compute the DOS for different number of k-points
- $20 \times 20 \times 20 \Rightarrow 40 \times 40 \times 40$ (step 10)
- For too small number of k-points unrealistic oscillations occur