Metals: K-points, broadening

Bloch Theorem

$$[\hat{H}, \hat{T}_R] = 0 \qquad \Longrightarrow \qquad \Psi_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r}) e^{i\mathbf{kr}}$$

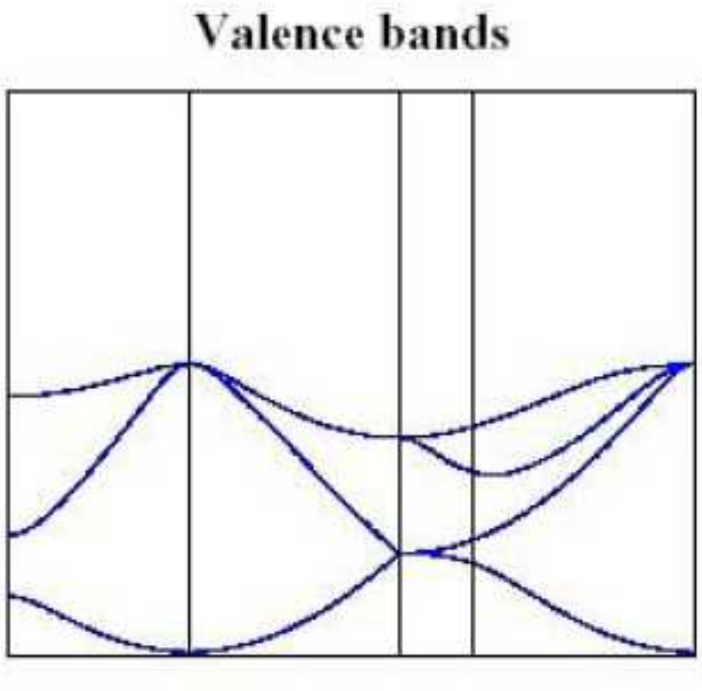
- n, $\mathbf{k}$ are quantum numbers (band index and crystal momentum)
- $u(\mathbf{r})$ is periodic : $u(\mathbf{r}) = u(\mathbf{r} + \mathbf{R})$

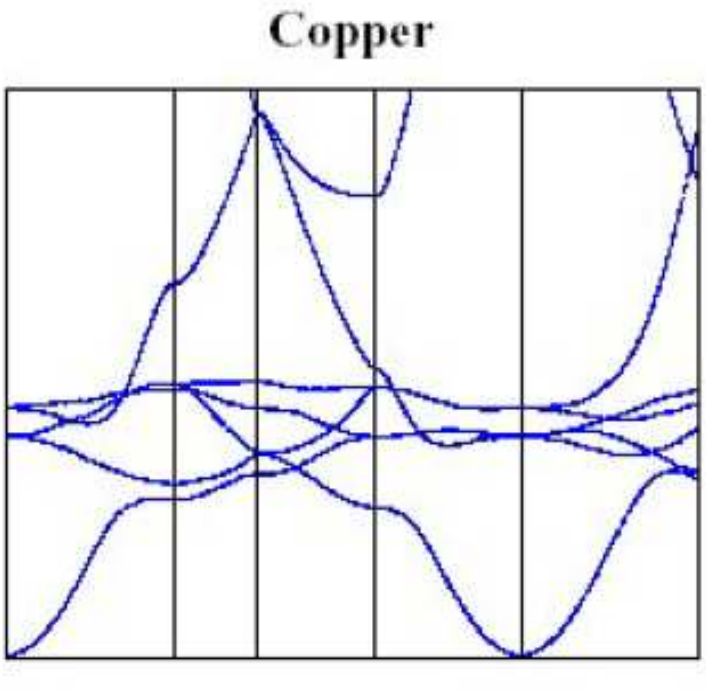
Brillouin Zone Integration

1. Sampling at one point (Gamma or Baldereschi point)

2. Sampling at regular grids (Monkhorst-Pack)

3. For metallic systems, integration of the discontinuity is improved introducing a fictitious electronic temperature

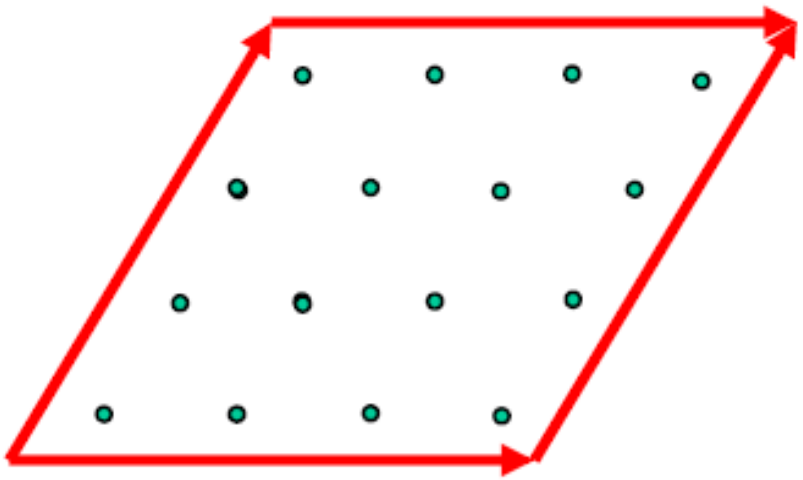




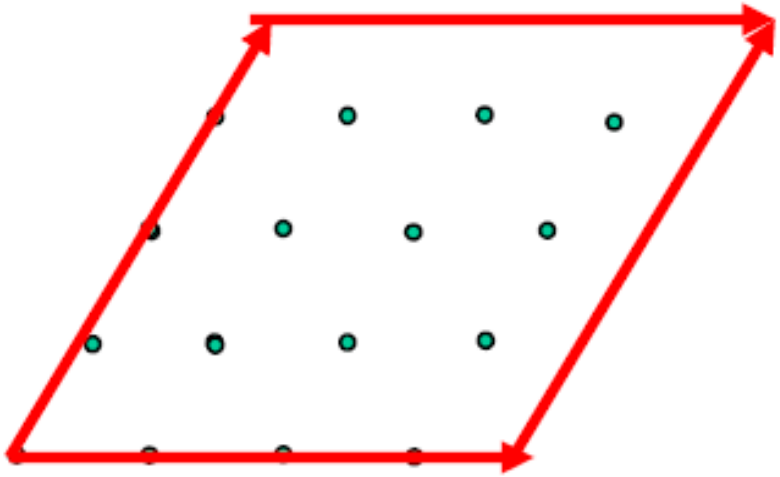
Monkhorst-Pack meshes

- regular equispaced meshes in the Brillouin Zone (generated automatically by PWscf - "automatic" keyword)

(4,4,4) shifted



(4,4,4) unshifted



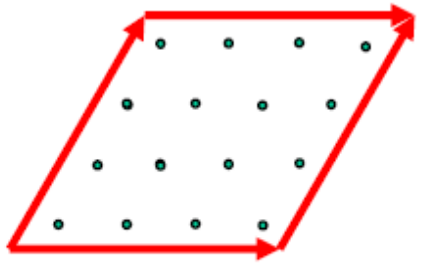
The K_POINTS input card

```
K_POINTS { tpiba | automatic | crystal | gamma }

gamma: use k = 0 (do not read anything after this card}

automatic: automatically generated uniform grid of k-points

     next card:
   nk1,nk2,nk3,k1,k2,k3

     nk1,nk2,nk3 as in Monkhorst-Pack grids
     k1,k2,k3 can be 0 (no offset)
                   or 1 (grid displaced by 1/2 step)

 ...
```

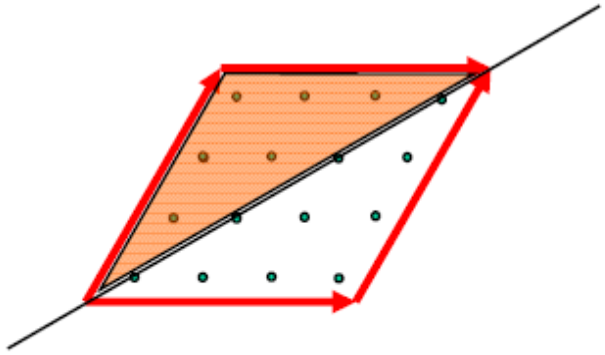
Exploiting symmetry

- Symmetry is exploited in order to reduce the number of inequivalent points to be considered.

$$\rho(\vec{r}) = \sum_{n,\vec{k}} \left\| \Psi_{n,\vec{k}}(\vec{r}) \right\|^2$$



$$\Psi_{n,\vec{k}}\left(S^{-1}\vec{r}\right) = \Psi_{n,S\vec{k}}(\vec{r})$$



$$\rho(\vec{r}) = \sum_{n,\vec{k}} \left\| \Psi_{n,\vec{k}}(\vec{r}) \right\|^2 = \sum_{n,S,\vec{k}_{irr}} \left\| \Psi_{n,S\vec{k}_{irr}}(\vec{r}) \right\|^2 =$$

$$= \sum_{n,S,\vec{k}_{irr}} \left\| \Psi_{n,\vec{k}_{irr}}\left(S^{-1}\vec{r}\right) \right\|^2$$

The K_POINTS input card (continued)

```
K_POINTS { tpiba | automatic | crystal | gamma }

 ...

crystal: read k-points in crystal coordinates
tpiba: read k-points in carthesian coordinates
       in unit of 2pi/a

     next cards:
   nks  (number of points supplied)
       followed by nks lines containing
   xk_x, xk_y, xk_z, wk
       special points in the irreducible BZ and weights
```

- It is assumed that the list of k-points has been reduced with the full symmetry of the Bravais lattice.

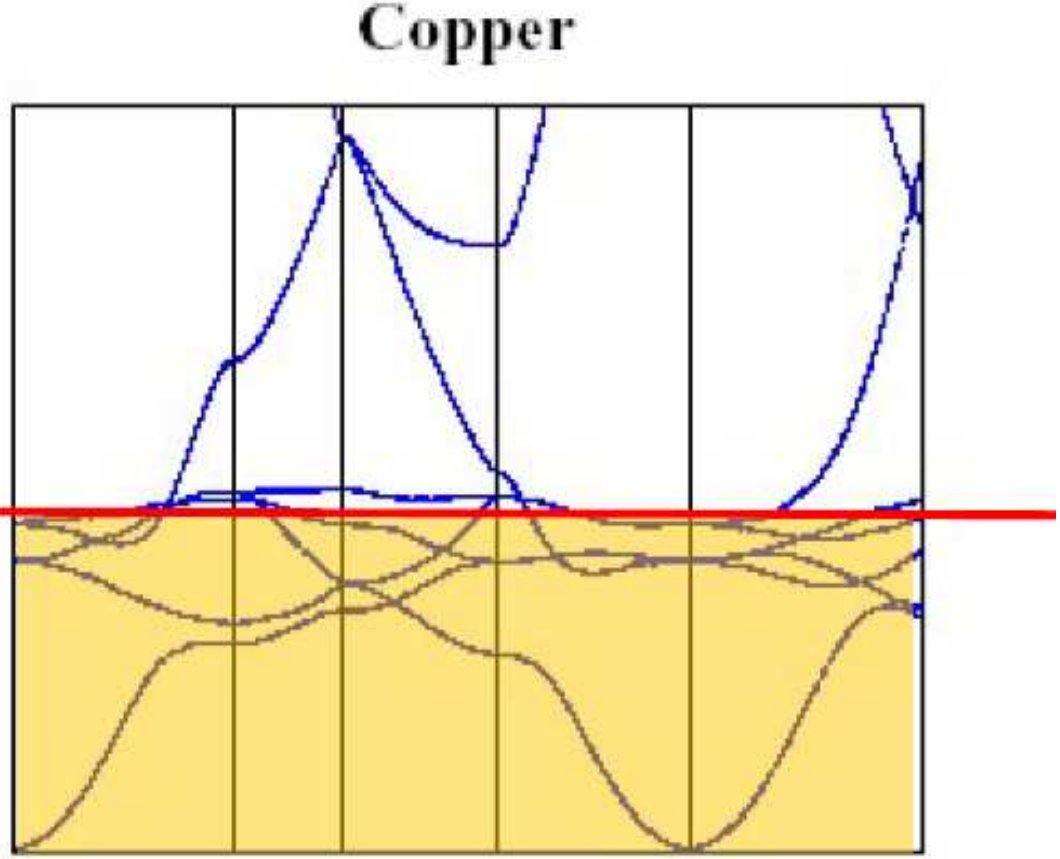
The K_POINTS input card (continued)

```
K_POINTS { tpiba | automatic | crystal | gamma }

 ...

crystal: read k-points in crystal coordinates
tpiba: read k-points in carthesian coordinates
       in unit of 2pi/a

     next cards:
   nks  (number of points supplied)
       followed by nks lines containing
   xk_x, xk_y, xk_z, wk
       special points in the irreducible BZ and weights
```

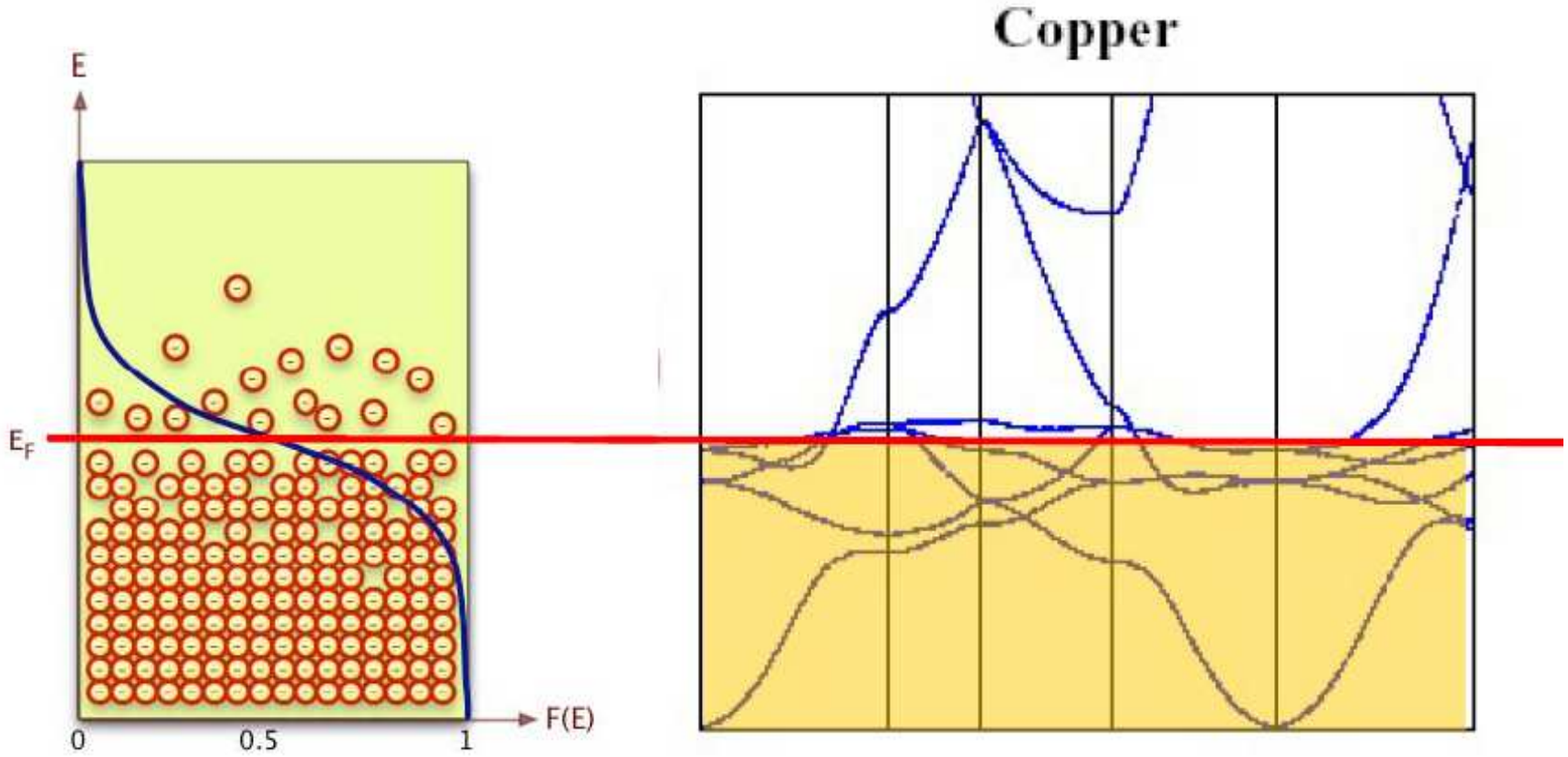
- If a lower symmetry is present, the needed new inequivalent points are generated and the corresponding weights redistributed.

Metals

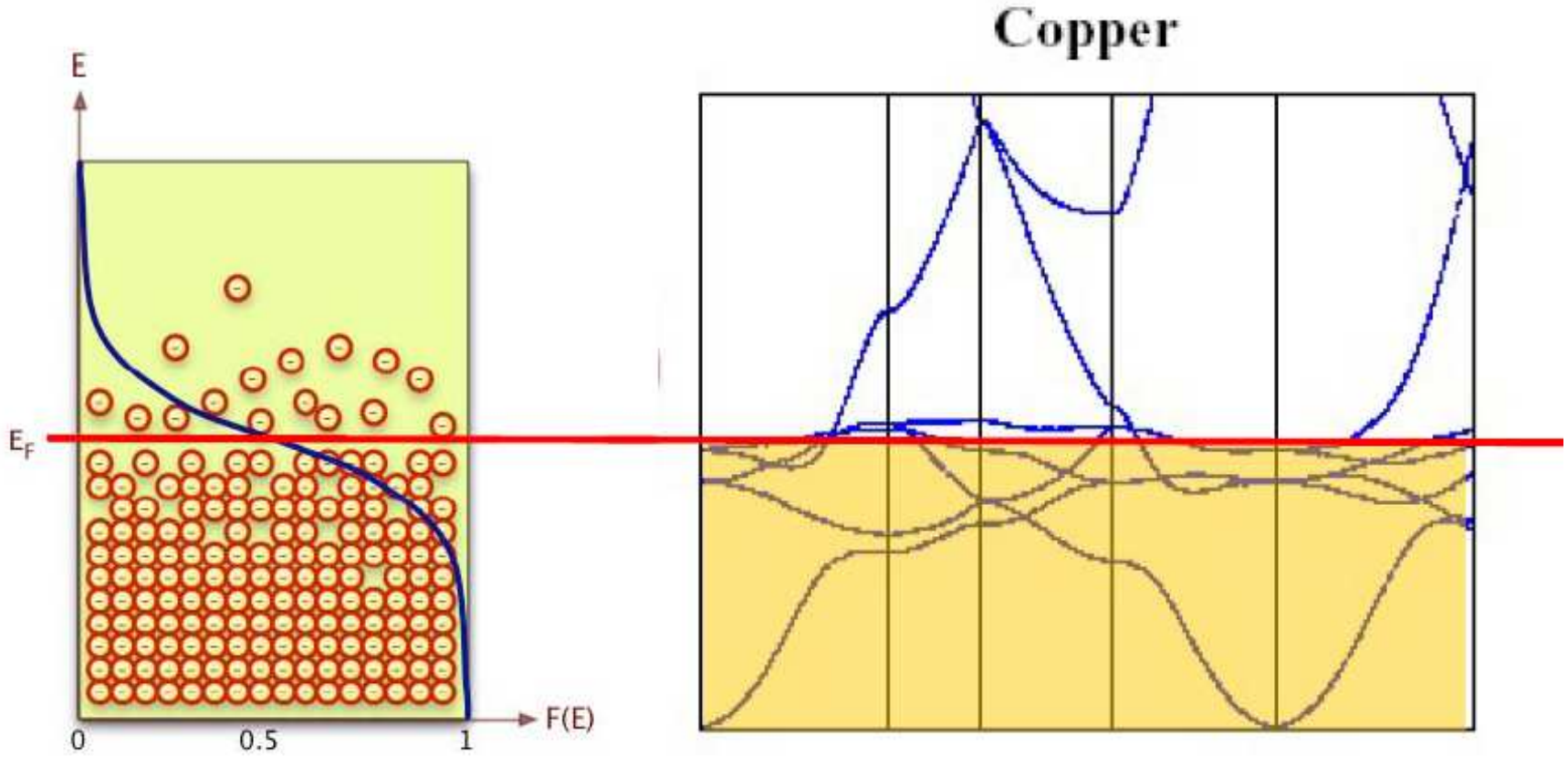
$$\rho(\vec{r}) = \sum_{n,\vec{k}} f_{n,\vec{k}} \left\| \Psi_{n,\vec{k}}(\vec{r}) \right\|^2$$



Metals



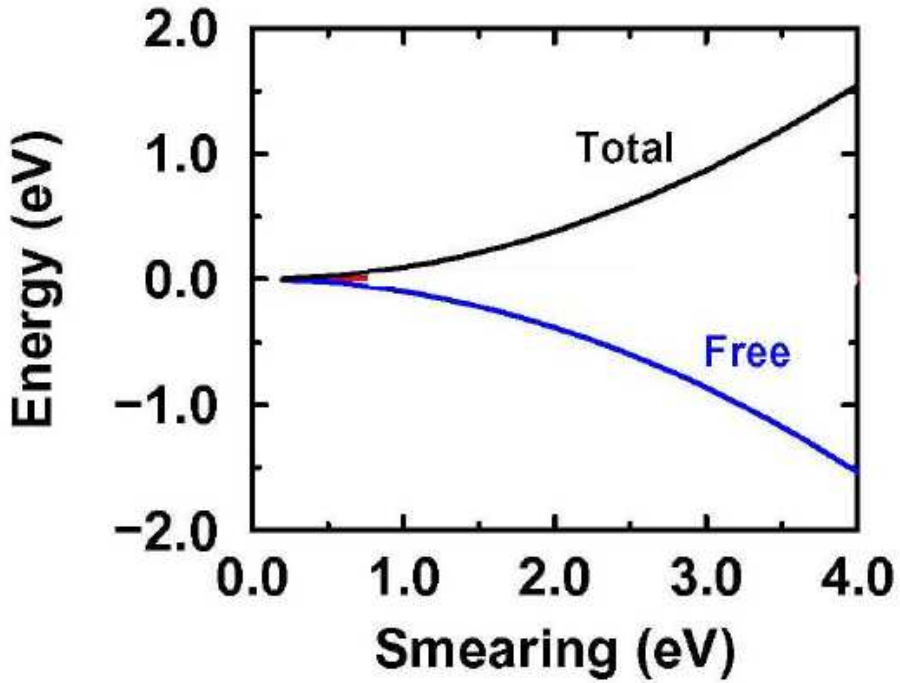
Metals



$$f_{n,\mathbf{k}} = \frac{1}{1 + exp(\beta(\varepsilon_{n,\mathbf{k}} - \varepsilon_F))}$$

Temperature and smearing

$$A\,[\,\sigma\,;\{\psi_i\},\{f_i\}] \;=\; \sum_i f_i\,\langle\psi_i|\hat{T}_e+\hat{V}_{nl}|\psi_i\rangle + E_{\mathrm{Hxc}}[n] - \sigma S[\,\{f_i\}\,]\,.$$



.

$$\frac{dA(\sigma)}{d\sigma} = -S = \sum_i \tilde{\theta}(\frac{\varepsilon_F - \varepsilon_i}{\sigma})$$

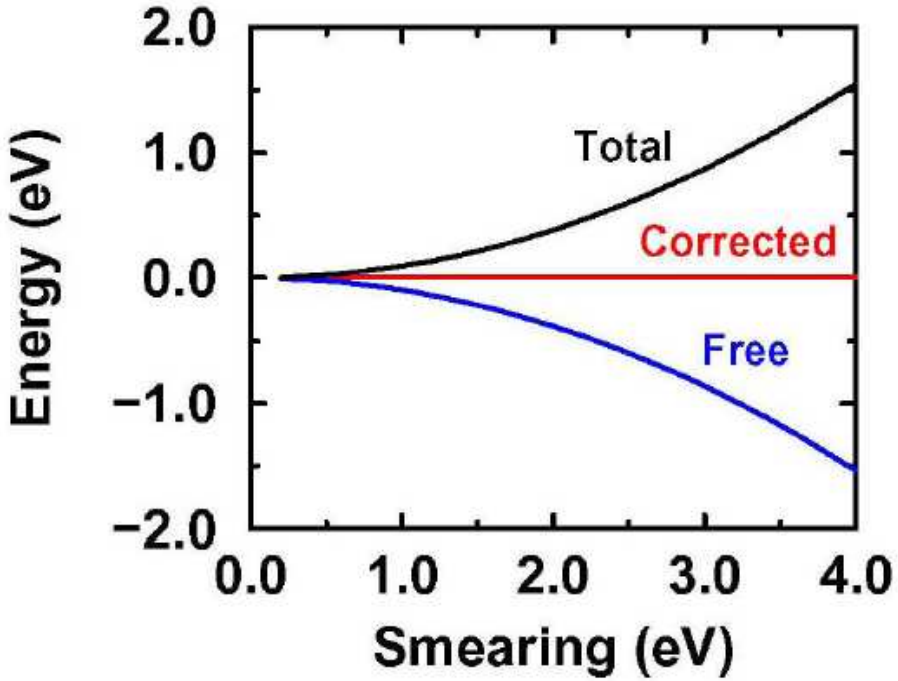
$$\frac{dA(\sigma)}{d\sigma} \approx -\sigma c_1 n(\varepsilon_F)$$

$$c_1 = \int x^2 \tilde{\delta}(x) dx; \quad \tilde{\delta}(x) = \frac{d\tilde{\theta}(x)}{dx}$$

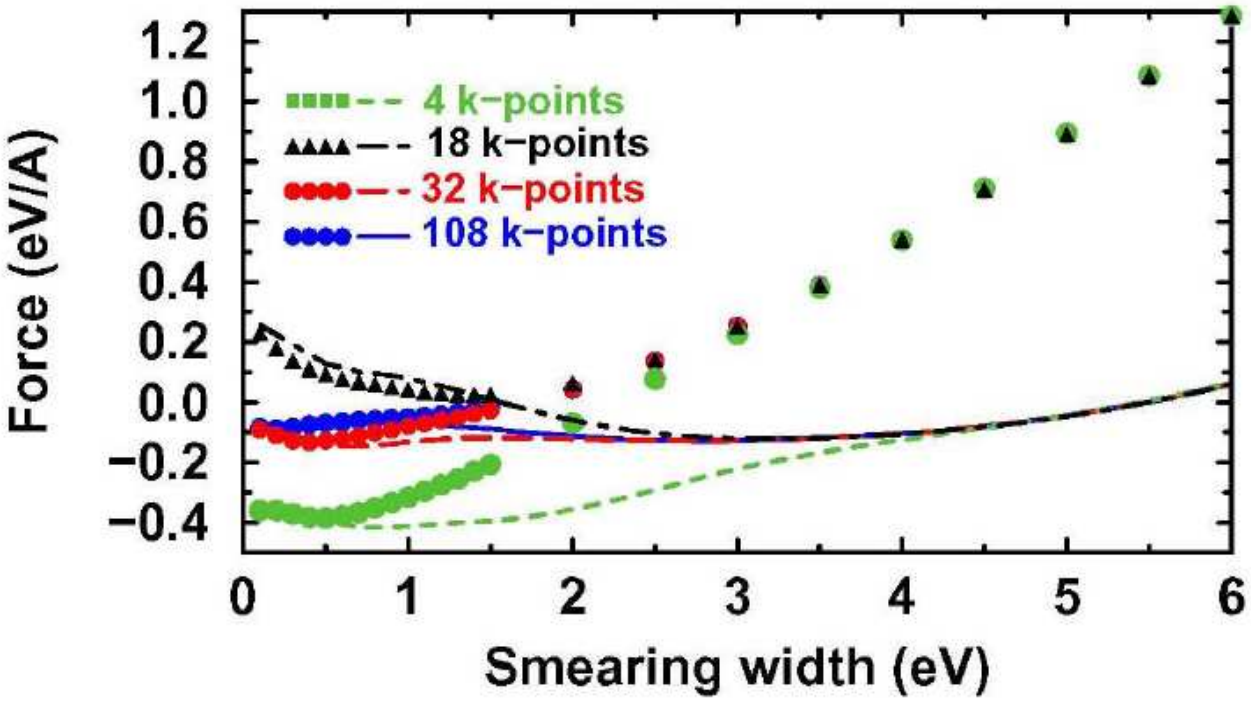
$$A(\sigma) \approx A(0) - \sigma^2 \frac{c_1}{2} n(\varepsilon_F), \qquad U(\sigma) \approx A(0) + \sigma^2 \frac{c_1}{2} n(\varepsilon_F)$$

Temperature and smearing

$$A\left[\sigma;\{\psi_i\},\{f_i\}\right] = \sum_i f_i \langle\psi_i|\hat{T}_e + \hat{V}_{nl}|\psi_i\rangle + E_{\mathrm{Hxc}}[n] - \sigma S[\{f_i\}]\,.$$



Temperature and smearing



.

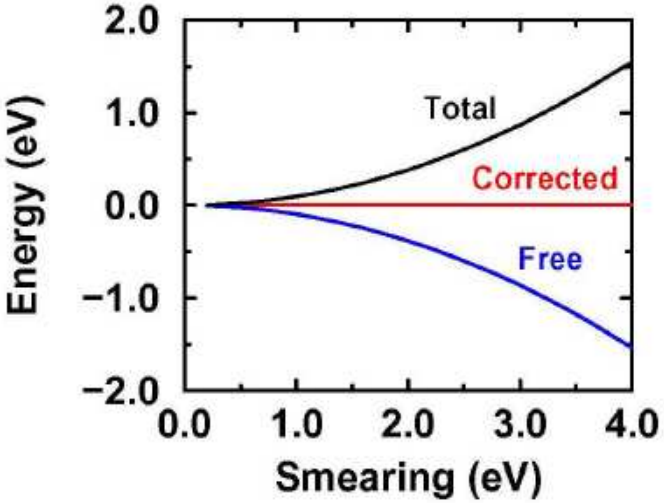
$$\frac{dA(\sigma)}{d\sigma} = -S = \sum_i \tilde{\theta}(\frac{\varepsilon_F - \varepsilon_i}{\sigma})$$

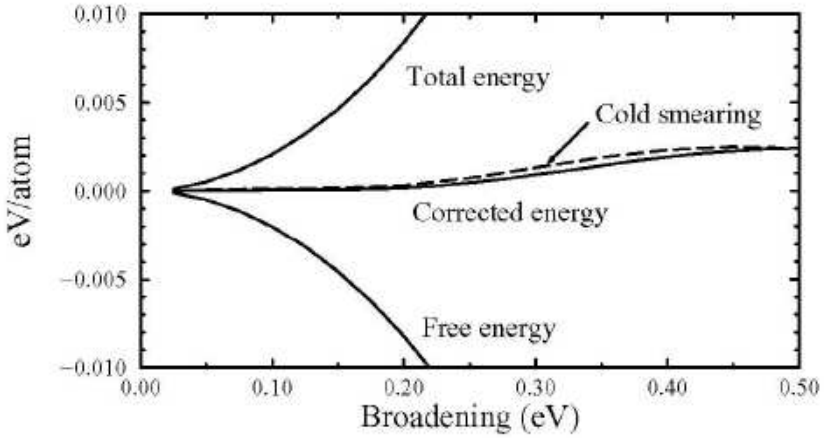
$$\frac{dA(\sigma)}{d\sigma} = -\sum_{k=0}^{\infty} \sigma^{2k+1} \frac{c_{k+1}}{2k+1!} \frac{d^{2k}n}{d\varepsilon^{2k}}\bigg|_{\varepsilon_F}$$

$$c_k = \int x^{2k}\tilde{\delta}(x)dx; \quad \tilde{\delta}(x) = \frac{d\tilde{\theta}(x)}{dx}$$

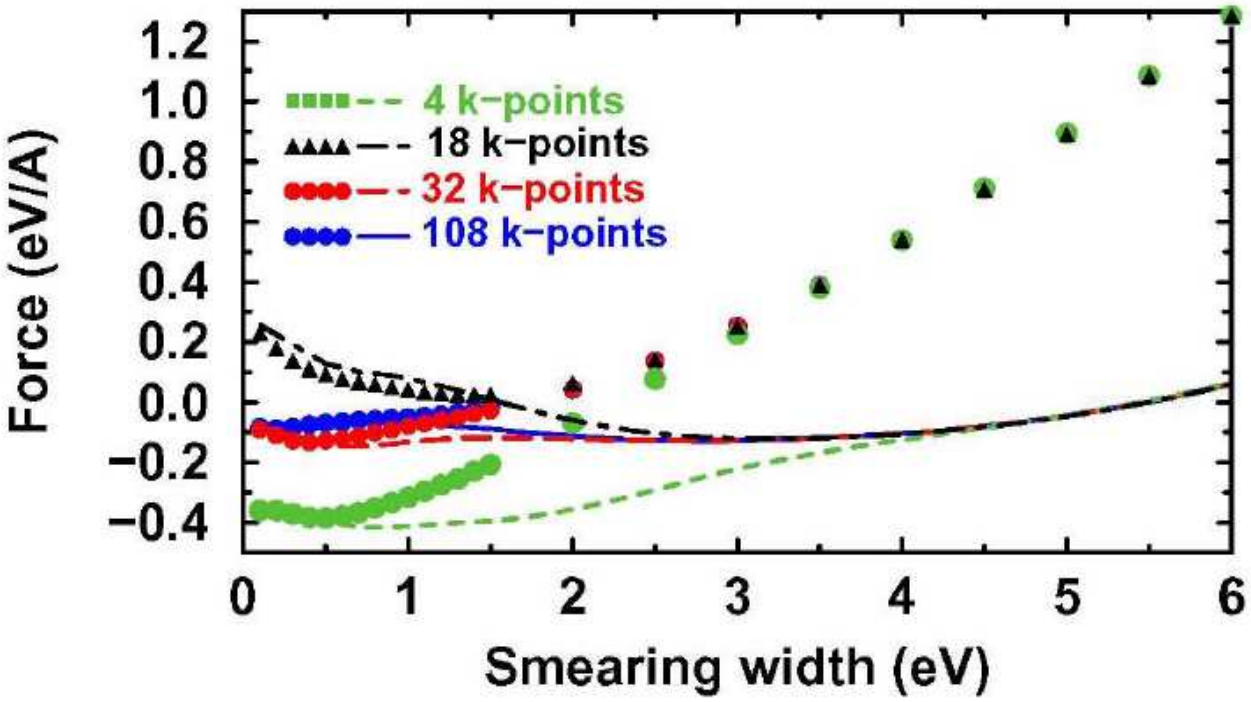
$$A(\sigma) = A(0) - \sum_{k=0}^{\infty} \sigma^{2k+2} \frac{c_{k+1}}{2k+2!} \frac{d^{2k}n}{d\varepsilon^{2k}}\bigg|_{\varepsilon_F}$$

Methfessel-Paxton, Marzari-Vanderbilt





Temperature and smearing



in the &SYSTEM namelist

```
occupation   CHARACTER
    'smearing': smearing for metals
                requires a value for degauss
    'tetrahedra': for metals and DOS calculations
                (see PRB 49, 16223 (1994))
                requires uniform grid of k-points,
                automatically generated
    'fixed': for insulator with gap
    'from_input': the occupation are read from input file.
                Presently works only with one-kpoint
                (LSDA allowed)
```

```
degauss         REAL (default = 0.d0 Ry)
     value of the smearing for brillouin-zone
     integration in metals.


smearing      CHARACTER
     'gaussian', 'gauss' :
             ordinary gaussian smearing (default)
     'methfessel-paxton', 'm-p', 'mp':
             Methfessel-Paxton first order smearing
             (see PRB 40, 3616 (1989))
     'marzari-vanderbilt', 'cold', 'm-v', 'mv':
             Marzari-Vanderbilt cold smearing
             (see PRL 82, 3296 (1999))
     'fermi-dirac','f-d','fd':
             smearing with Fermi-Dirac function
```

THE END