Metales y sistemas magnéticos

Eduardo Menendez, GNM, Universidad de Chile. http://www.gnm.cl

Plan

Metales a temperatura finita
Metales a 0K. Metodo de smearing.
Sistemas magnéticos.

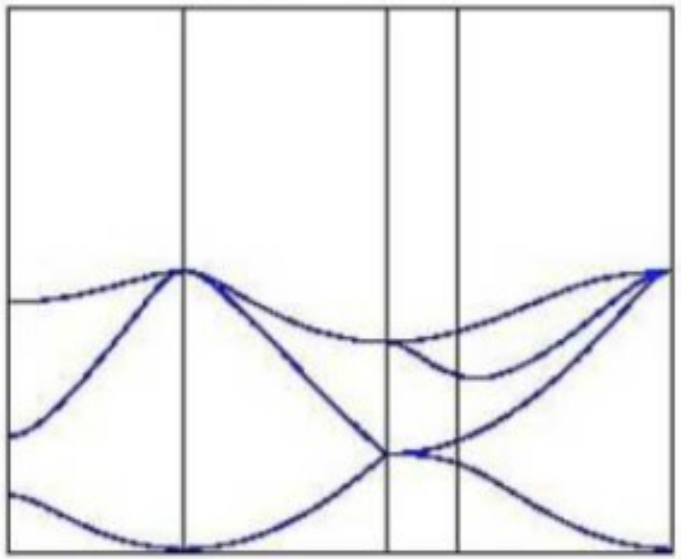
Brillouin Zone Integration

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

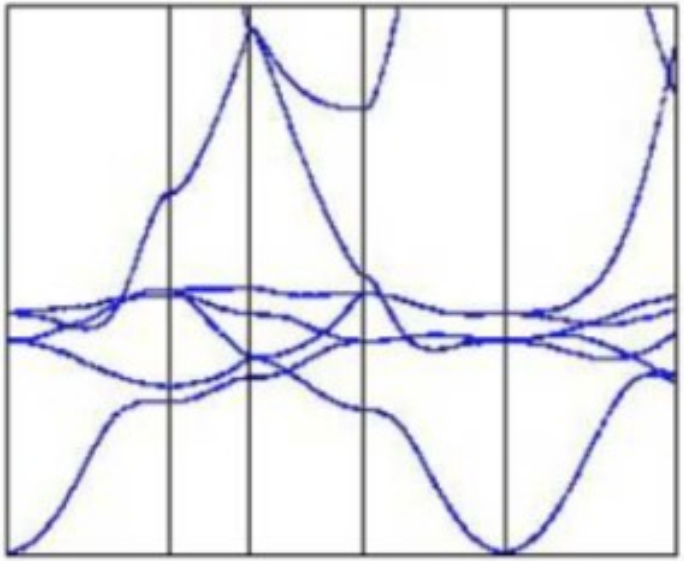
2. Sampling at regular grids (Monkhorst-Pack)

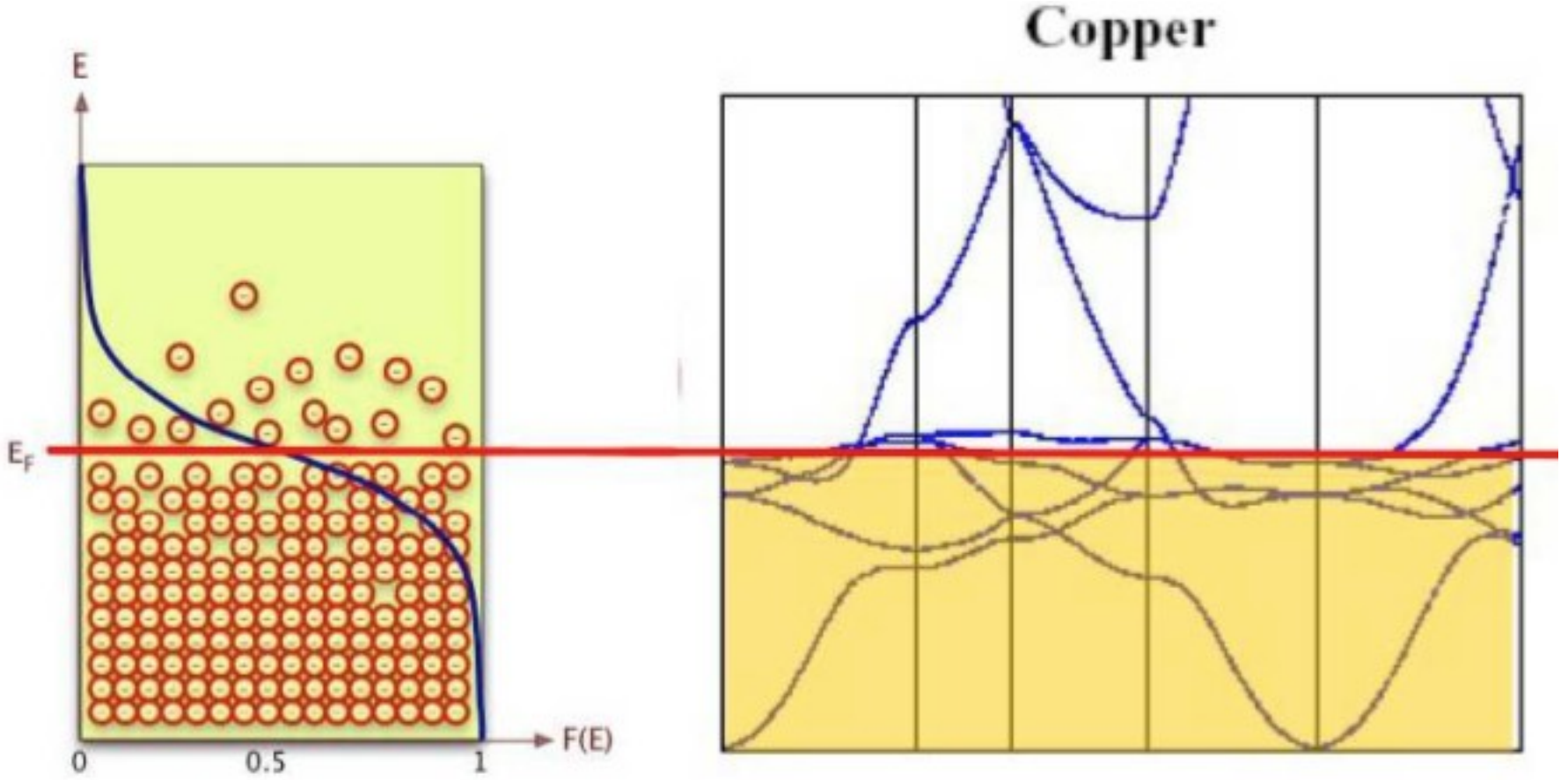
3. For metallic systems, integration of the discontinuity is improved introducing a fictitious electronic temperature

Valence bands



Copper





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

Temperatura

$$f_i = \frac{1}{\exp[(\varepsilon_i - \mu)/k_B T] + 1}$$

$$n(\vec{r}) = \sum_i^{\infty} f_i |\psi_i(\vec{r})|^2$$

$$E(T) = \sum_i f_i \varepsilon_i - \frac{1}{2}\int n(\vec{r}) V_H(\vec{r}) d^3\vec{r} + E_{xc}[n] - \int n(r) v_{xc}(r) d^3\vec{r}.$$

$$F = E - TS$$

$$S = -\sum_i \left[f_i \ln f_i + (1 - f_i) \ln(1 - f_i) \right].$$

Necesidad del smearing en metales (T= 0K)

$$\sum_n \frac{1}{\Omega_{BZ}} \int_{\Omega_{BZ}} \epsilon_{n\mathbf{k}}\, \Theta(\epsilon_{n\mathbf{k}} - \mu)\, \mathrm{d}\mathbf{k}, \longrightarrow \sum_{\mathbf{k}} w_{\mathbf{k}} \epsilon_{n\mathbf{k}}\, \Theta(\epsilon_{n\mathbf{k}} - \mu),$$

La suma converge lentamente con el numeo de k-points en los metales. Esto ocurre porque para los k crcanos a la superficie de Fermi, los numeros de ocupacion saltan entre 0 y 1. El truco es remplazar la funcion de salto por una función mas suave, que haga suaves los cambios de ocupación al variar los niveles de energía.

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F(T) &= E(0) - \alpha T^2 \\
E(0) &= \frac{1}{2}(E(T) + F(T)) + O(T^4).
\end{aligned}
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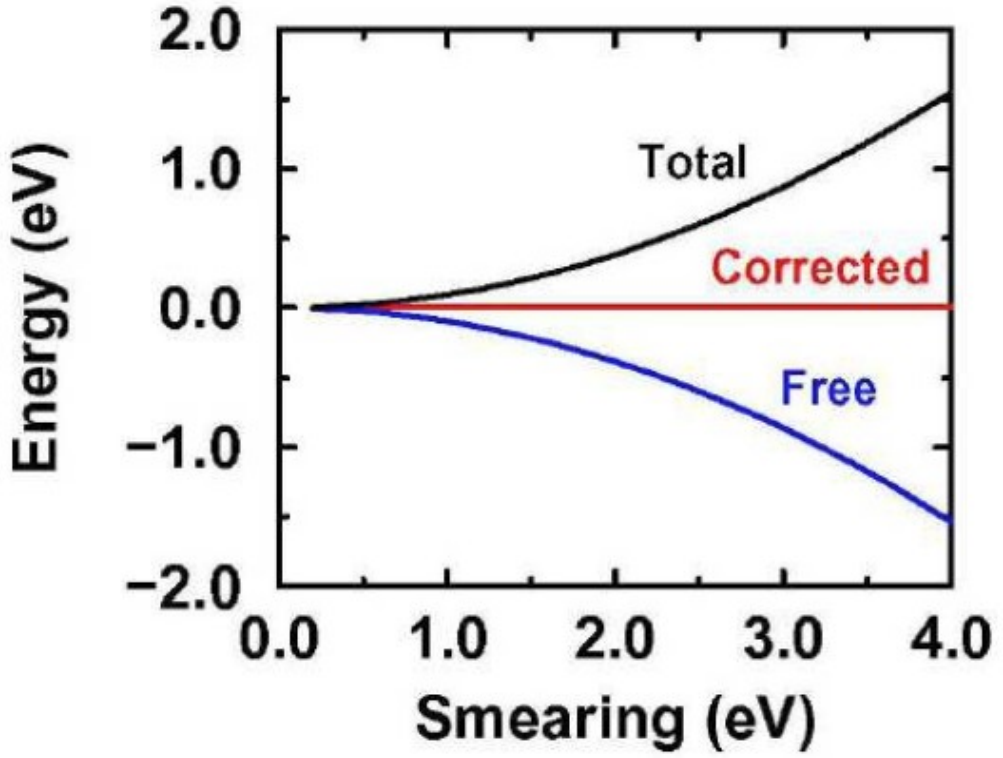
$$A\left[\sigma;\{\psi_i\},\{f_i\}\right] = \sum_i f_i \langle\psi_i|\hat{T}_e + \hat{V}_{nl}|\psi_i\rangle + E_{\mathrm{Hxc}}[n] - \sigma S[\{f_i\}]\,.$$



Temperatura

Las fuerzas de Hellman-Feynman corresponden a F(T), no a E(0).

$$\vec{F} = -\nabla F(T)$$

Metales: TS<1meV/atomo

Ahorro CPU,RAM $\rightleftharpoons$ Precision

Pocos k $\rightleftharpoons$ Baja T

Alta T $\rightleftharpoons$ Muchos k

Metales

- Fermi smearing es ineficiente. Solo se usa para calcular energia libre verdadera.
- Otros métodos: gaussiano, Methfessel-Paxton,cold smearing.
  `smearing='gaussian','mp',degauss=0.02`
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  Phys. Rev. B 65, 035111 (2001), Smearing scheme finite-temperature electronic calculations

El método de tetrahedros es una interpolación de las energias en puntos intermedios que no estan en la malla de puntos k. Es lo mejor para calcular energía.

Smearing

in the &SYSTEM namelist

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                requires a value for degauss
    'tetrahedra': for metals and DOS calculations
                (see PRB 49, 16223 (1994))
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El método de tetrahedros es bueno para la energía, mas no da las fuerzas correctas. Si necesita fuerzas, use occupation='smearing', smearing='mp',degauss=?

```
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     value of the smearing for brillouin-zone
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     'fermi-dirac','f-d','fd':
            smearing with Fermi-Dirac function
```

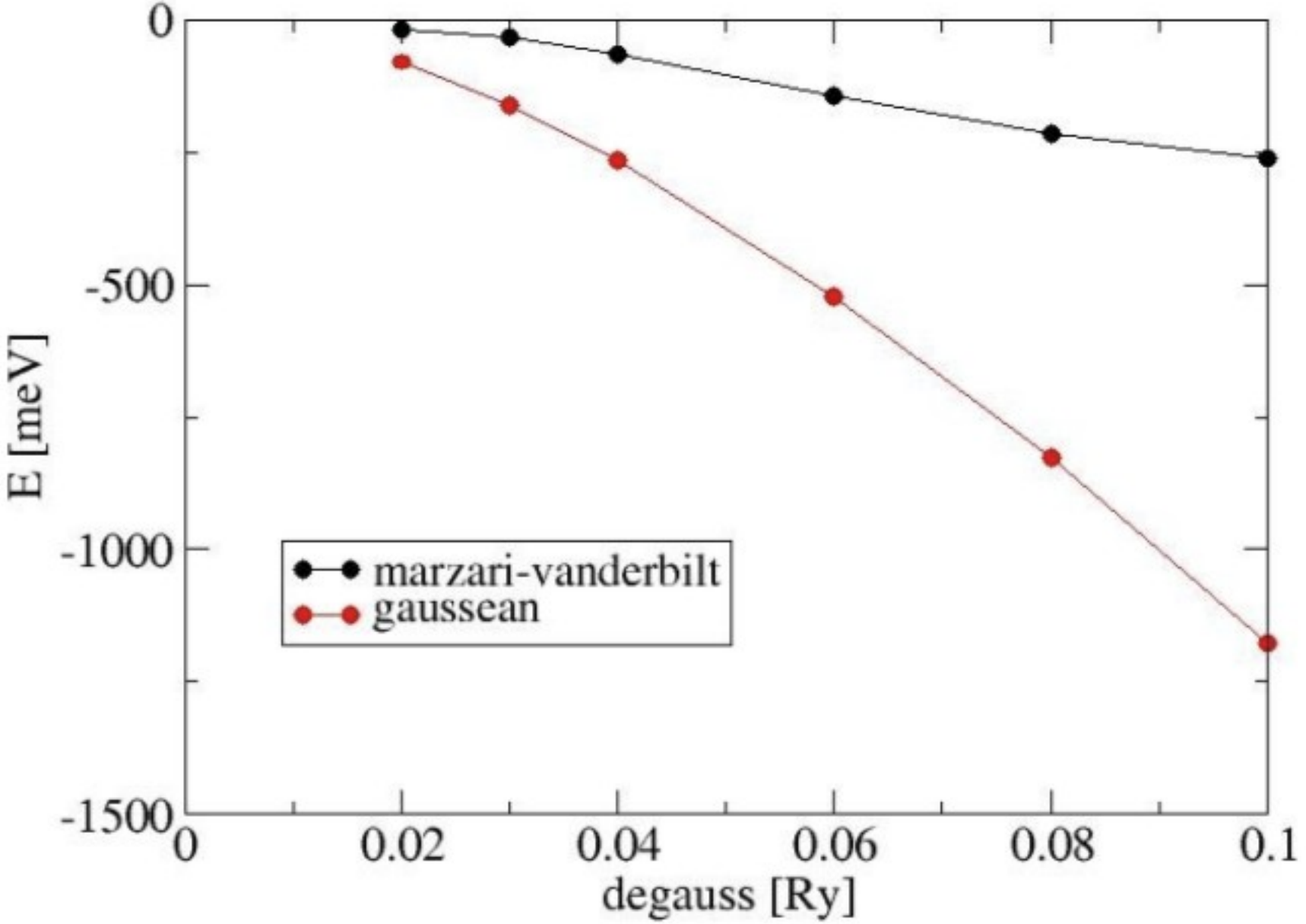
0
-500
-1000
-1500
E [meV]
0
0.02
0.04
0.06
0.08
0.1
degauss [Ry]
marzari-vanderbilt
gaussean

sistemas magnéticos

So far in this course: we "neglected" spin of the electrons:

$$n(\boldsymbol{r}) = 2 \sum_{i=1}^{N_{el}/2} |\psi_i(\boldsymbol{r})|^2$$

Implicitly, we have assumed that spin-up and spin-down wavefunctions are the same:

$$\psi_i^{\uparrow}(\boldsymbol{r}) = \psi_i^{\downarrow}(\boldsymbol{r})$$

Advantage: we need only N_{el} /2 orbitals

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For the case of spin-polarized systems, we drop this constraint and Use N orbitals:

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sistemas magnéticos

Look at how the total energy depends on the two charge densities:

$$E[n^{\uparrow}, n^{\downarrow}] = E_{kin} + E_{ext}[n^{\uparrow}+n^{\downarrow}] + E_{Har}[n^{\uparrow}+n^{\downarrow}] + E_{xc}[n^{\uparrow}, n^{\downarrow}]$$

Calculate the functional derivative in order to obtain the Hamiltonian:

$$\frac{\delta E}{\delta n^{\uparrow}(\boldsymbol{r})} \neq \frac{\delta E}{\delta n^{\downarrow}(\boldsymbol{r})}$$

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Since we have:

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sistemas magnéticos

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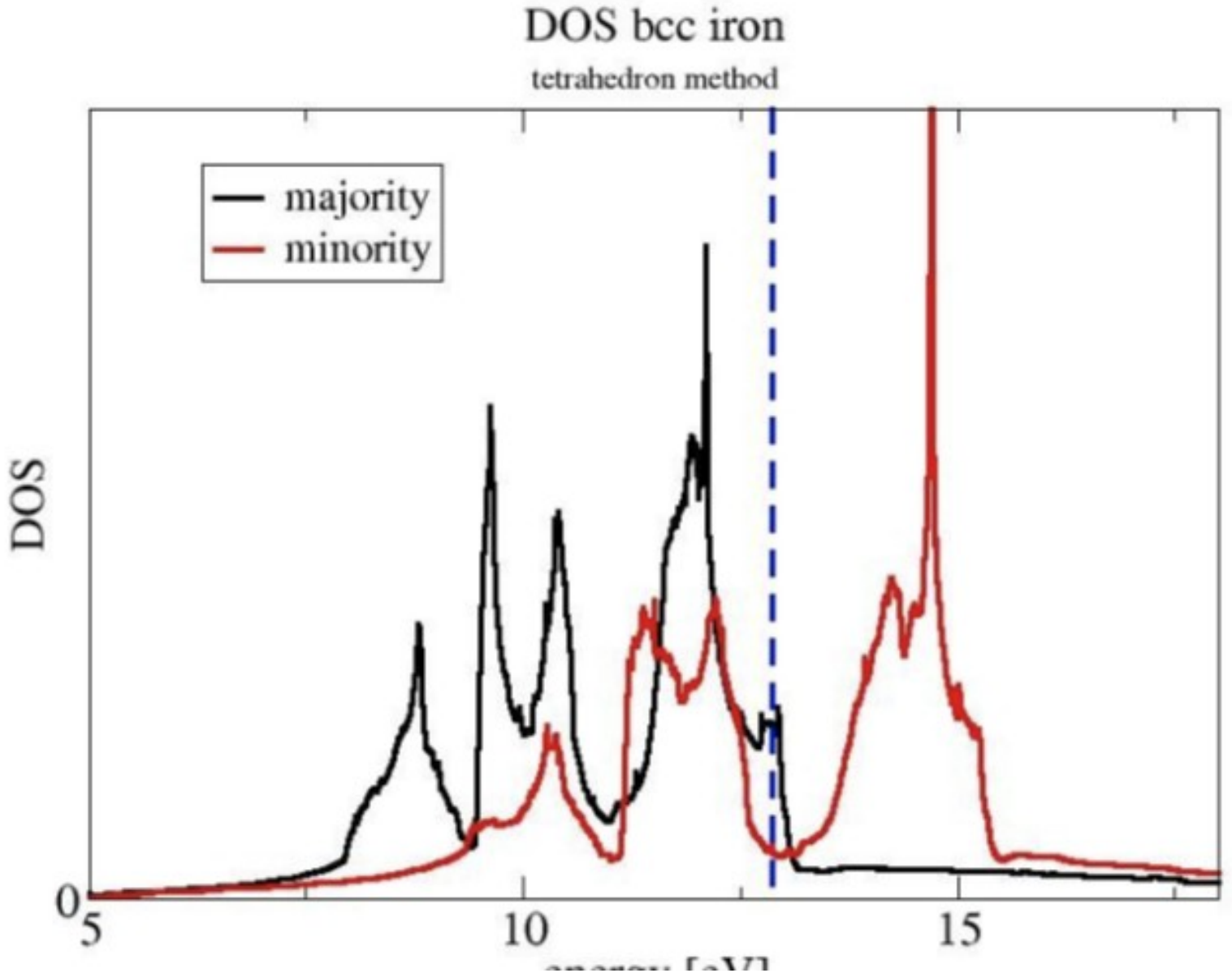
Densidad de estados



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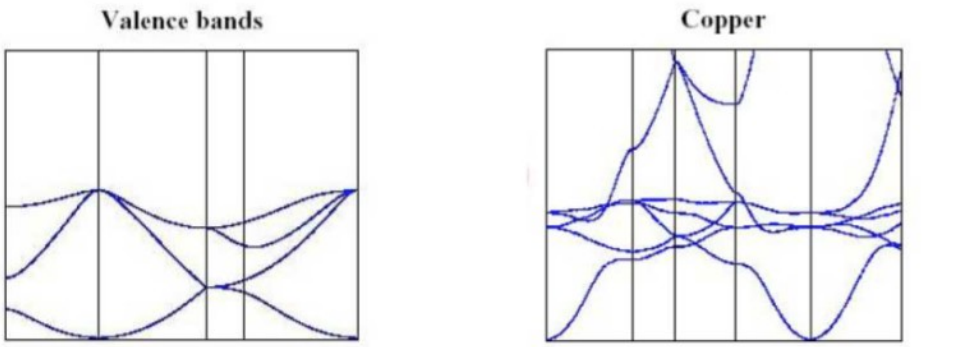

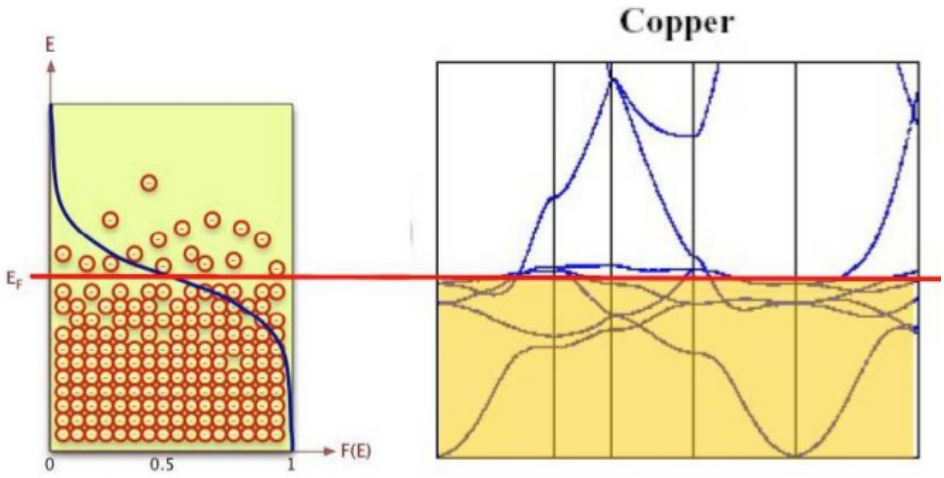

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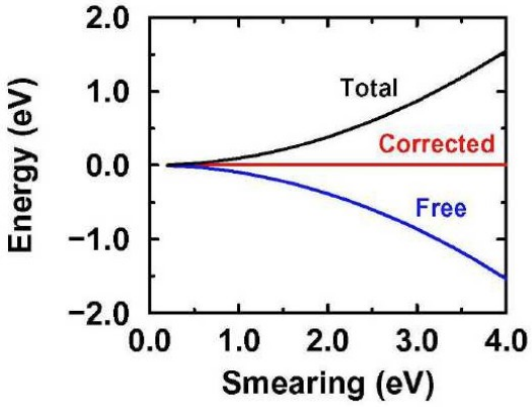

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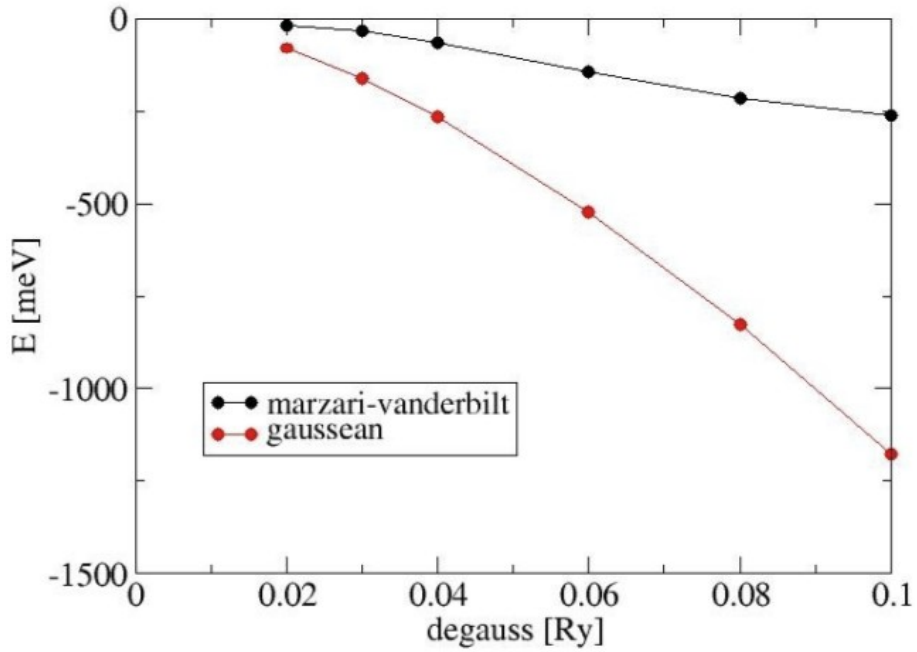
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sistemas magnéticos

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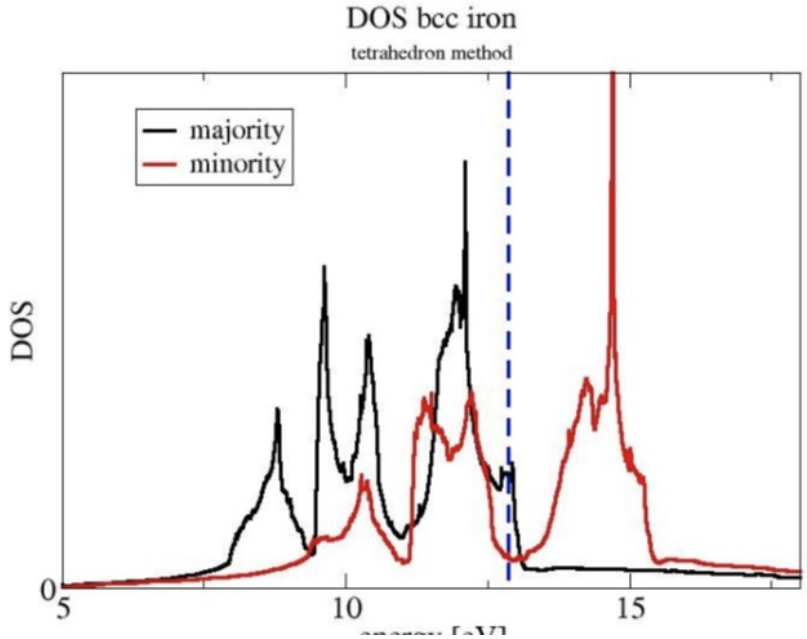

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