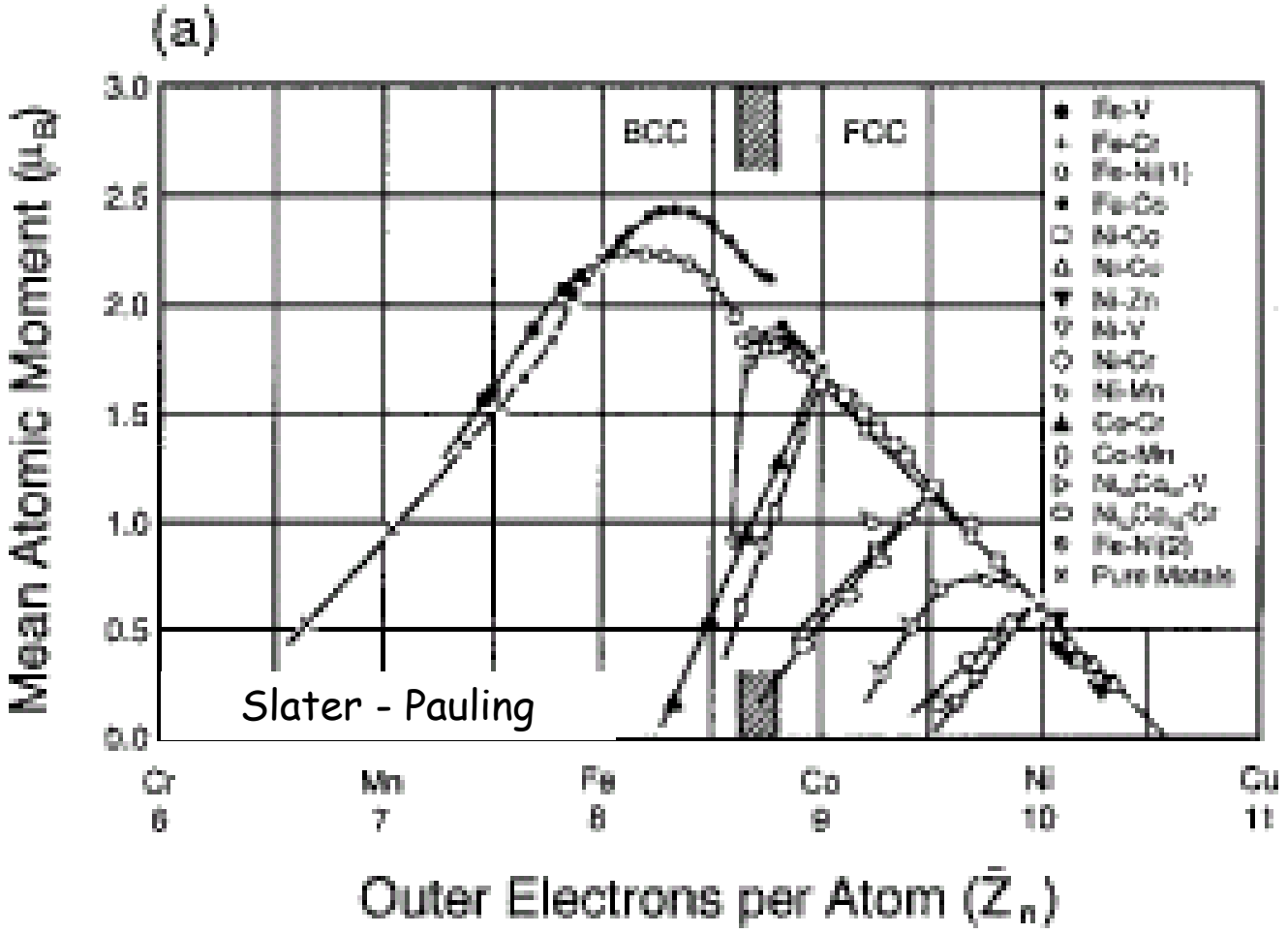
Intercambio en bandas

Intercambio

e^- itinerantes - metales



Intercambio

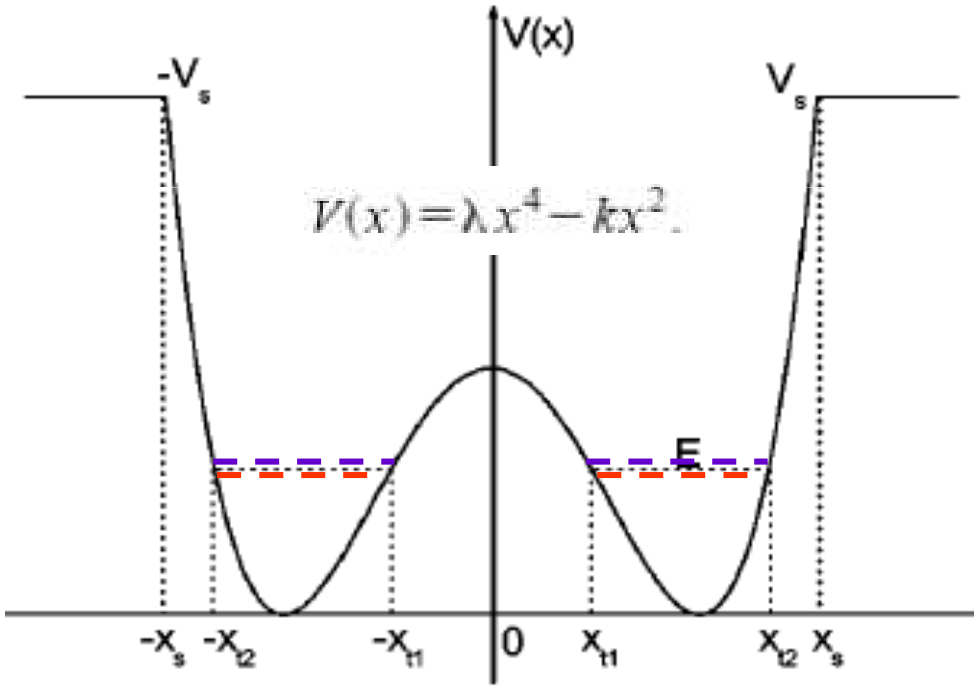
Desdoblamiento en energía de los niveles atómicos

PHYSICAL REVIEW A 67, 062112 (2003)

Energy splitting in symmetric double-well potentials

Feng Zhou, Zhuangqi Cao, and Qishun Shen
Institute of Optics and Photonics, Shanghai Jiao Tong University, Shanghai 200230, China

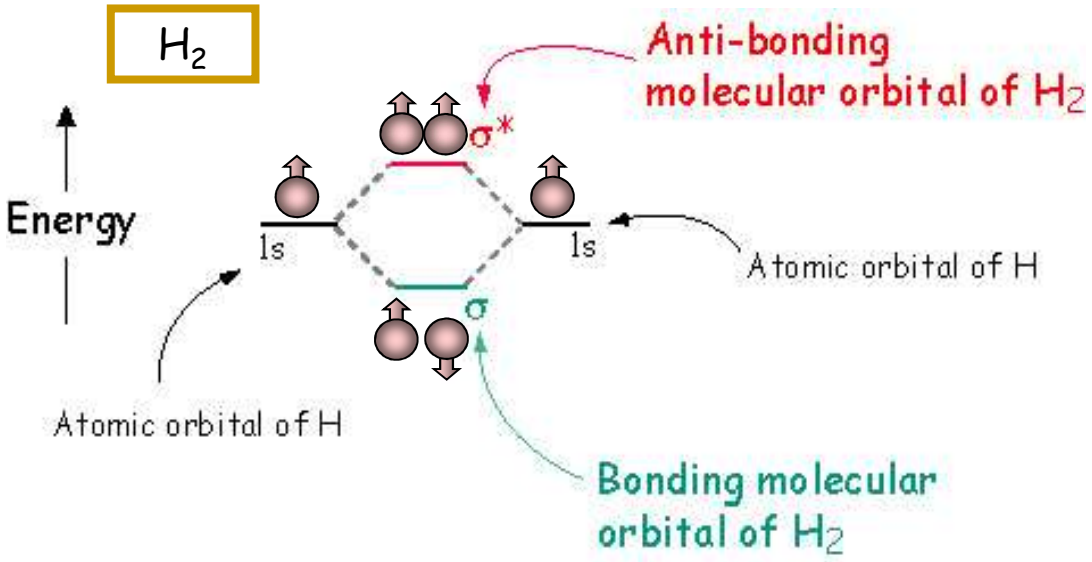
(Received 24 January 2003; published 30 June 2003)

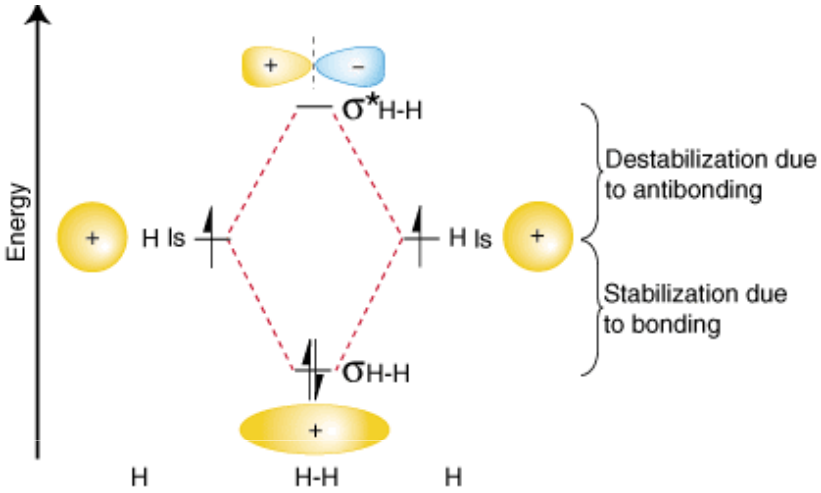


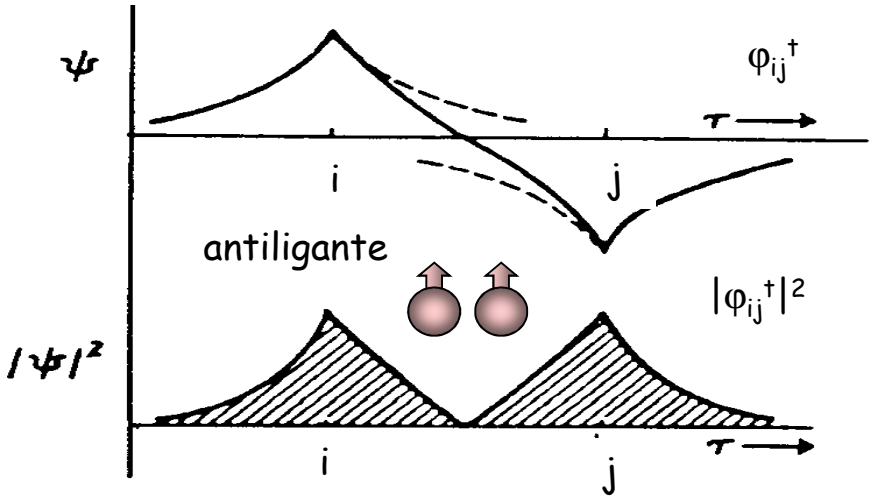
λ	Exact
0.02	1.39352758504 1.39352758715
0.04	1.37112223656 1.37130846161
0.10	1.23450716279 1.34694086892
0.15	1.06249924796 1.42108689054
0.20	0.94175034208 1.53553020408

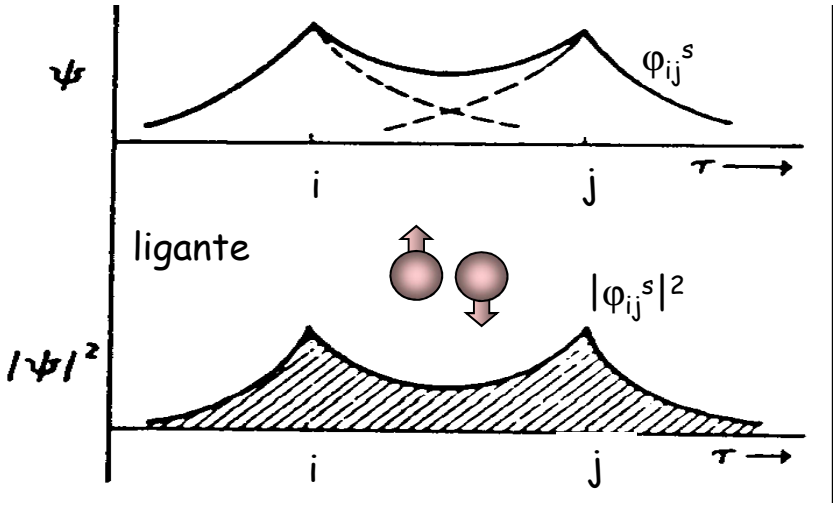
Intercambio y superintercambio

1 - moléculas y bandas



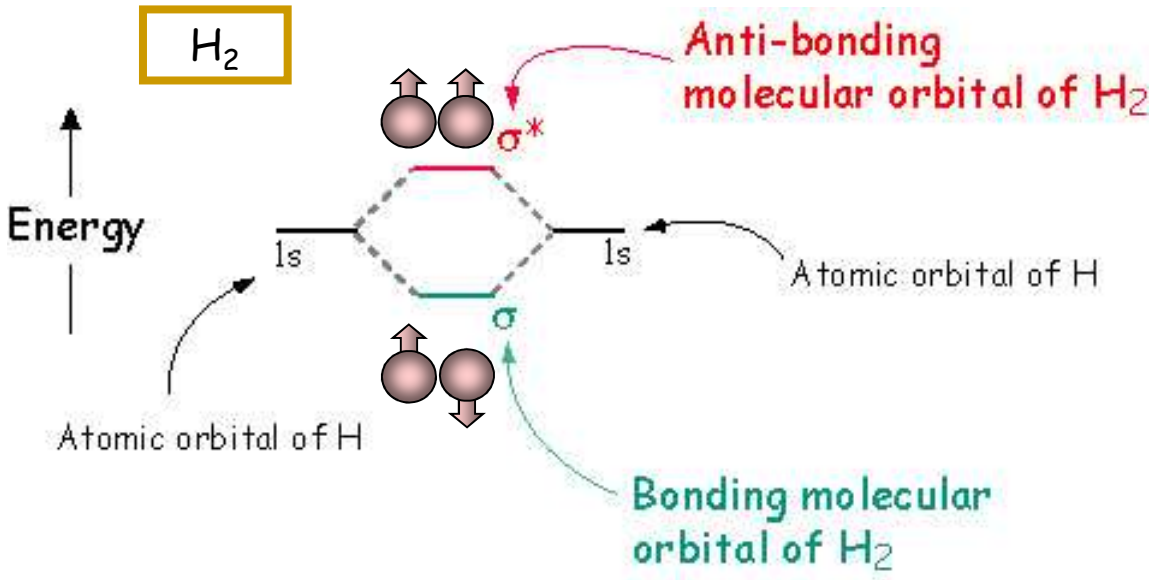


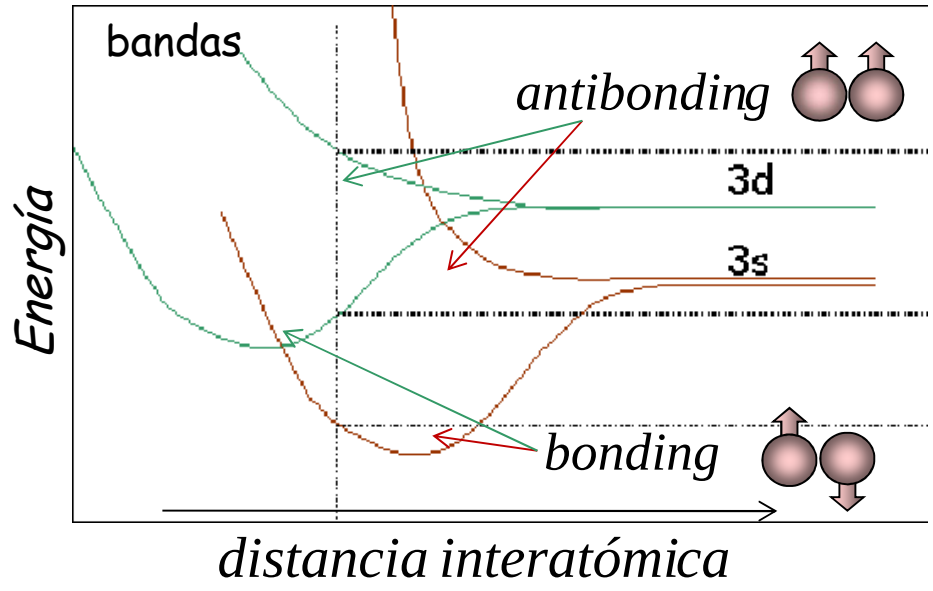




Intercambio y superintercambio

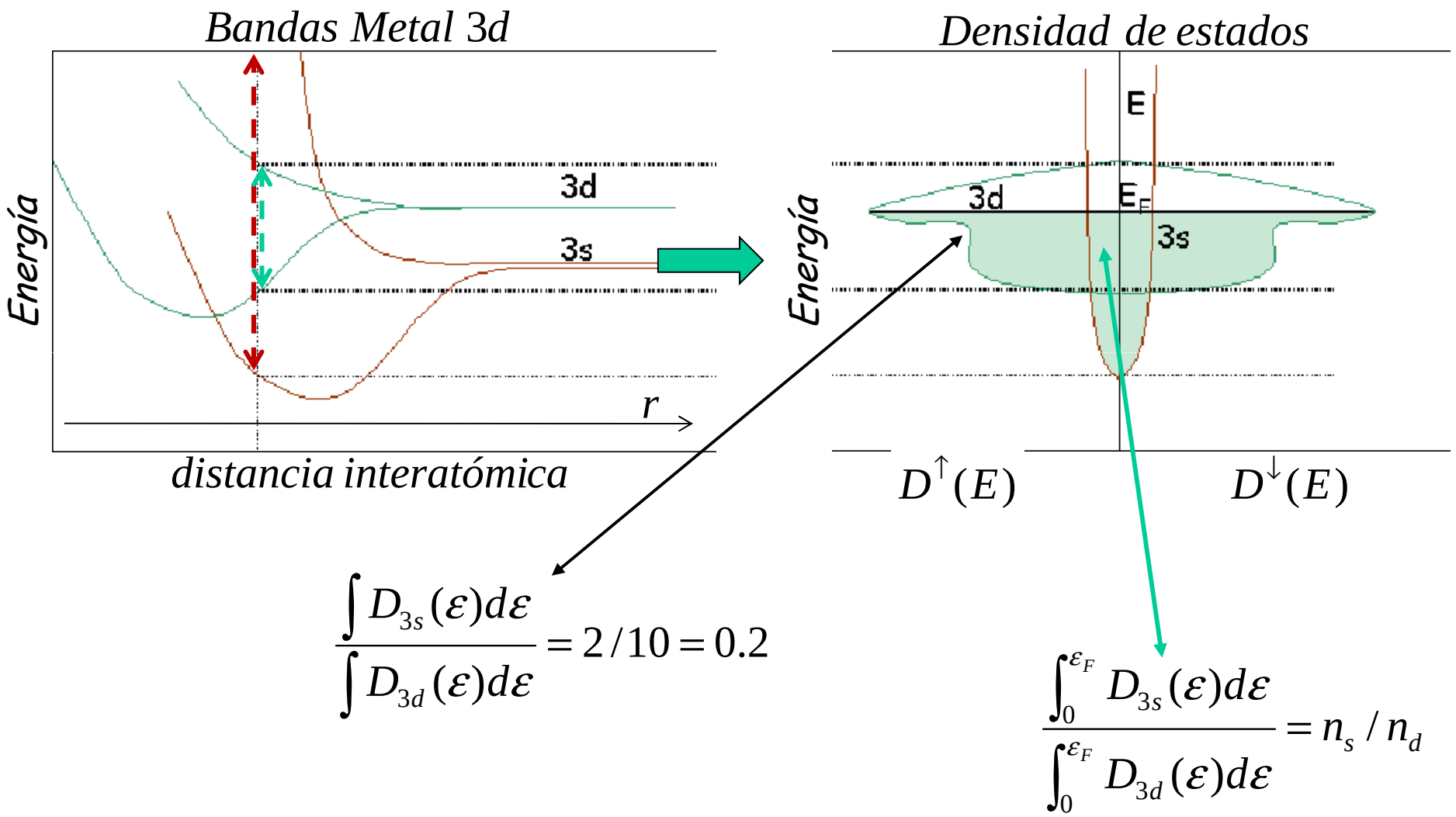
1 – moléculas y bandas





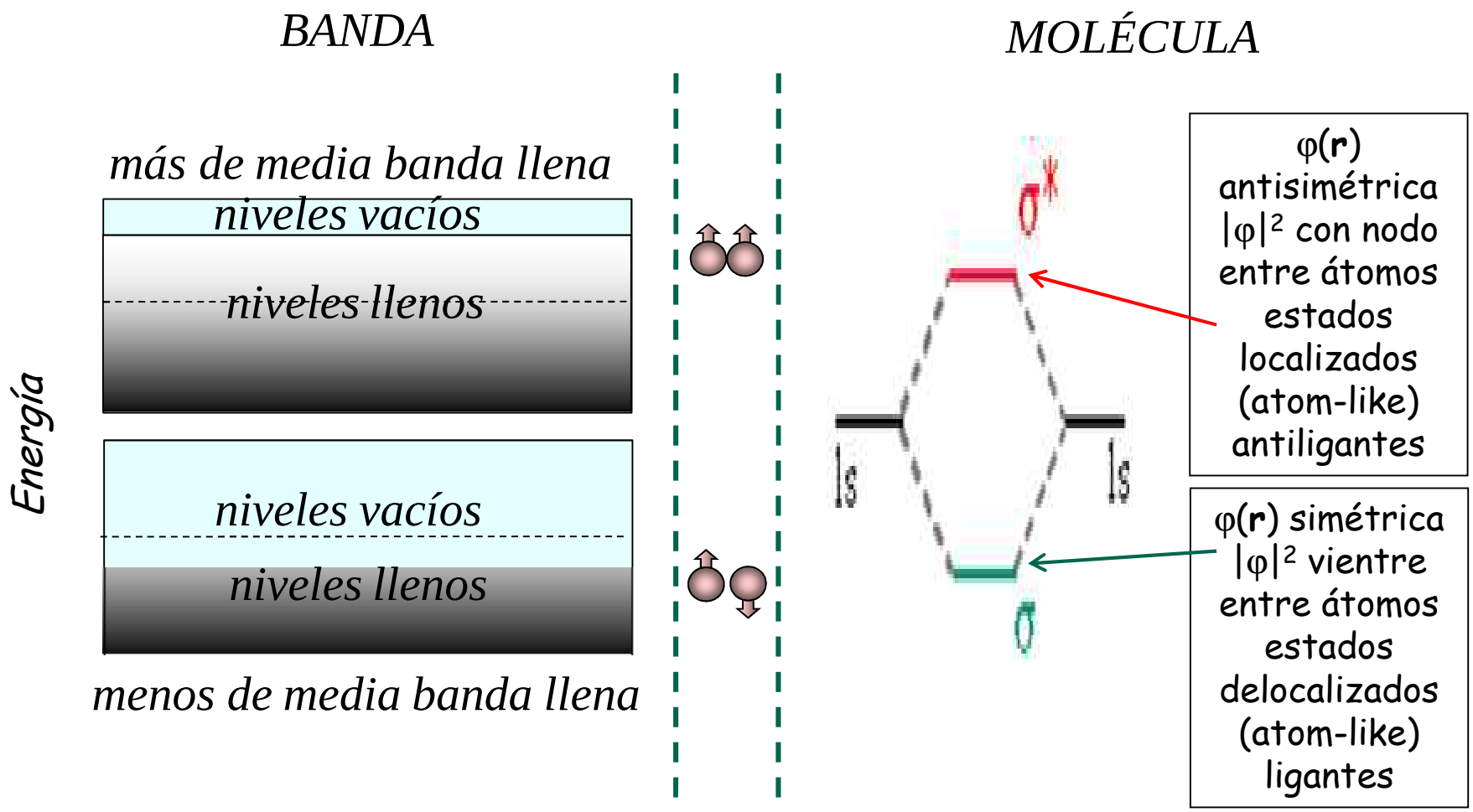
Interpretación de la curva de Slater - Pauling

bandas



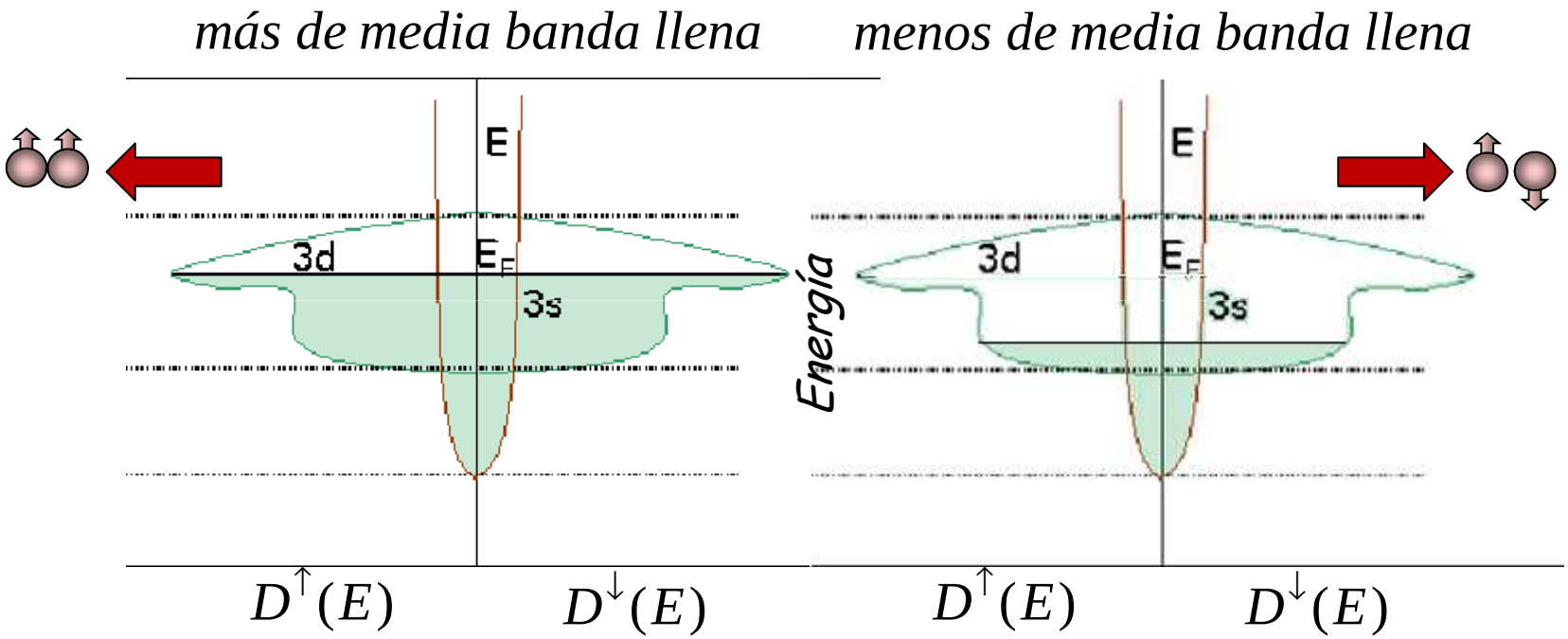
Interpretación de la curva de Slater - Pauling

1 - bandas y moléculas



Interpretación de la curva de Slater - Pauling

bandas

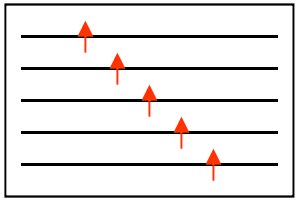


Interpretación de la curva de Slater - Pauling

2 - intercambio

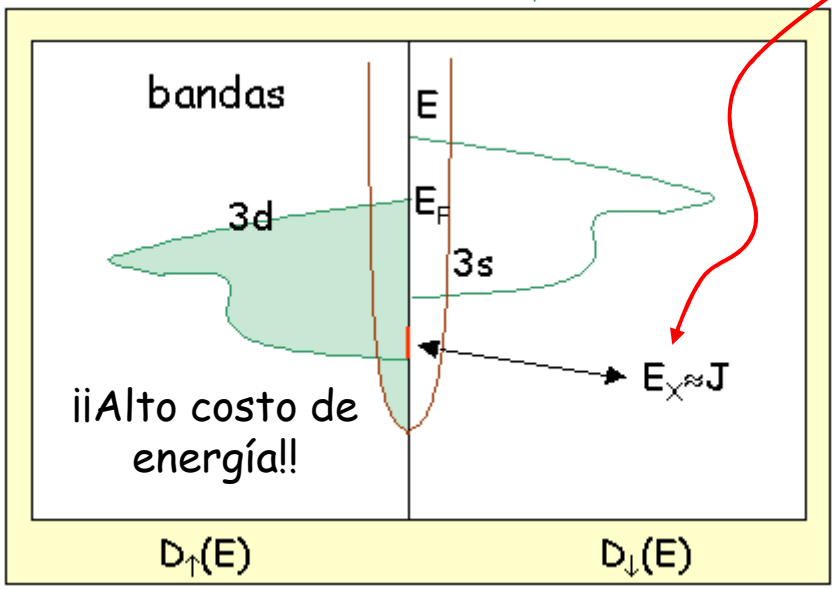
Campo molecular de Weiss ⟺ intercambio ⟺ $E_{ij} = K_{ij} \pm J_{ij}$

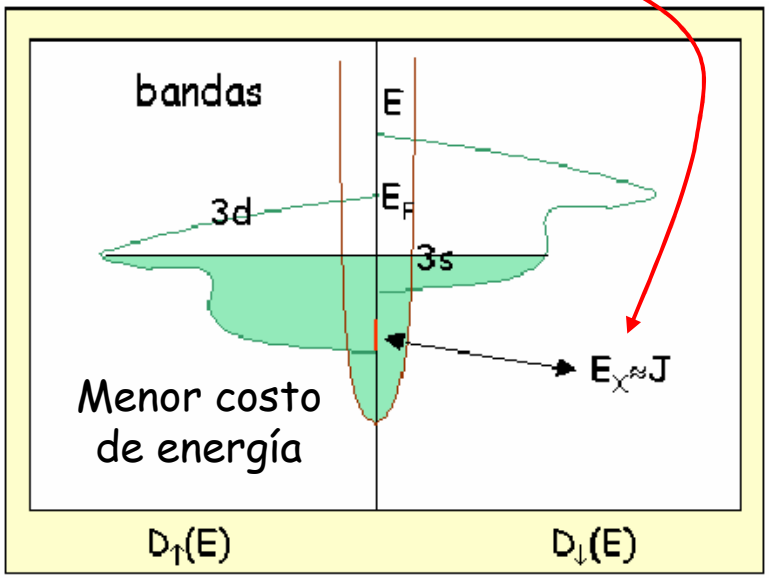
Estados atómicos degenerados – reglas de Hund



Máximo S, mínima superposición orbital

¿puede aplicarse a bandas?





Interpretación de la curva de Slater - Pauling

¿Cuanto cuesta agregar Δn electrones a la banda ↑?

$$D(\varepsilon) = \frac{dn}{d\varepsilon} \approx \frac{\Delta n}{\Delta \varepsilon} \Rightarrow \Delta\varepsilon = \frac{\Delta n}{D(\varepsilon_F)}$$

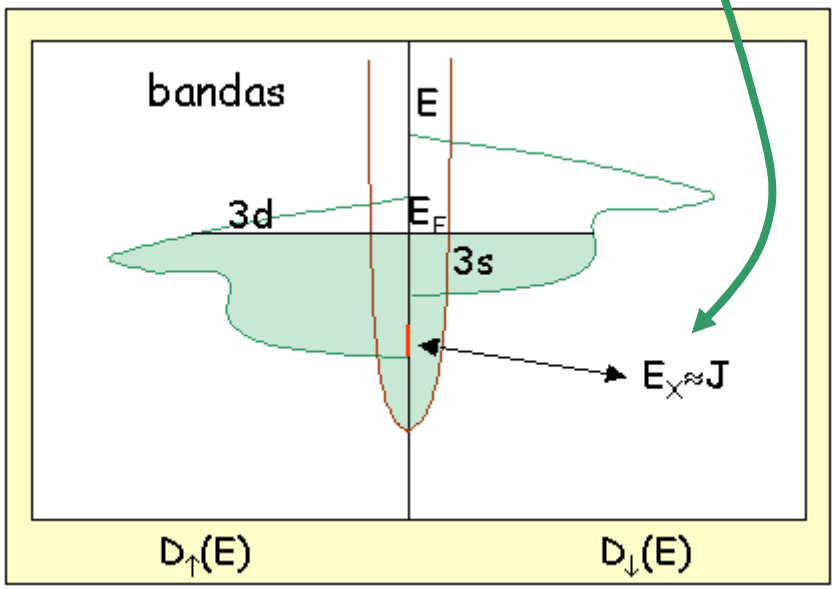
Si hay intercambio toda la subbanda reduce su energía en J

J debe ser suficiente para **compensar** Δε

$$\frac{J}{\Delta\varepsilon} > 1 \Rightarrow \frac{JD(\varepsilon_F)}{\Delta n} > 1 \xrightarrow{\Delta n \geq 1} JD(\varepsilon_F) > 1$$

$$JD(\varepsilon_F) > 1$$

$$J > 1/D(\varepsilon_F)$$

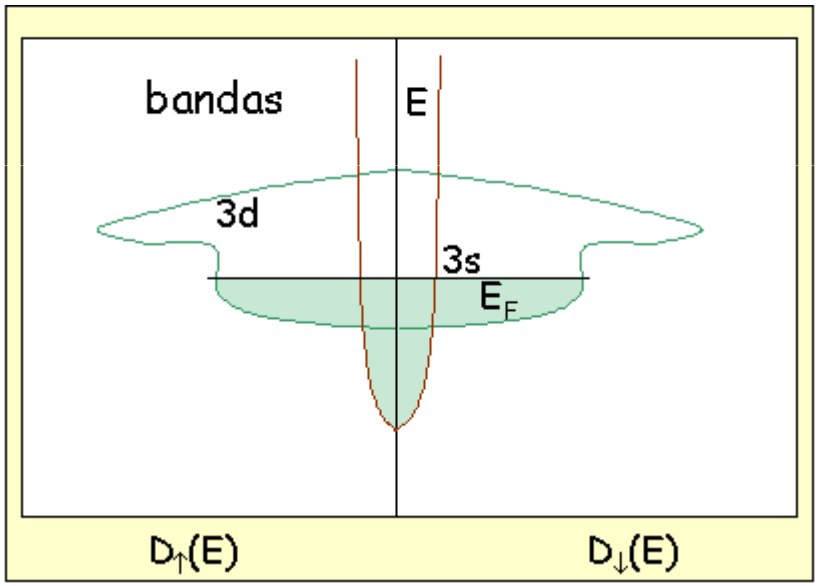


Criterio de Stoner para la existencia de magnetismo en conductores

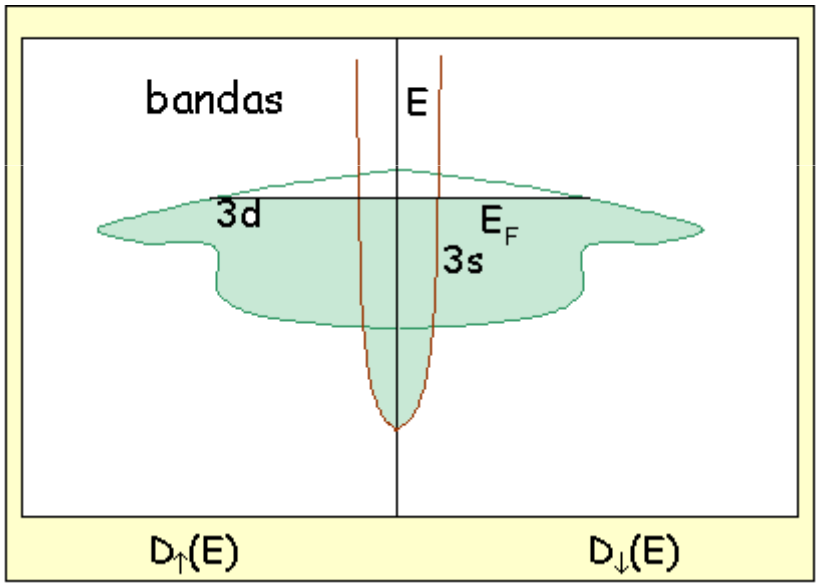
Interpretación de la curva de Slater - Pauling

3 – V, Cr, Mn vs. Fe, Co, Ni

V, Cr, Mn
Menos de la mitad de la banda 3d llena
Estados ligantes
antiferromagnetismo

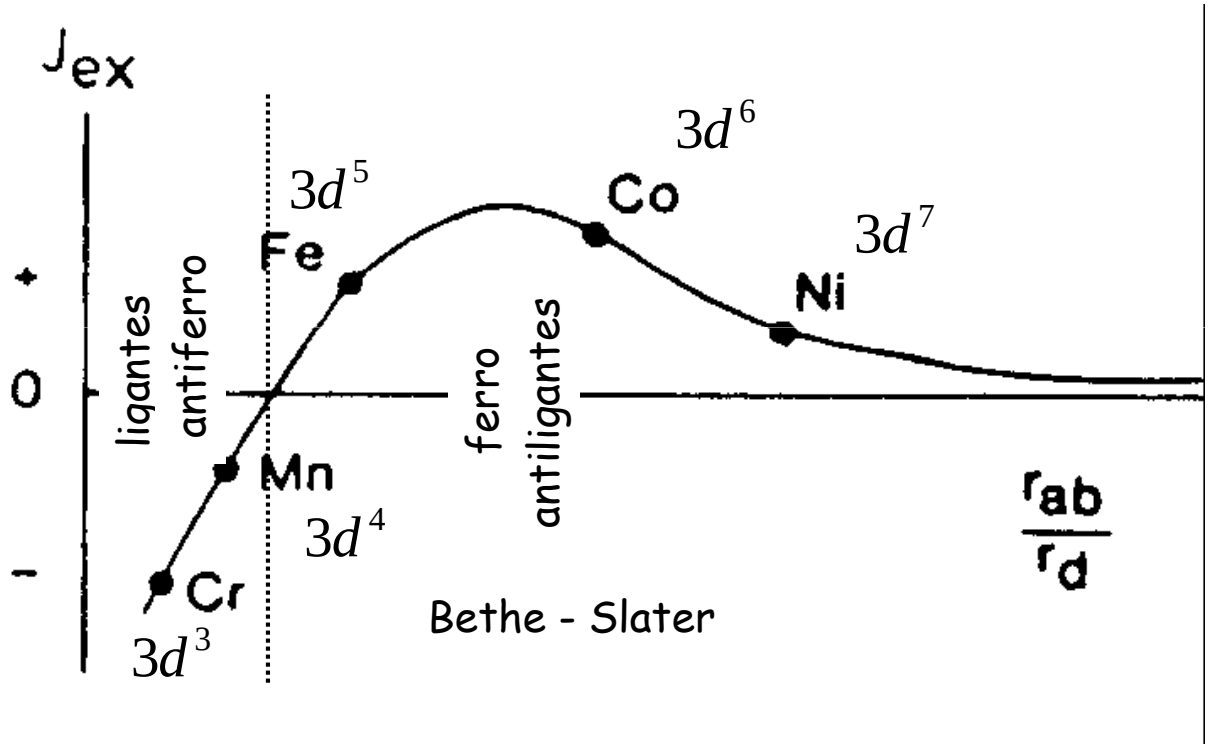


Fe, Co, Ni
Más de la mitad de la banda 3d llena
Estados antiligantes
ferromagnetismo



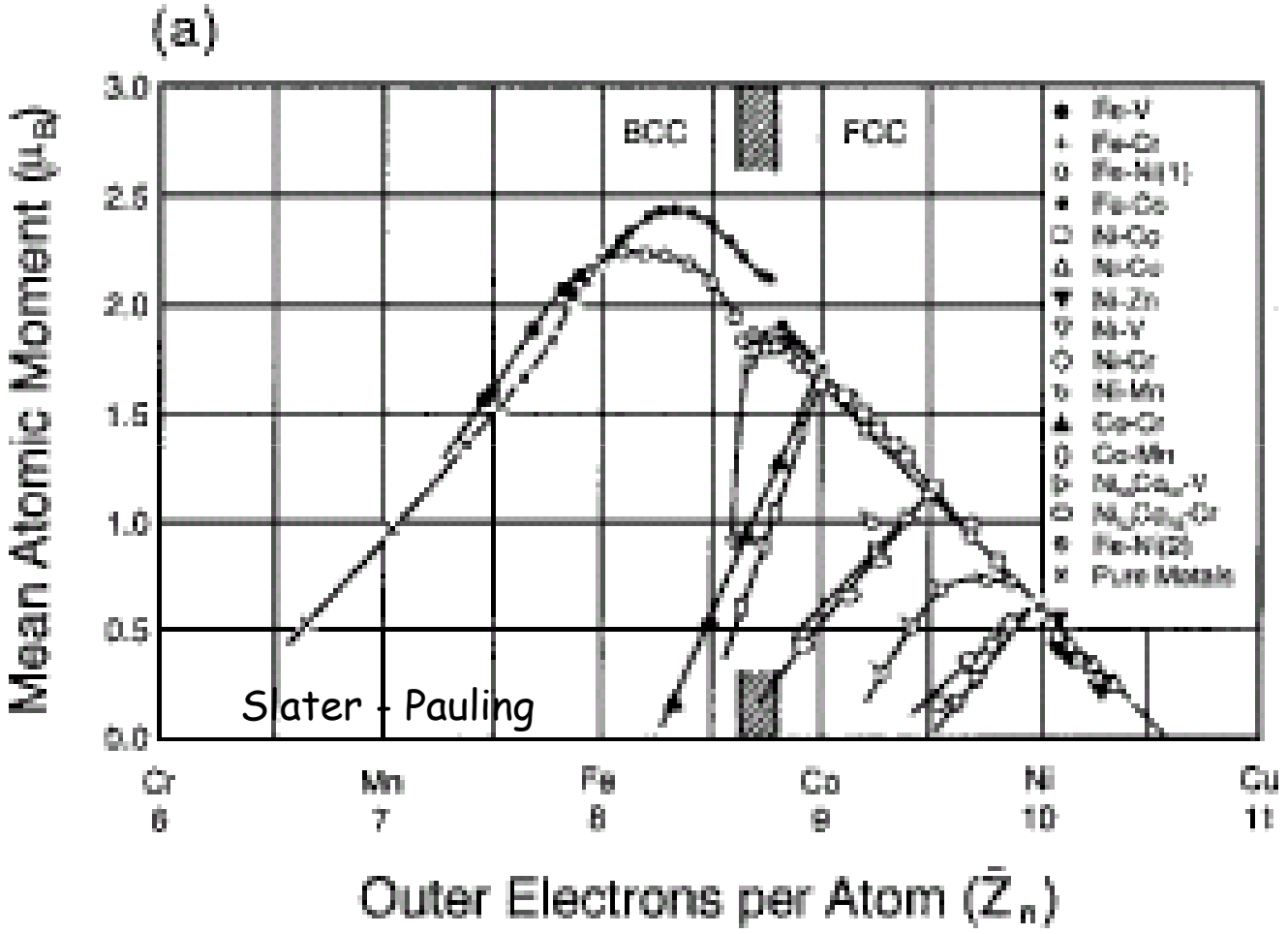
Covalencia → delocalización parcial de los electrones → disminución de $D(\varepsilon)$
Creación de ligaduras → electrones apareados en arreglos antiferro
Reduce o imposibilita el magnetismo

curva de Bethe – Slater. Metales de transición

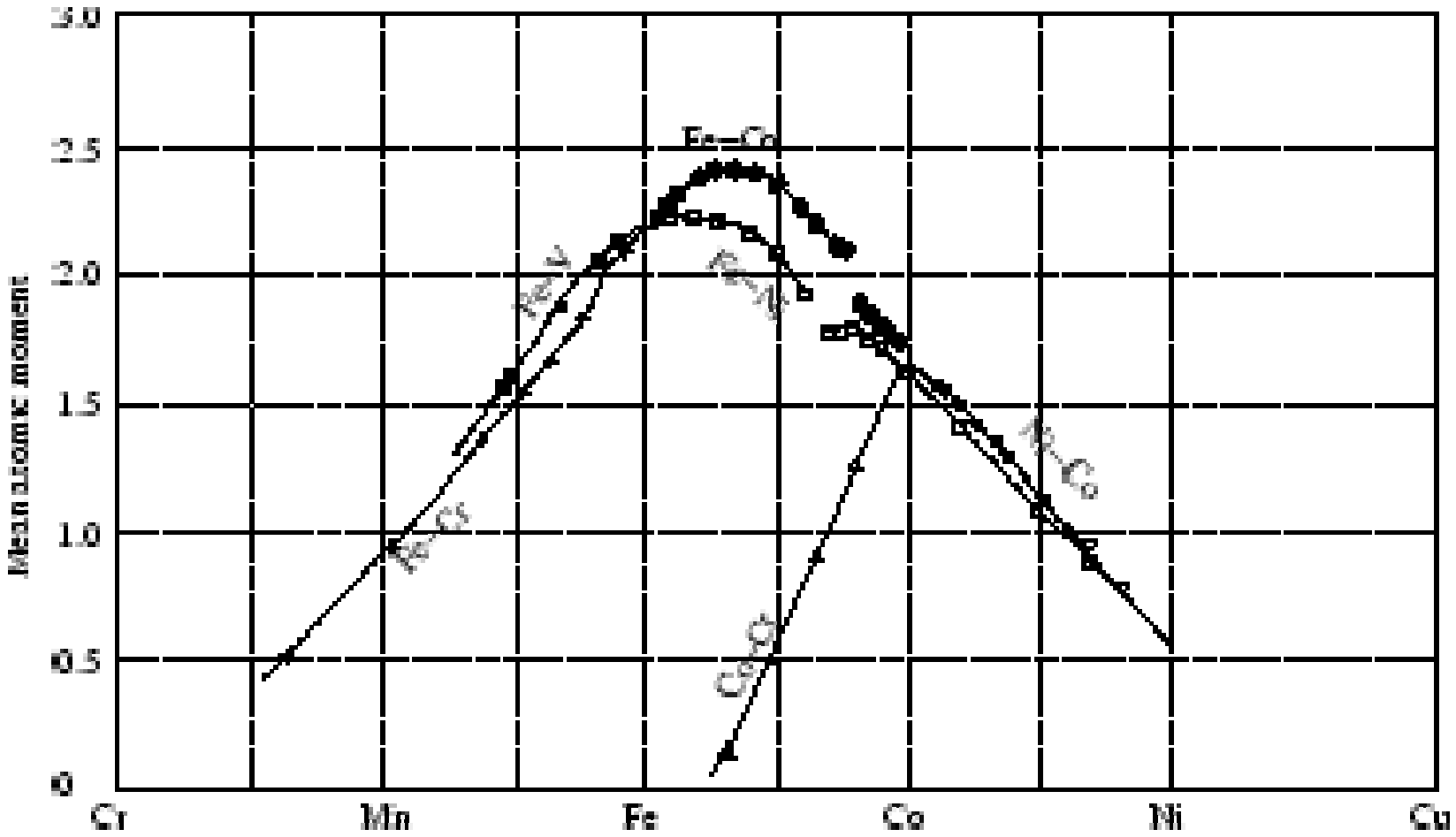


Modelo de bandas rígidas

Interpretación de la curva de Slater - Pauling



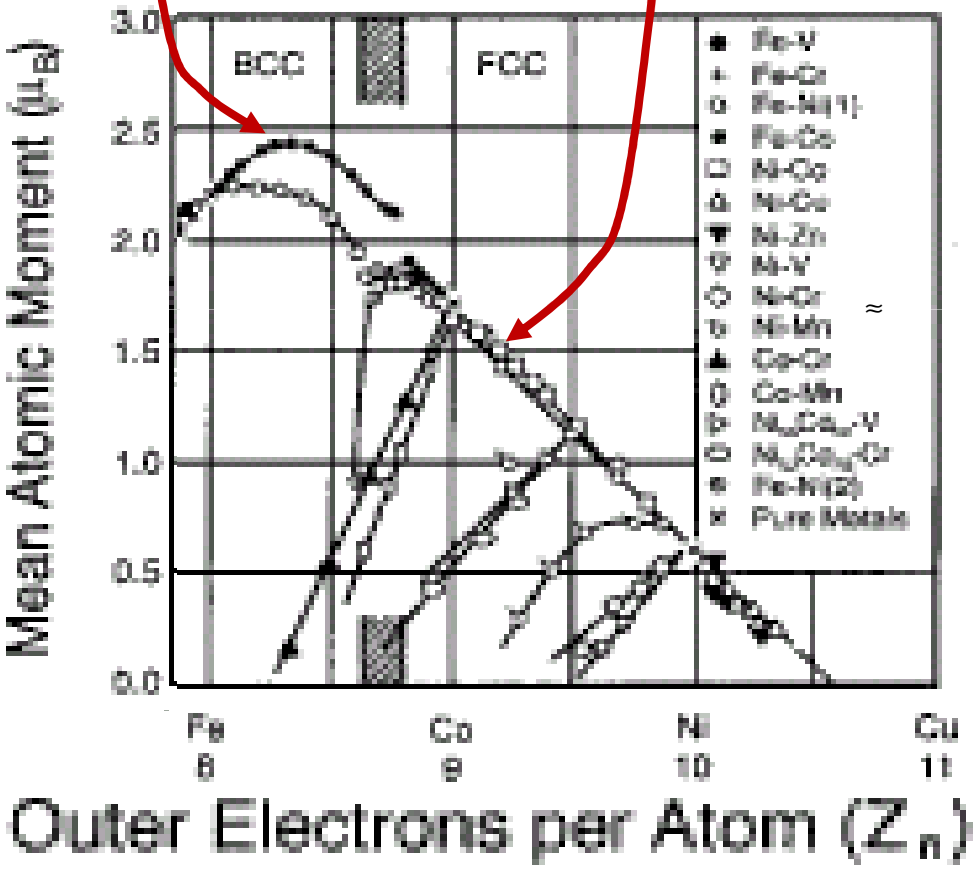
Interpretación de la curva de Slater - Pauling



Interpretación de la curva de Slater – Pauling. Modelo de bandas rígidas

máximo

pendiente $\frac{\partial \overline{m}}{\partial Z} \approx -1\mu_B / e^-$



Fe

8 electrones externos

$$n_{e^- ext}(MT_{3d}) = n_s + n_d = 8$$

Medidas de transporte

$$n_s(Fe) = n_s^{\uparrow} + n_s^{\downarrow} \approx 1$$

$$n_d(Fe) = n_d^{\uparrow} + n_d^{\downarrow} \approx 7$$

Fe

$$n_s(Fe) = n_s^{\uparrow} + n_s^{\downarrow} \approx 1$$

$$n_d(Fe) = n_d^{\uparrow} + n_d^{\downarrow} \approx 7$$

e^- *s* muy poco polarizados

$$n_s^{\uparrow} \approx n_s^{\downarrow} \approx 0.5$$

Medidas magnéticas $m_{Fe} = 2.2\mu_B$

$$n_d^{\uparrow} - n_d^{\downarrow} \approx 2.2$$

$$n_d^{\uparrow}(Fe) \approx 4.6; n_d^{\downarrow}(Fe) \approx 2.4$$

Ni

10 electrones externos

$$n_{e^- ext}(MT_{3d}) = n_s + n_d = 10$$

Medidas de transporte

$$n_s(Ni) = n_s^{\uparrow} + n_s^{\downarrow} \approx 0.6$$

$$n_d(Ni) = n_d^{\uparrow} + n_d^{\downarrow} \approx 9.4$$

Ni

$$n_s(Ni) = n_s^{\uparrow} + n_s^{\downarrow} \approx 0.6$$
$$n_d(Ni) = n_d^{\uparrow} + n_d^{\downarrow} \approx 9.4$$

e^- s muy poco polarizados

$$n_s^{\uparrow} \approx n_s^{\downarrow} \approx 0.3$$

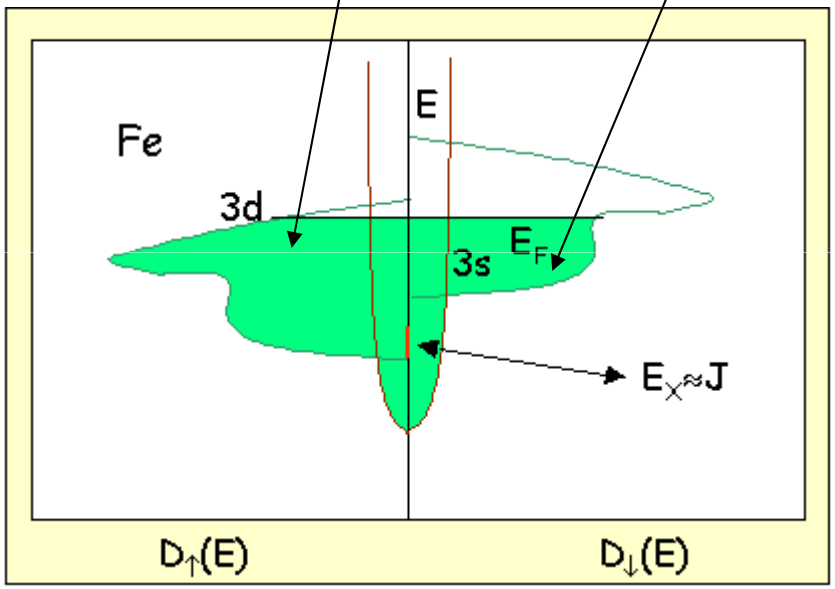
Medidas magnéticas $m_{Ni} = 0.6\mu_B$

$$n_d^{\uparrow} - n_d^{\downarrow} \approx 0.6$$

$$n_d^{\uparrow}(Ni) \approx 5.0; n_d^{\downarrow}(Ni) \approx 4.4$$

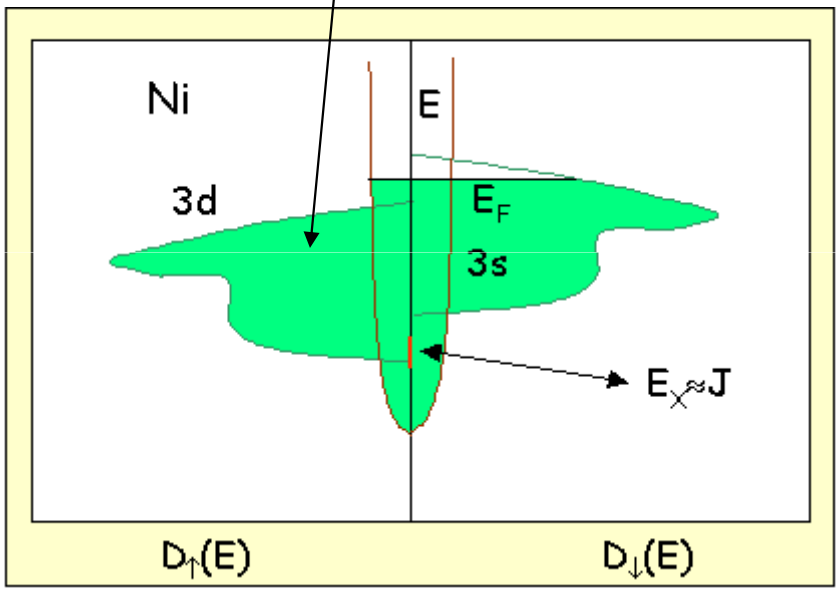
Sub-banda ↑ llena

$n_d^{\uparrow}(Fe) \approx 4.6; n_d^{\downarrow}(Fe) \approx 2.4$



Sub-banda 3d↑ semillena

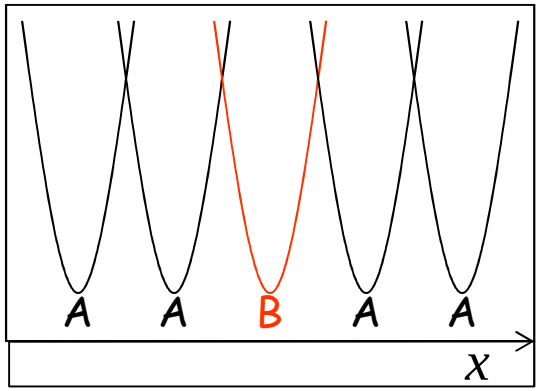
$n_d^{\uparrow}(Ni) \approx 5.0; n_d^{\downarrow}(Ni) \approx 4.4$



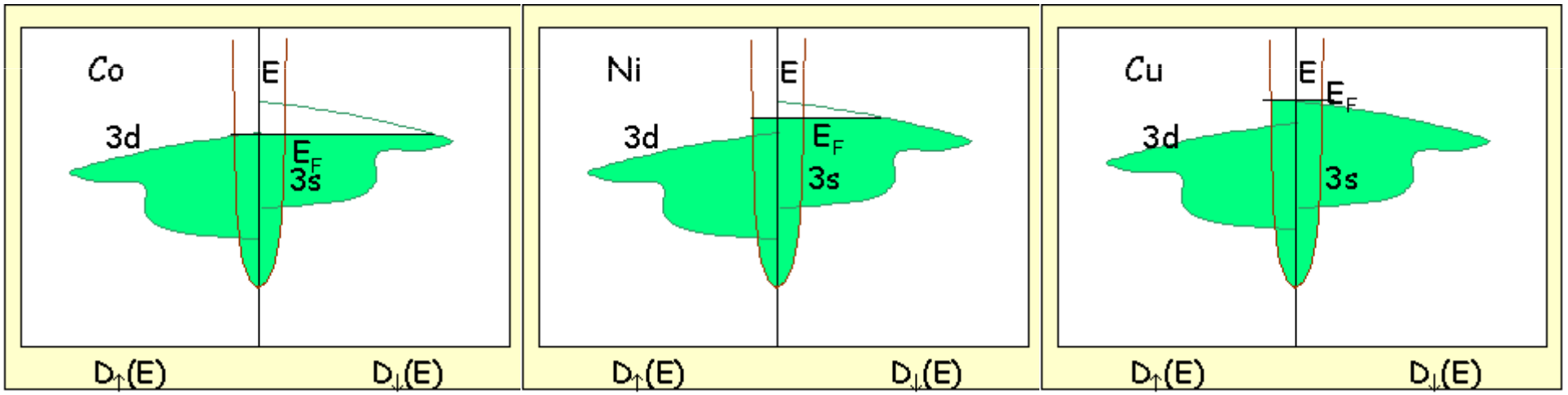
Sub-banda 3d↑ llena

hipótesis del modelo – aleaciones $A_{1-x}B_x$

B perturba poco el potencial periódico



Co → Cu sub-banda ↑ llena, $n_{d\uparrow} = 5$



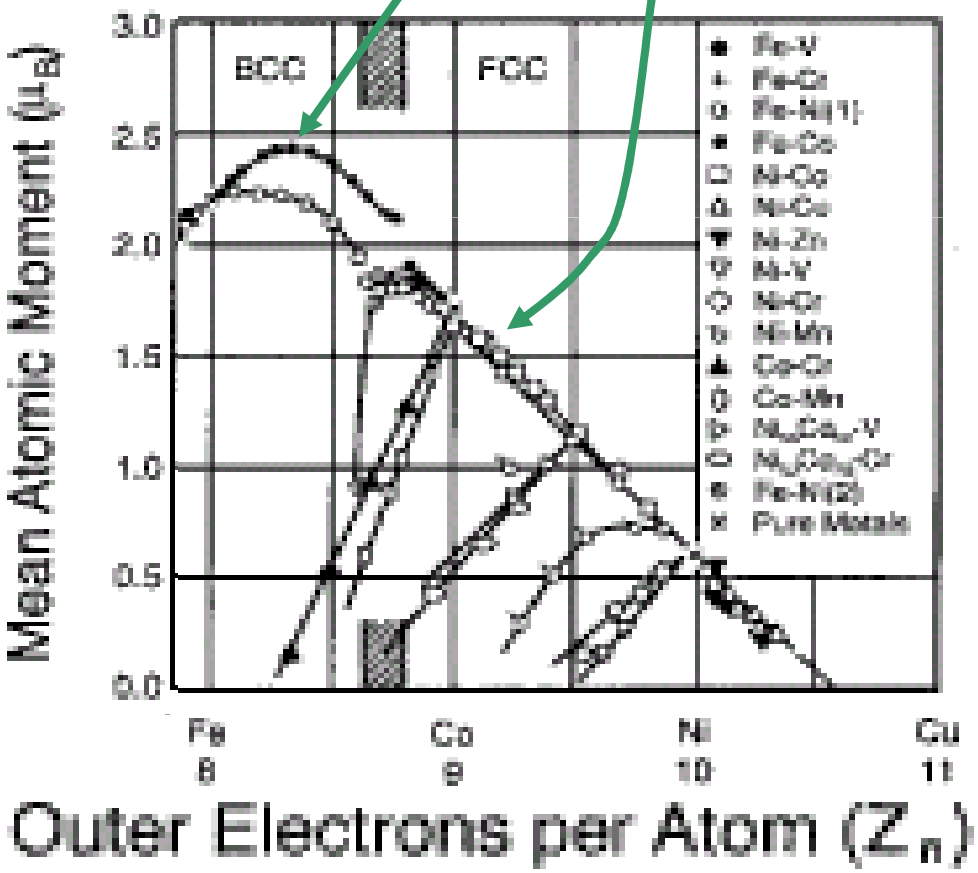
$m_{Co} = 1.7\mu_B$ $m_{Ni} = 0.6\mu_B$ $m_{Cu} = 0\mu_B$

$$m_{MT} = (n_d^{\uparrow} - n_d^{\downarrow})\mu_B = (5 - n_d^{\downarrow})\mu_B = (10 - n_d)\mu_B$$

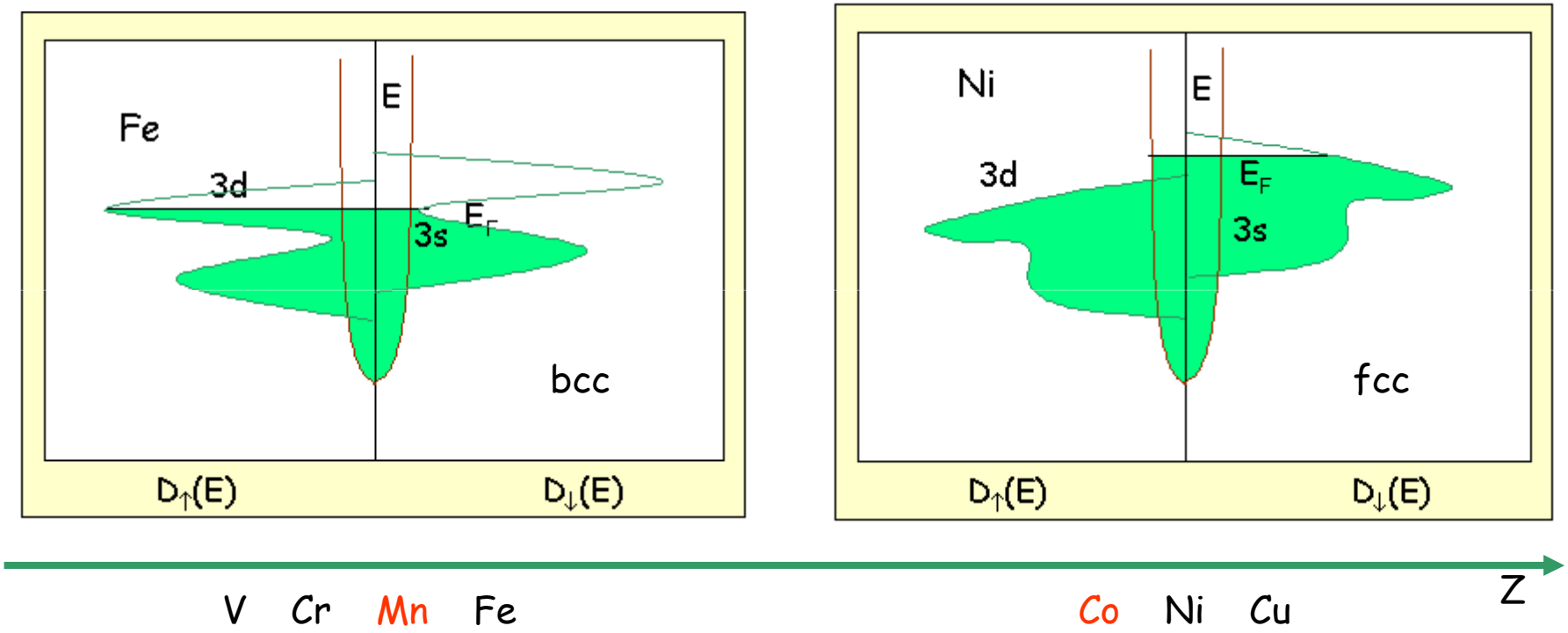
$$n_d^{\downarrow} = n_d - 5$$

Si n_d = 7.5: Momento medio $\overline{m}_{Fe_{0.5}Co_{0.5}} = (10 - n_d)\mu_B = 2.5\mu_B$

pendiente $\frac{\partial \overline{m}}{\partial Z} = \frac{\partial \overline{m}}{\partial n_d} = -1\mu_B / e^-$

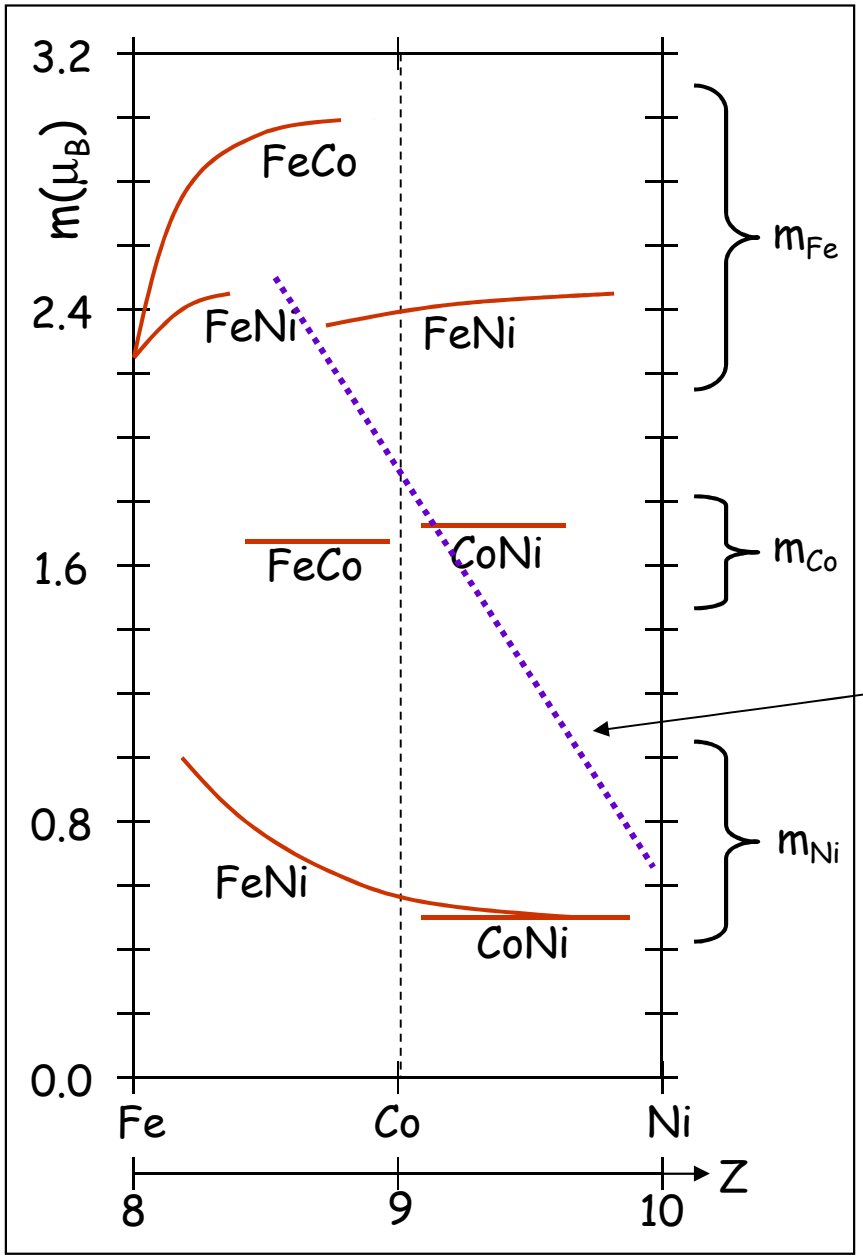


Influencia de la estructura



Momentos medios vs, momentos locales

Dispersión de neutrones



Momentos locales en sitios de Fe, Co y Ni de aleaciones FeCo, FeNi y CoNi

Momentos medios

Collins y Forsyth, Phil. Mag. **8**, 401 (1963)