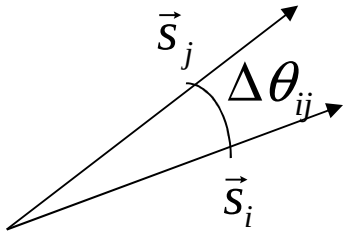
Intercambio – tratamiento continuo

Intercambio

Teoría del continuo - micromagnetismo

$$E_X = -2J_{ij}\vec{s}_i \cdot \vec{s}_j = -2s^2 J \cos\Delta\theta_{ij}$$

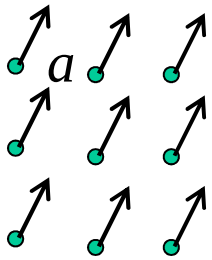


En un dominio $\cos\Delta\theta_{ij} = \left(1 - sen^2\left(\Delta\theta_{ij}\right)\right)^{1/2} \approx 1 - \frac{\left(\Delta\theta_{ij}\right)^2}{2}$

$$E_X = -2s^2 J \cos\Delta\theta_{ij} \approx -s^2 J\left(\Delta\theta_{ij}\right)^2 + cte$$

celdas cúbicas

$$\Delta\theta_{ij} \equiv \frac{\Delta\theta}{át} = \Delta x \frac{\Delta\theta}{\Delta x} \approx \alpha a \frac{\partial\theta}{\partial x}$$

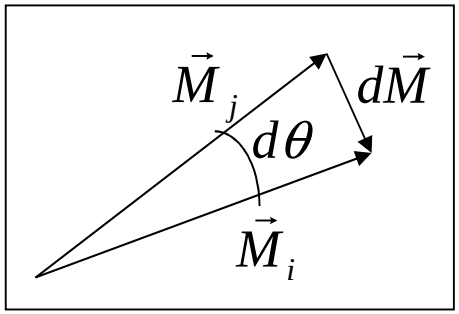


α depende del tipo de celda cúbica

$$\Delta E_X^{ij} \approx s^2 J\left(\Delta\theta_{ij}\right)^2 = s^2 J\alpha^2 a^2\left(\frac{\partial\theta}{\partial x}\right)^2$$

Teoría del continuo - micromagnetismo

$$\Delta E_X^{ij} \approx s^2 J \theta_{ij}^2 = s^2 J \alpha^2 a^2 \left(\frac{\partial \theta}{\partial x}\right)^2$$



$$dM \approx M d\theta \Rightarrow d\theta \approx \frac{dM}{M}$$

$$\frac{d\theta}{dx} = \frac{1}{M}\frac{dM}{dx} \Rightarrow \left(\frac{d\theta}{dx}\right)^2 = \frac{1}{M^2}\left(\frac{dM}{dx}\right)^2 \xrightarrow{3d} \left(\frac{d\theta}{dx}\right)^2 = \left(\frac{\vec{\nabla} M}{M}\right)^2$$

$$\Delta E_X^{ij} \approx s^2 J \alpha^2 a^2 \left(\frac{\vec{\nabla} M}{M}\right)^2$$

$$\varepsilon_X = \frac{\Delta E_X^{ij}}{V} \approx \frac{\alpha^2}{\beta}\frac{s^2 J}{a}\left(\frac{\vec{\nabla} M}{M}\right)^2 = A\left(\frac{\vec{\nabla} M}{M}\right)^2$$

β depende del tipo de celda cúbica

Cte de "Stiffnes"

$$A = \frac{\alpha^2}{\beta}\frac{s^2 J}{a}$$

Teoría del continuo - micromagnetismo

Cte de "Stiffnes"

$$A = \frac{\alpha^2}{\beta}\frac{s^2 J}{a}$$

Tipo de celda cúbica

- sc → $\alpha = 1$ → $A = \dfrac{s^2 J}{a}$
- bcc → $\alpha = \sqrt{2}$ → $A = \dfrac{2s^2 J}{a}$
- fcc → $\alpha = 2$ → $A = \dfrac{4s^2 J}{a}$

Intercambio

Teoría del continuo - micromagnetismo

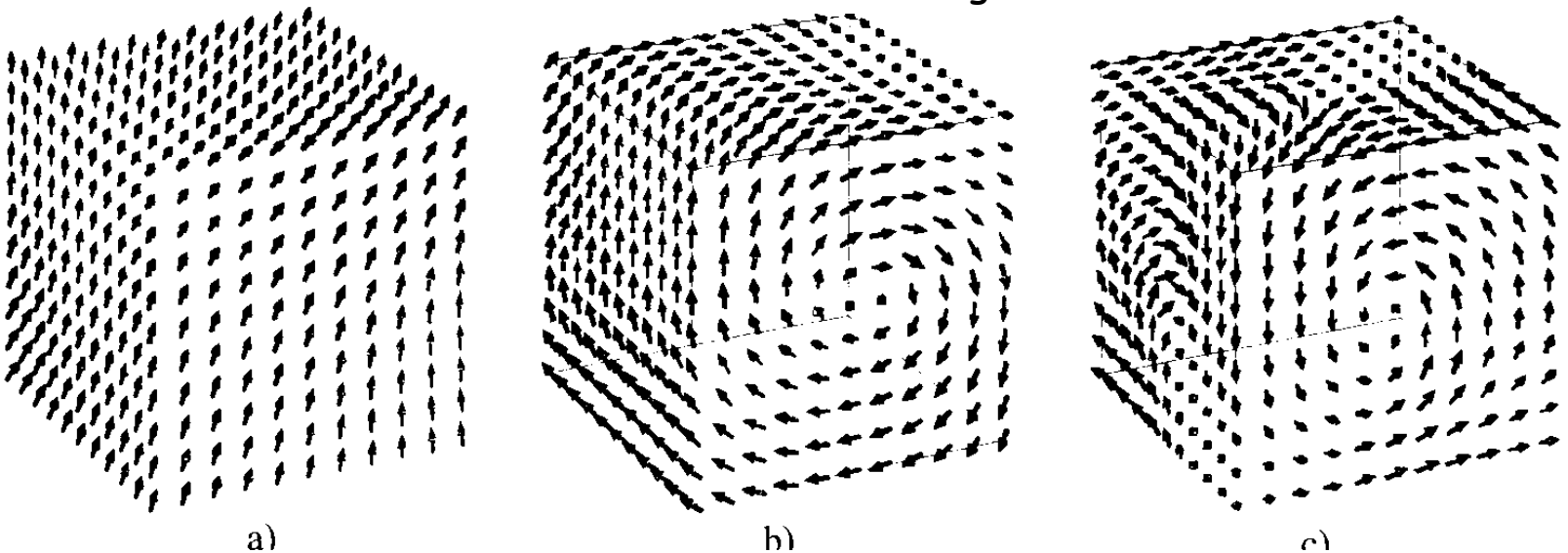
$$\varepsilon_X = A\left(\frac{\vec{\nabla}M}{M}\right)^2$$

Energía de "stiffness" por unidad de volumen

$$E_X = A\int\left(\frac{\vec{\nabla}M}{M}\right)^2 dV = A\int\left[\vec{\nabla}(\vec{m})\right]^2 dV$$

Integral extendida a todo el cuerpo

Soluciones de mínima energía

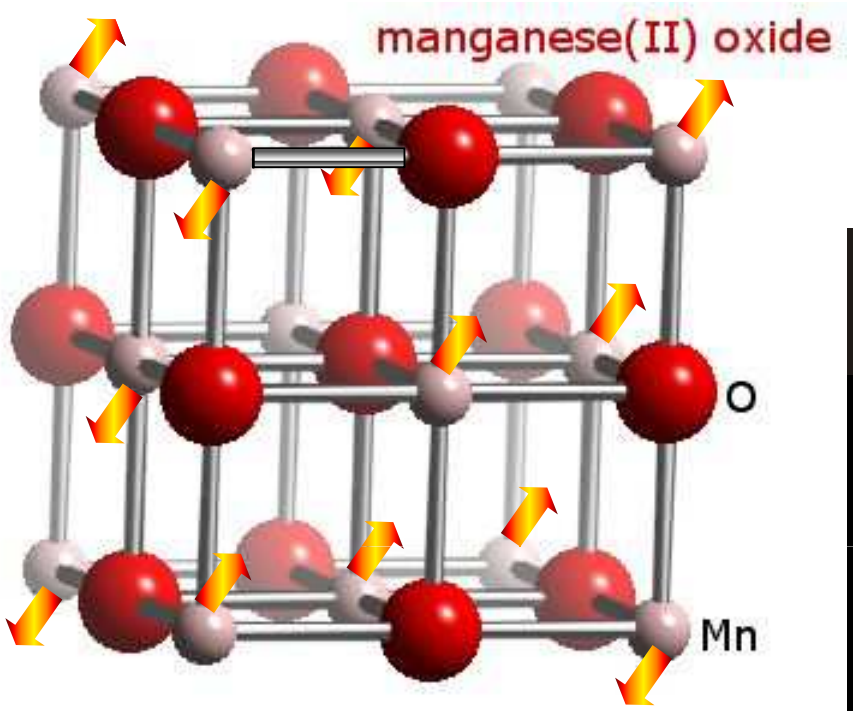


Superintercambio (a)

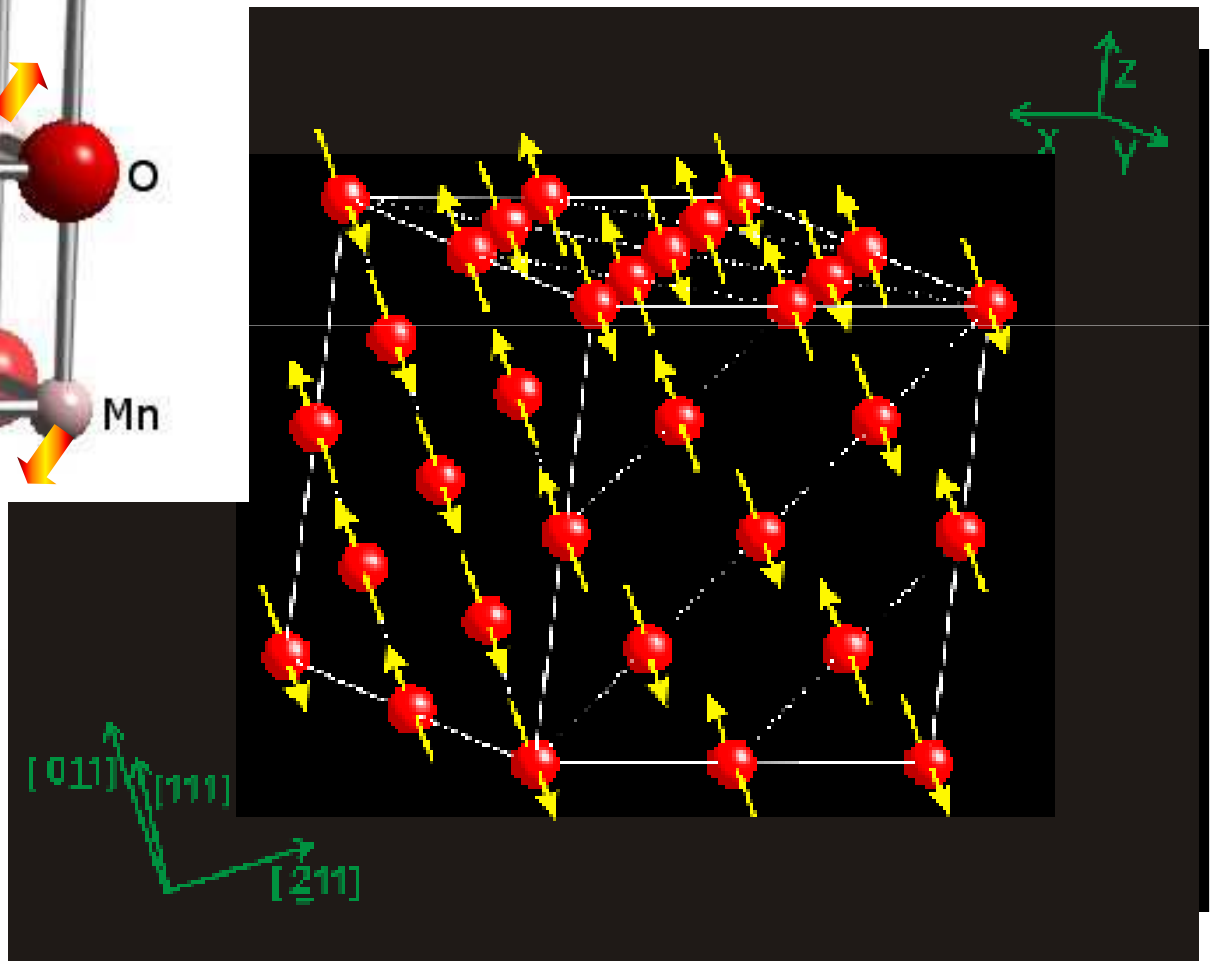
Intercambio y superintercambio

Orbitales atómicos y campo cristalino

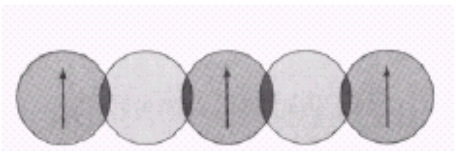
Ejemplo: MnO



Antiferromagneto T_N =118 K
estructura F (m3m) (12)
momentos magnéticos paralelos a planos (111)
planos (111) vecinos están ordenados AFM

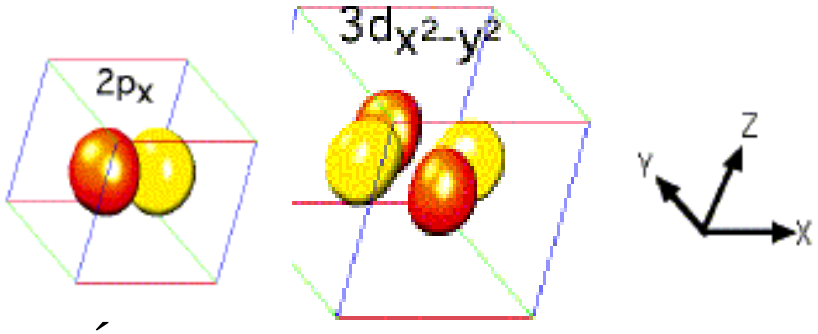


Superexchange.
A magnetic ion induces a spin polarisation in other magnetic ion which is coupled by their common non-magnetic neighbour.

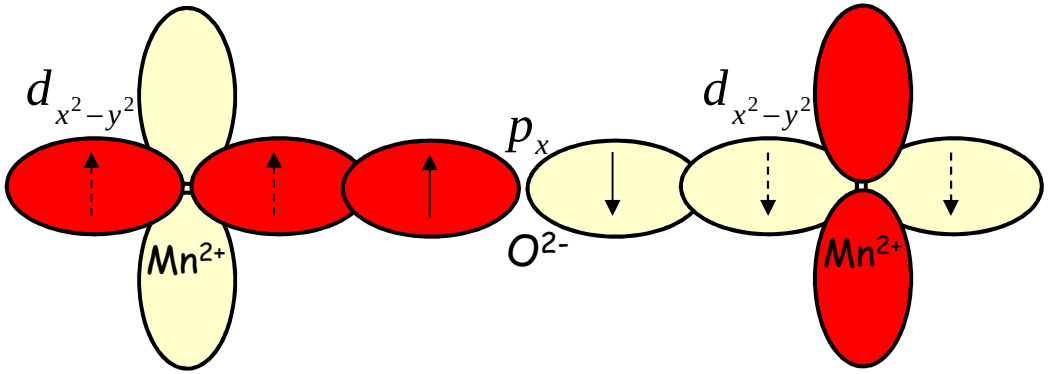


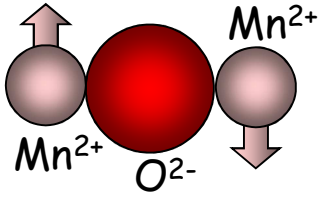
Intercambio y superintercambio

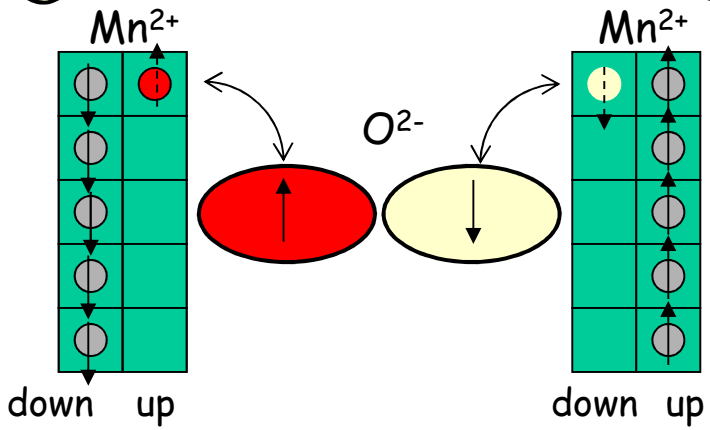
MnO



oxígeno *manganeso*







$$[Mn^0] = [Ar]3s^2 3d^5 4s^2$$

$$[Mn^{2+}] = [Ar]3s^2 3d^5$$

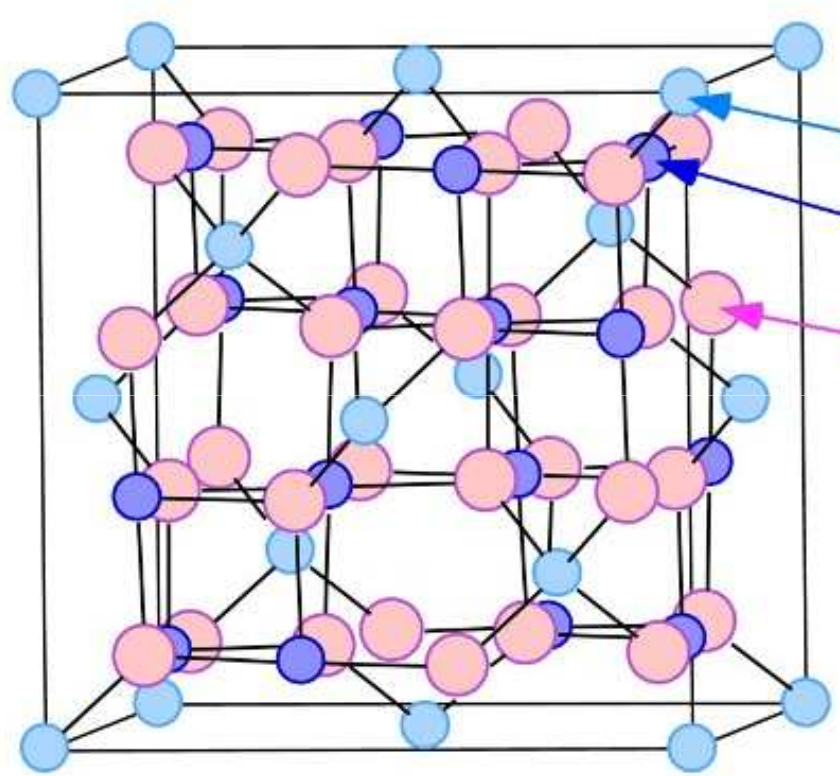
Intercambio y superintercambio

Magnetita: espinela de Fe

$$Fe_3O_4 = Fe^{2+}O.Fe_2^{3+}O_3$$

óxido	estructura	Estructura magnética	m(μ_B)	σ(emu/g)	T_N(K)
Fe_3O_4 magnetita	espinela	ferri	4.1 por form	96	858

Magnetita o espinela de Fe

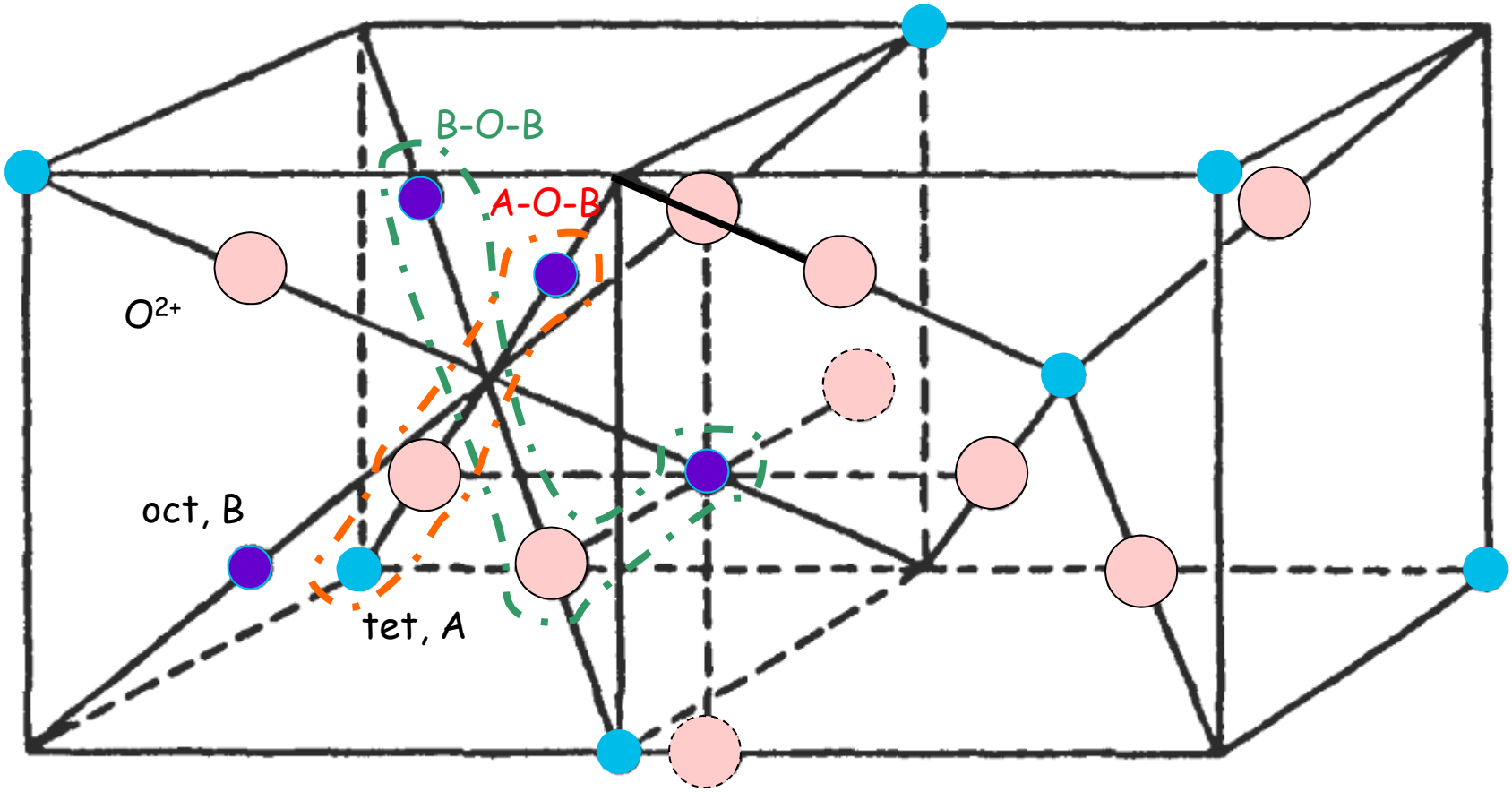


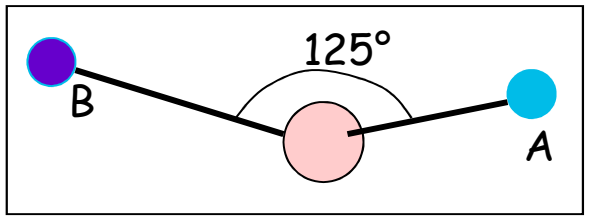
$$Fe_3O_4 = Fe^{2+}O.Fe_2^{3+}O_3$$

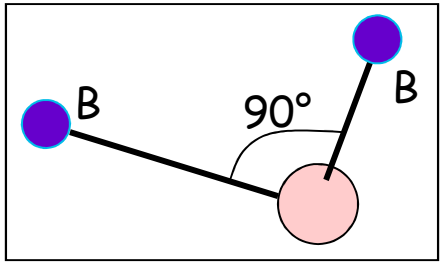
$$\langle \vec{m} \rangle_{Fe_3O_4} \approx m_{Fe^{3+}}(\Uparrow) + m_{Fe^{3+}}(\Downarrow) + m_{Fe^{2+}}(\uparrow) \approx m_{Fe^{2+}}(\uparrow) = 4\mu_B \vec{u}_z$$

Intercambio y superintercambio

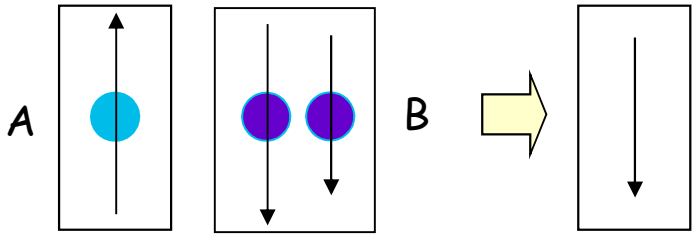
Magnetita o espinela de Fe







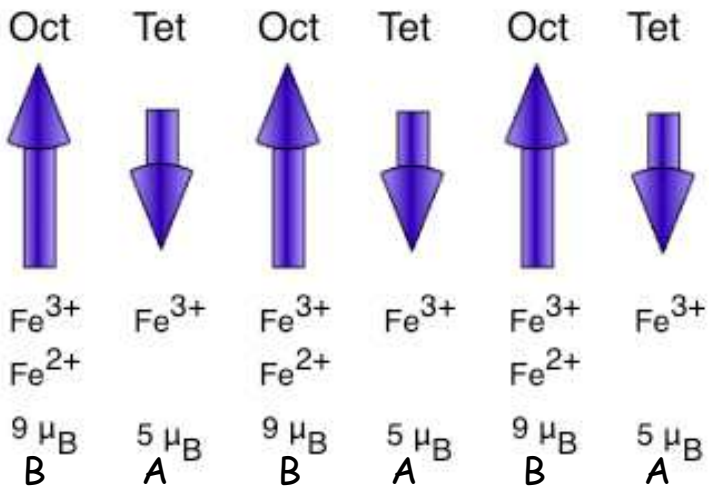
$J_{AB} >> J_{BB}$



Intercambio y superintercambio

Magnetita o espinela de Fe

$$Fe_3O_4 = Fe^{2+}O.Fe_2^{3+}O_3$$



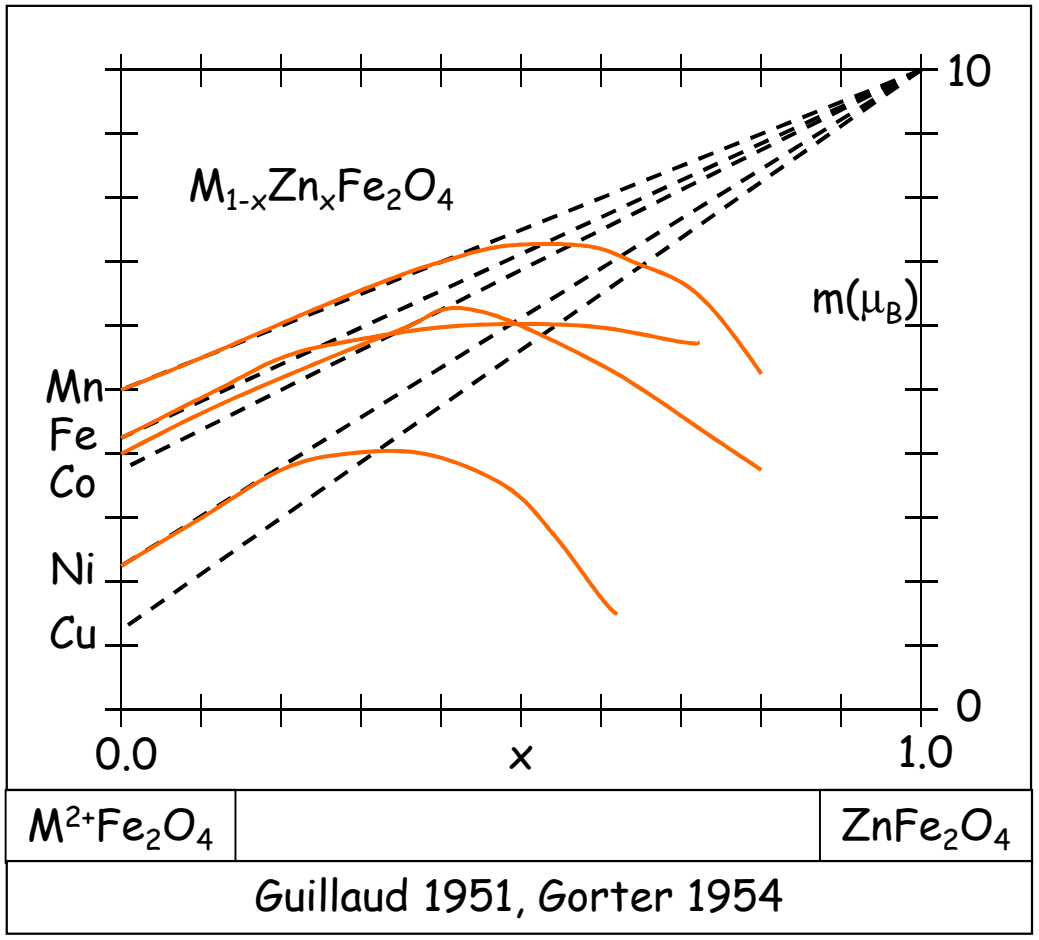
inversa		normal	
A tetraedral	B octaedral	A tetraedral	B octaedral
Fe^{3+} ($+5\mu_B$)	$Fe^{2+}Fe^{3+}$ [$-(4+5)\mu_B$]	Fe^{2+} ($+4\mu_B$)	$2Fe^{3+}$ [$2(-5)\mu_B$]

Intercambio y superintercambio

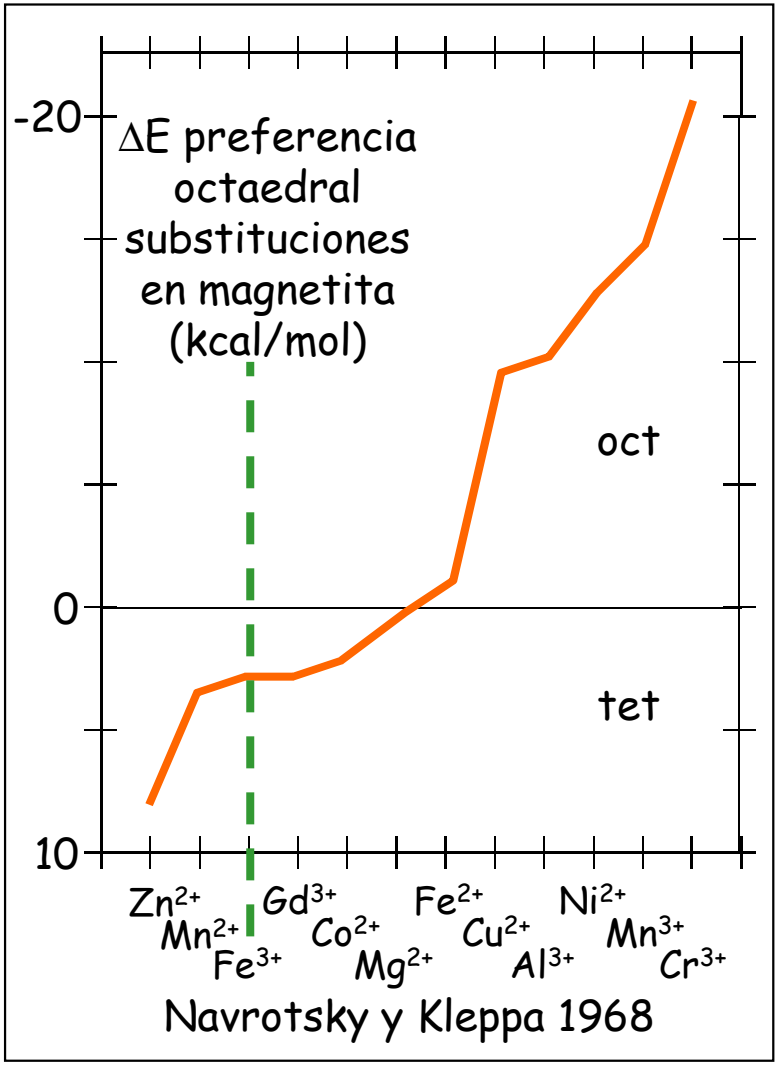
Espinelas $M^{2+}Fe_2O_4$

Un resultado inesperado

reemplazo de Fe por Zn



Guillaud 1951, Gorter 1954

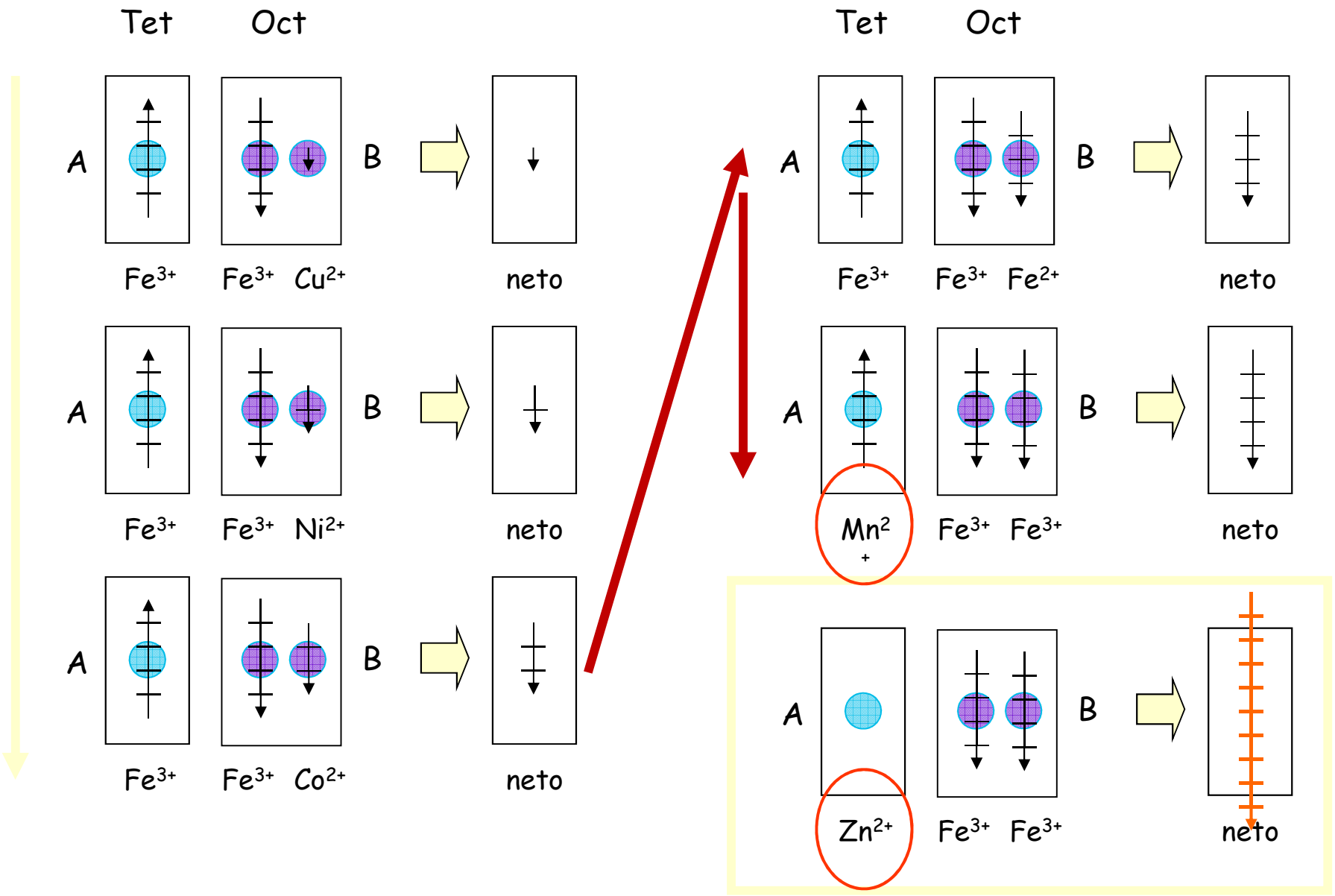


Navrotsky y Kleppa 1968

Intercambio y superintercambio

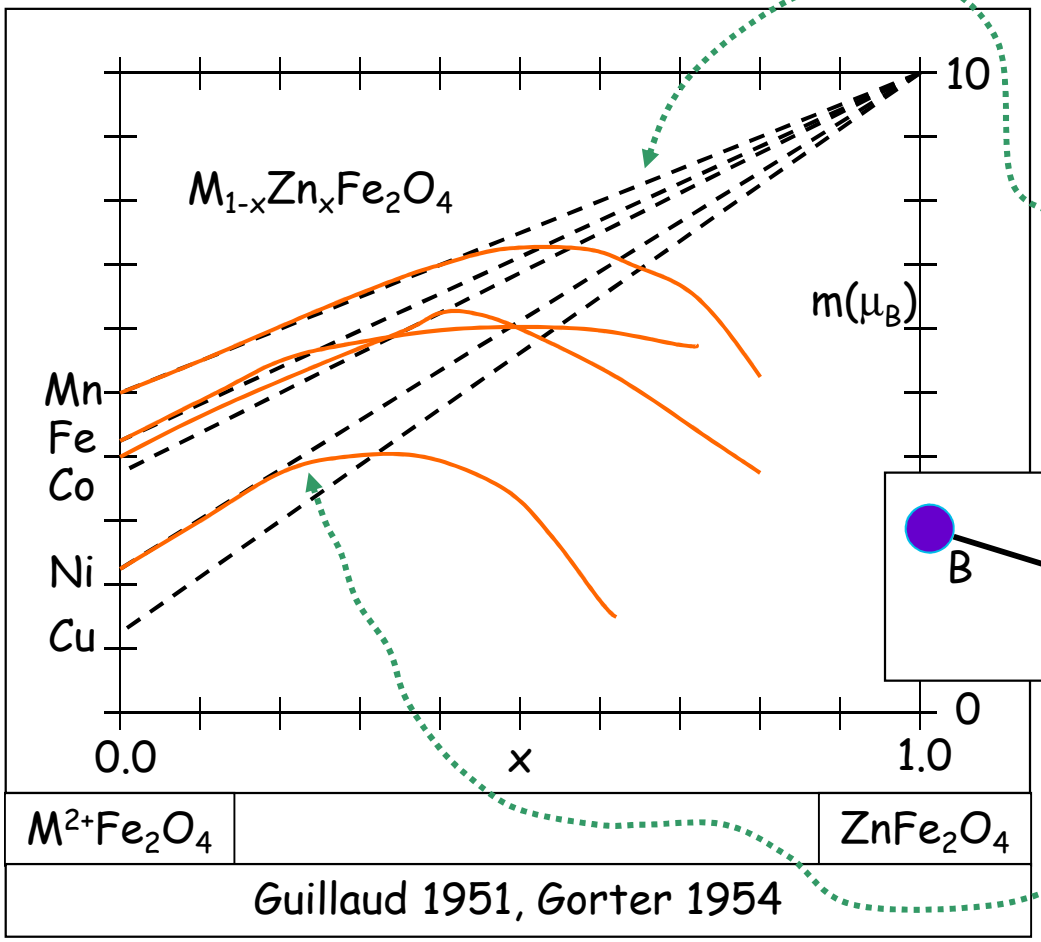
Espinelas $M^{2+}Fe_2O_4$

$$J_{AB} >> J_{BB}$$



Intercambio y superintercambio

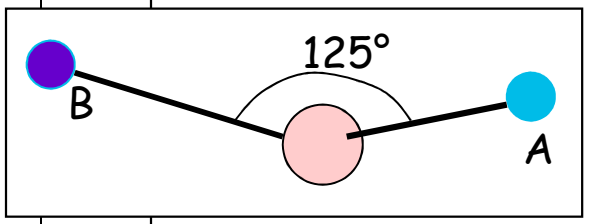
Espinelas $M^{2+}Fe_2O_4$

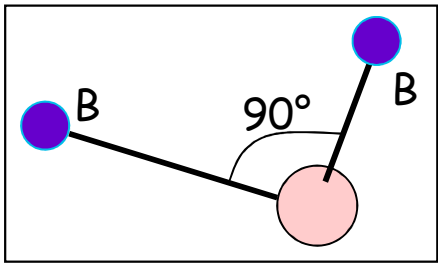


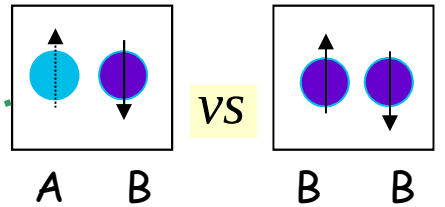
$$M = Cu, Ni, Co, Fe, Mn$$

$$m_{FU} = 5(1+x) + m_M(1-x) - 5(1-x)$$

$$m_{FU} = 10x + m_M(1-x)$$







$$J_{AB} >> J_{BB}$$

Intercambio y superintercambio

Espinelas