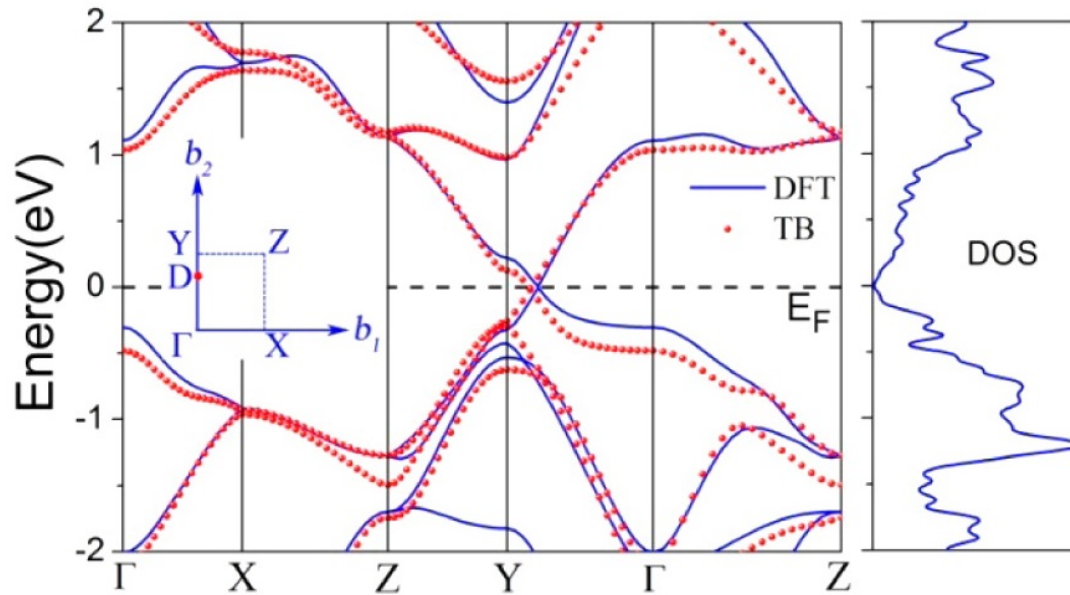


# Capítulo 6: Electrones en un potencial periódico - Teoría de bandas



Desde un punto de vista fundamental, se debe resolver el siguiente problema para obtener los niveles de energía de los electrones en un cristal:

$$H\Psi = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_i^2 \Psi - Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r}_i - \mathbf{R}|} \Psi \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \Psi = E\Psi.$$

donde  $\Psi(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2, \dots, \mathbf{r}_N s_N)$

Diferentes aproximaciones que se utilizan conducen a la ecuación de Schrodinger para 1 electrón en un potencial efectivo :

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})$$

one electron  
approximation

donde  $U(\vec{r} + \vec{R}) = U(\vec{r})$ ,  $\forall \vec{R} \in \text{Red de Bravais.}$

Ejemplo:

$$H\Psi = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_i^2 \Psi - Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r}_i - \mathbf{R}|} \Psi \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \Psi = E\Psi.$$

$$U^{\text{ion}}(\mathbf{r}) = -Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r} - \mathbf{R}|}.$$

Aproximación:

$$U^{\text{el}}(\mathbf{r}) = -e \int d\mathbf{r}' \rho(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|}.$$

En el marco de la one electron approximation:

$$\rho(\mathbf{r}) = -e \sum_i |\psi_i(\mathbf{r})|^2,$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\mathbf{r}) + U^{\text{ion}}(\mathbf{r})\psi_i(\mathbf{r}) + \left[ e^2 \sum_j \int d\mathbf{r}' |\psi_j(\mathbf{r}')|^2 \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right] \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}).$$

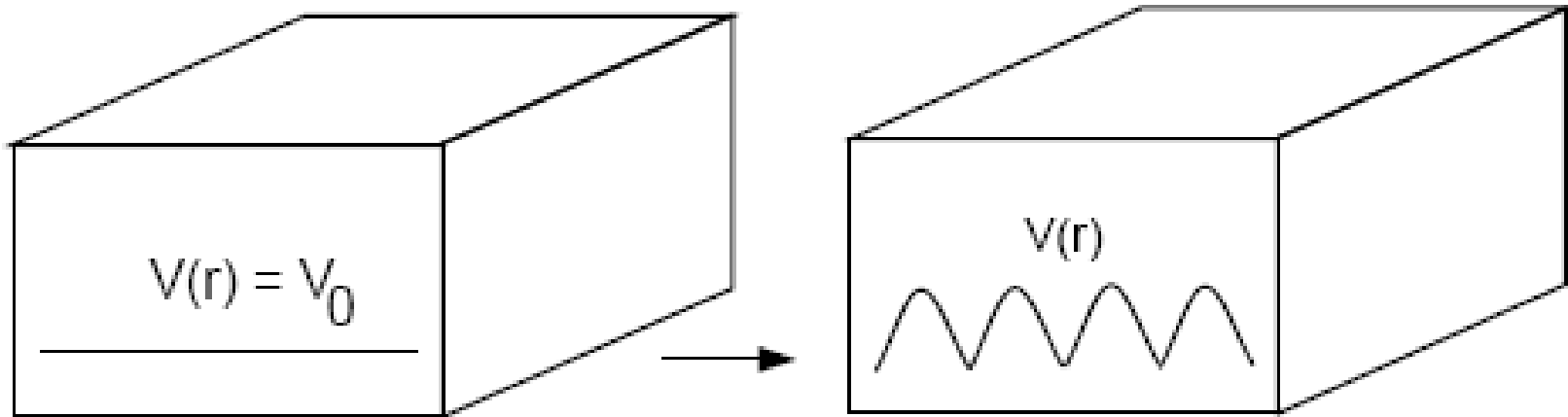
**Ecuaciones de Hartree**

$$U(\mathbf{r}) = U^{\text{ion}}(\mathbf{r}) + U^{\text{ee}}(\mathbf{r})$$

Se resuelven en forma autoconsistente  $U^{\text{ee}}(\Psi) !!!$

$$\check{H}\Psi(\vec{r}) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right] \Psi(\vec{r}) = \epsilon\Psi(\vec{r})$$

donde  $U(\vec{r} + \vec{R}) = U(\vec{r})$ ,  $\forall \vec{R} \in \text{Red de Bravais}$ .



$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e} (k_x^2 + k_y^2 + k_z^2)$$

?



Por lo tanto, es de suma importancia el problema de un electrón en un potencial periódico:

$$\hat{H}\Psi(\vec{r}) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right] \Psi(\vec{r}) = \epsilon\Psi(\vec{r})$$

donde  $U(\vec{r} + \vec{R}) = U(\vec{r})$ ,  $\forall \vec{R} \in \text{Red de Bravais}$ .

## Teorema de Bloch

Las soluciones son del forma

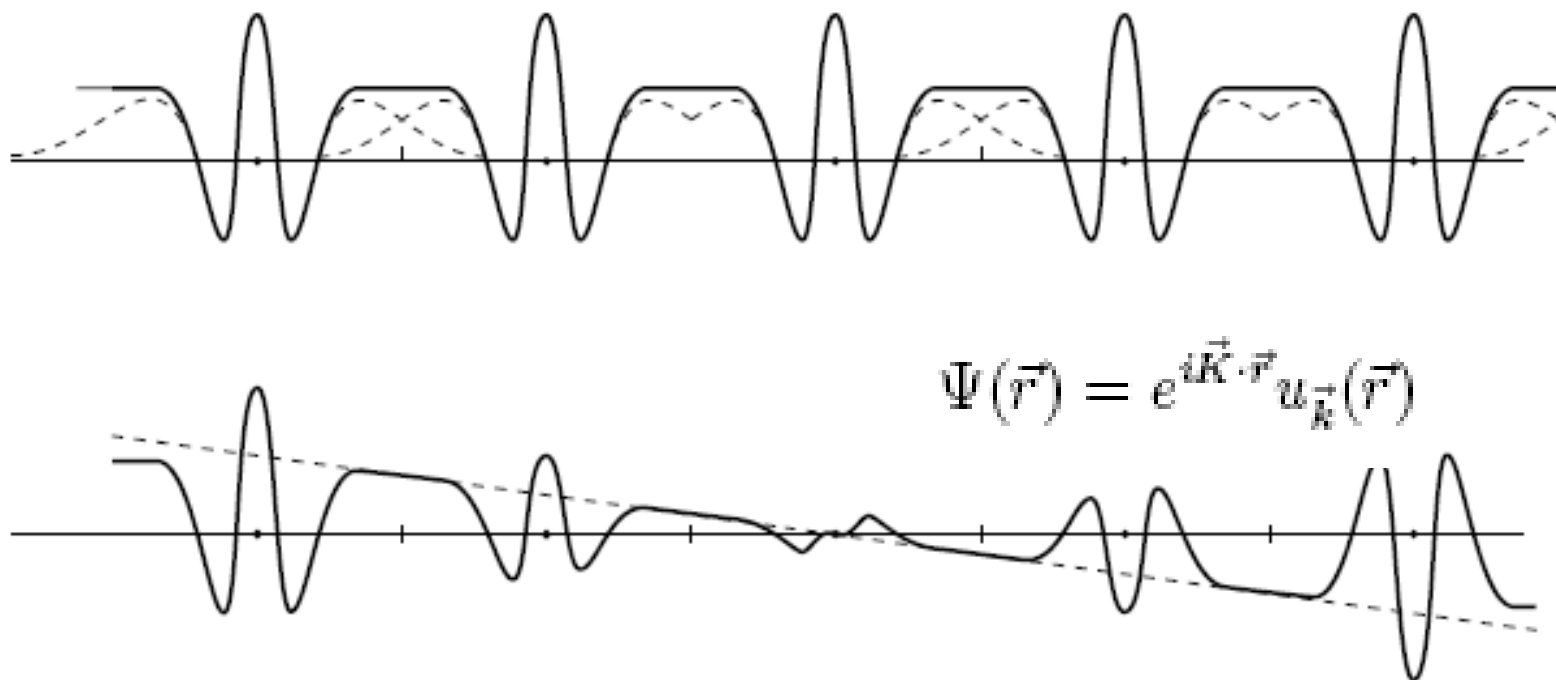
$$\Psi(\vec{r}) = e^{i\vec{K} \cdot \vec{r}} u_{\vec{K}}(\vec{r})$$

donde

$$u_{\vec{K}}(\vec{r} + \vec{R}) = u_{\vec{K}}(\vec{r}) \quad \text{para todo } \vec{R} \in \text{red de Bravais}$$

**Notemos que**

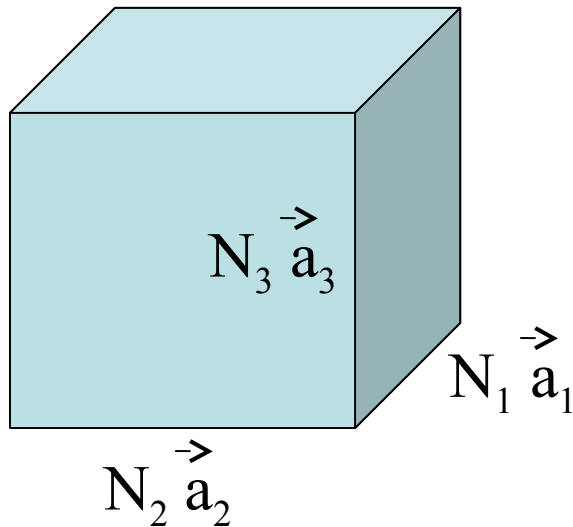
$$\Psi(\vec{r} + \vec{R}) = e^{i\vec{K} \cdot \vec{R}} \Psi(\vec{r})$$



**Fig. 17.1.** A lattice-periodic function  $u(x)$  and the real part of the corresponding Bloch function

## Condiciones periódicas de contorno (Born-von Karman)

Sean  $\vec{a}_1, \vec{a}_2, \vec{a}_3$  vectores primitivos, definamos



$$N \equiv N_1 N_2 N_3$$

Número de  
celdas

$$\Psi(\vec{r} + N_i \vec{a}_i) = \Psi(\vec{r}), \quad i = 1, 2, 3.$$

$$\Psi(\vec{r} + N_i \vec{a}_i) = \underbrace{e^{i\vec{K} \cdot N_i \vec{a}_i}}_1 \Psi(\vec{r}) \quad i = 1, 2, 3$$

$$N_i \vec{K} \cdot \vec{a}_i = 2\pi m_i, \quad m_i \in \mathbb{Z}$$

Los valores permitidos de  $\mathbf{k}$  son:

$$\mathbf{k} = \sum_{i=1}^3 \frac{m_i}{N_i} \mathbf{b}_i,$$

## Comentarios:

1- El número de  $k$  permitidos que pertenecen a la primer zona de Brillouin es igual al número de celdas del cristal  $N$ .

2- El volumen del espacio  $k$  asociado a cada punto  $k$  permitido es:

$$\Delta k = \frac{\mathbf{b}_1}{N_1} \cdot \left( \frac{\mathbf{b}_2}{N_2} \times \frac{\mathbf{b}_3}{N_3} \right) = \frac{1}{N} \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3).$$

Pero: 
$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

El volumen de la celda primitiva de la red directa  $v = V/N$

$$\Delta k = \frac{(2\pi)^3}{V}$$

**Lo mismo que  
para el gas de  $e^-$**

$$g(k) = \frac{2}{(2\pi)^3}$$

3-  $\Psi(\vec{r}) = e^{i\vec{K}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$  no son autofunciones del momento lineal

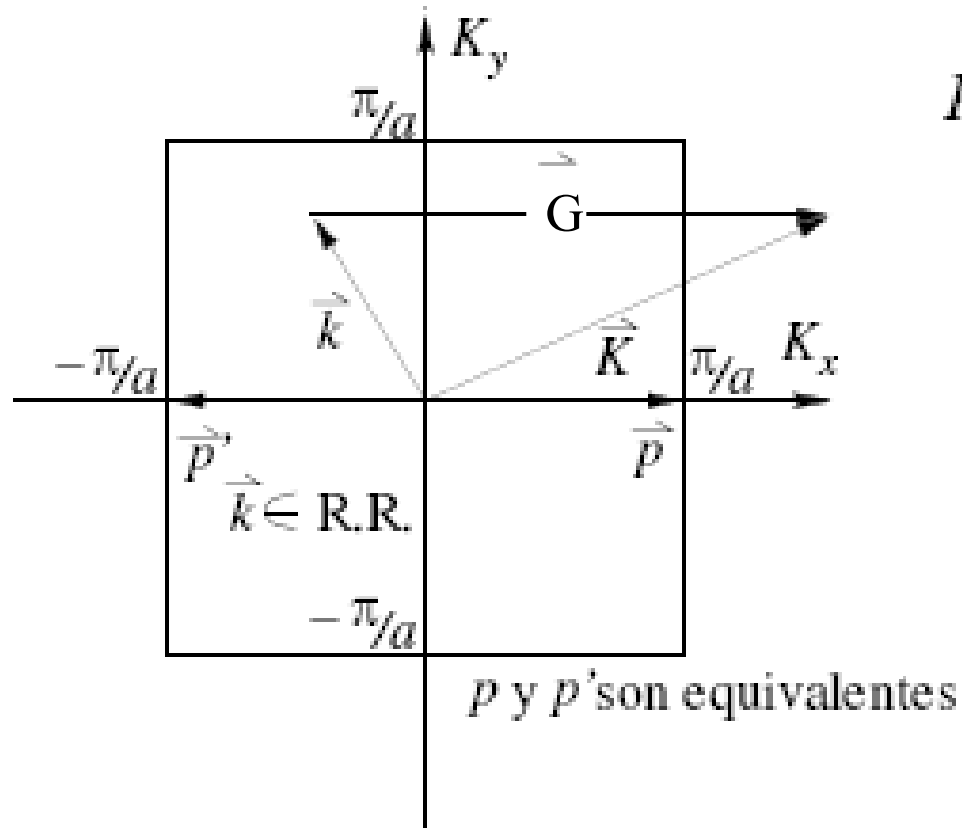
$$\begin{aligned} -i\hbar\vec{\nabla}\Psi(\vec{r}) &= -i\hbar\vec{\nabla}(e^{i\vec{K}\cdot\vec{r}} u_{\vec{k}}) \\ &= \hbar\vec{K} e^{i\vec{K}\cdot\vec{r}} u_{\vec{k}} - i\hbar e^{i\vec{K}\cdot\vec{r}} \vec{\nabla} u_{\vec{k}} \end{aligned}$$

4- El vector  $\vec{K}$  siempre se puede restringir a la 1 zona de Brillouin.

En efecto, todo vector  $\vec{K}$  se puede escribir:

$$\vec{K} = \vec{k} + \vec{G}$$

Donde  $\vec{G}$  pertenece a la red recíproca y  $\vec{k}$  a la 1ZB.



$$\vec{K} = \vec{k} + \vec{G}$$

Si para  $\vec{K}$  se cumple  $\Psi(\vec{r} + \vec{R}) = e^{i\vec{K} \cdot \vec{R}} \Psi(\vec{r})$

Esta condición también se cumple para  $\vec{k}$  ya que

$$e^{i\vec{G} \cdot \vec{R}} = 1$$

## Demostración del Teorema de Bloch

Expando la función de onda en una base de ondas planas (satisfacen las condiciones periódicas de contorno)

$$\psi(\mathbf{r}) = \sum_{\mathbf{q}} c_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}}.$$

Como  $U(\mathbf{r})$  es periódico:  $U(\mathbf{r}) = \sum_{\mathbf{K}} U_{\mathbf{K}} e^{i\mathbf{K} \cdot \mathbf{r}}.$

donde  $U_{\mathbf{K}} = \frac{1}{v} \int_{\text{cell}} d\mathbf{r} e^{-i\mathbf{K} \cdot \mathbf{r}} U(\mathbf{r}).$

- Se fija el nivel de energía /  $U_0 = \frac{1}{v} \int_{\text{cell}} d\mathbf{r} U(\mathbf{r}) = 0.$

$$- U_{-\mathbf{K}} = U_{\mathbf{K}}^*.$$

-Para cristales con simetría de inversión:  $U_{-\mathbf{K}} = U_{\mathbf{K}} = U_{\mathbf{K}}^*$

$$U(\mathbf{r}) = U(-\mathbf{r}),$$

$$\frac{p^2}{2m}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = \sum_{\mathbf{q}} \frac{\hbar^2}{2m} q^2 c_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (1)$$

$$\begin{aligned} U\psi &= \left( \sum_{\mathbf{K}} U_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}} \right) \left( \sum_{\mathbf{q}} c_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \right) \\ &= \sum_{\mathbf{K}\mathbf{q}} U_{\mathbf{K}} c_{\mathbf{q}} e^{i(\mathbf{K}+\mathbf{q})\cdot\mathbf{r}} = \sum_{\mathbf{K}\mathbf{q}'} U_{\mathbf{K}} c_{\mathbf{q}'-\mathbf{K}} e^{i\mathbf{q}'\cdot\mathbf{r}}. \end{aligned} \quad (2)$$

$\nearrow$   
 $\mathbf{K}+\mathbf{q}=\mathbf{q}'$

Cambio los índices de suma  $\mathbf{K}\mathbf{q}'$  por  $\mathbf{K}'\mathbf{q}$

(1) + (2) :

$$\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \left\{ \left( \frac{\hbar^2}{2m} q^2 - \varepsilon \right) c_{\mathbf{q}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'} c_{\mathbf{q}-\mathbf{K}'} \right\} = 0.$$



Como la base es ortogonal y completa:

$$\left( \frac{\hbar^2}{2m} q^2 - \varepsilon \right) c_{\mathbf{q}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'} c_{\mathbf{q}-\mathbf{K}'} = 0.$$

Se puede escribir  $\mathbf{q} = \mathbf{k} - \mathbf{K}$ , con  $\mathbf{k}$  pertenece a la 1ZB

$$\left( \frac{\hbar^2}{2m} (\mathbf{k} - \mathbf{K})^2 - \varepsilon \right) c_{\mathbf{k}-\mathbf{K}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'} c_{\mathbf{k}-\mathbf{K}-\mathbf{K}'} = 0,$$

Haciendo el cambio  $\mathbf{K}' \rightarrow \mathbf{K}' - \mathbf{K}$ ,

$$\left( \frac{\hbar^2}{2m} (\mathbf{k} - \mathbf{K})^2 - \varepsilon \right) c_{\mathbf{k}-\mathbf{K}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'-\mathbf{K}} c_{\mathbf{k}-\mathbf{K}'} = 0.$$

**Ecuación de Schrodinger en el espacio  $\mathbf{k}$**

Dado un  $\mathbf{k}$  dentro de la 1ZB, la ecuación anterior acopla solamente

$$\mathbf{k}, \mathbf{k} - \mathbf{K}', \mathbf{k} - \mathbf{K}'', \dots,$$

Problema original  $\longrightarrow$  N problemas independientes  
(N valores de  $\mathbf{k}$  dentro de la 1ZB)

Entonces:

$$\psi_{\mathbf{k}} = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}} e^{i(\mathbf{k}-\mathbf{K}) \cdot \mathbf{r}}.$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \left( \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}} e^{-i\mathbf{K} \cdot \mathbf{r}} \right),$$

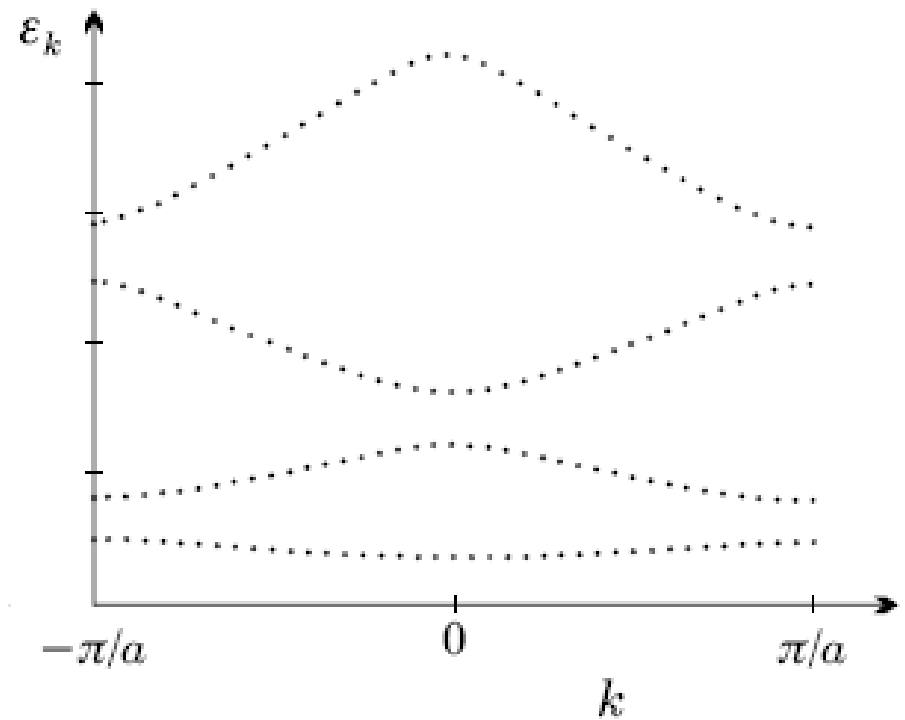
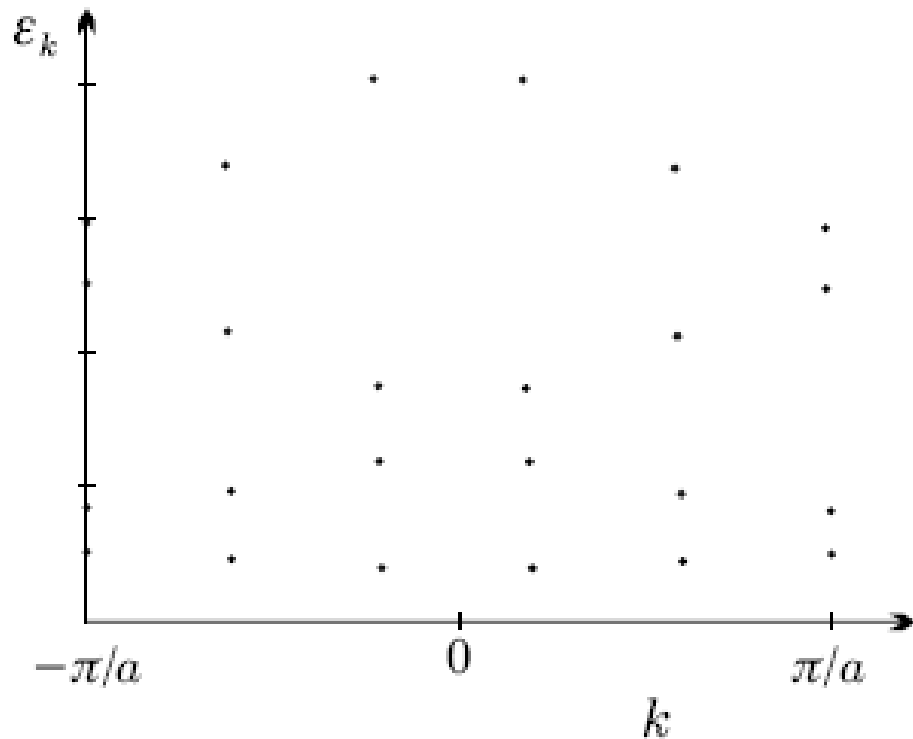
Queda demostrado el teorema de Bloch, ya que la función

$$u(\mathbf{r}) = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}} e^{-i\mathbf{K} \cdot \mathbf{r}} \quad \text{es una función periódica}$$

5- Fijado  $k$ , existen diferentes soluciones

$$\varepsilon_{nk}$$

$$\psi_{nk}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r})$$



Se puede demostrar que:

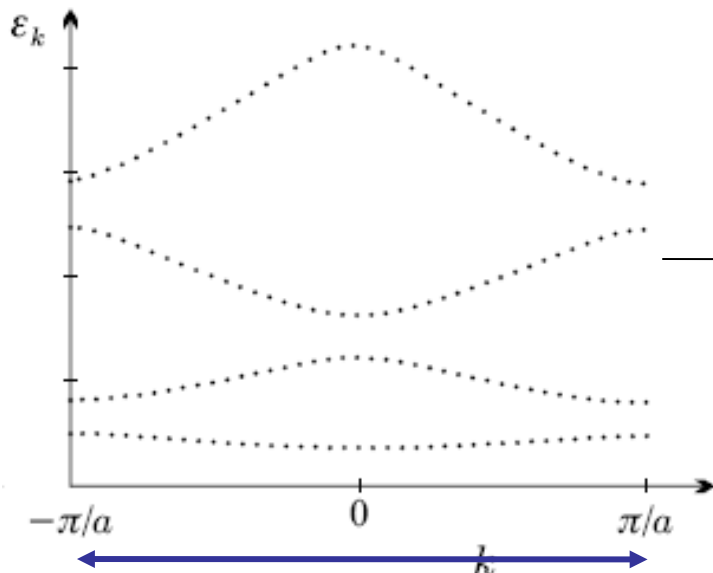
$$\psi_{n, \mathbf{k} + \mathbf{K}}(\mathbf{r}) = \psi_{n\mathbf{k}}(\mathbf{r}):$$
$$\epsilon_{n, \mathbf{k} + \mathbf{K}} = \epsilon_{n\mathbf{k}}.$$

El conjunto de todas las energías y autoestados del sistema se obtiene resolviendo el problema para los  $\mathbf{k}$  dentro de la 1ZB

Para  $n$  fijo,  $\epsilon_{n\mathbf{k}}$  es una función “continua” de  $\mathbf{k}$  —————>

$$\epsilon_n(\mathbf{k})$$

**Banda**



~  $10^{23}$  puntos  $\mathbf{k}$   
dentro de la 1ZB

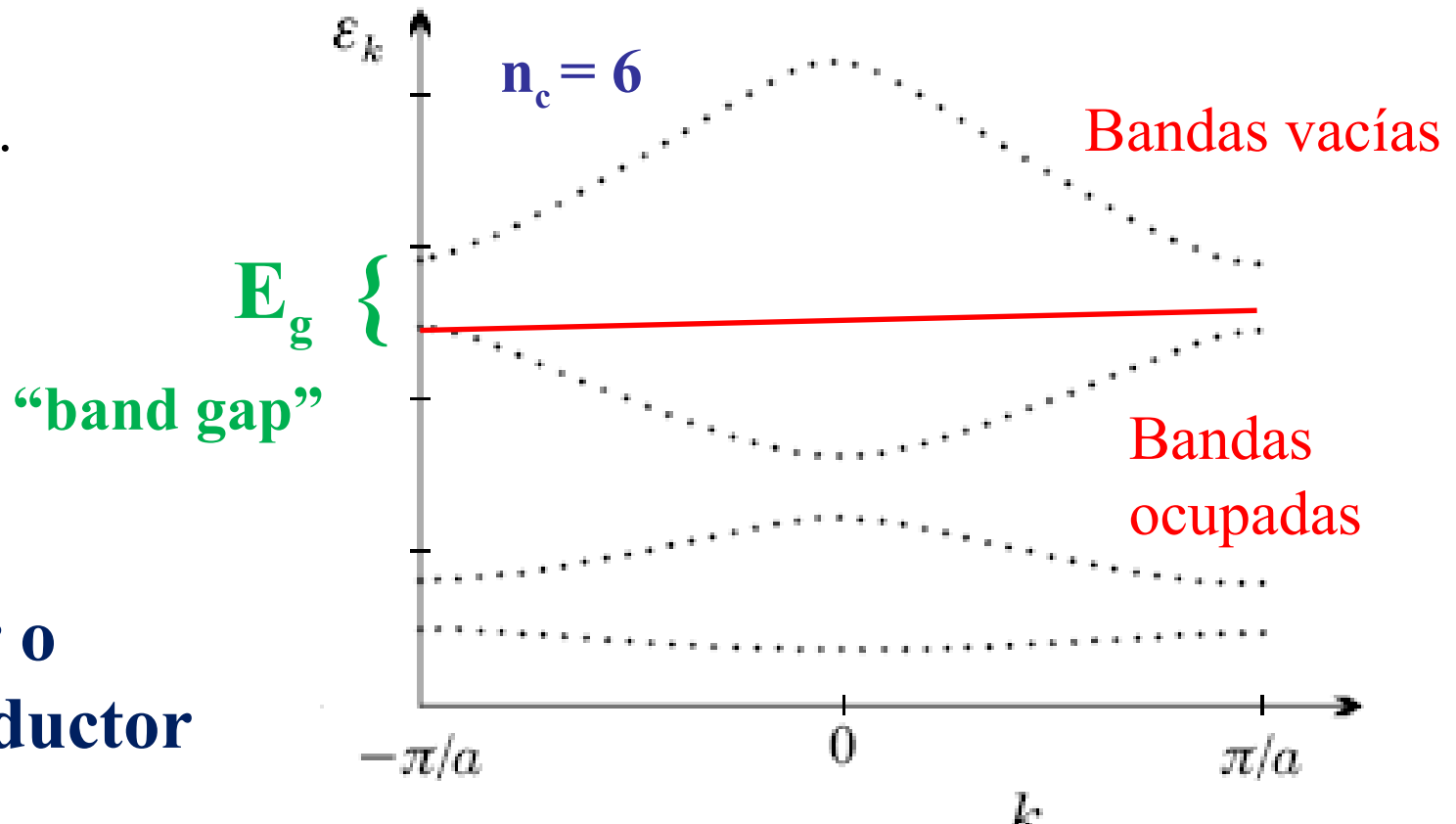
**N valores permitidos de  $\mathbf{k}$**

El estado fundamental de  $N_e$  electrones se obtiene ocupando con 2 electrones ( $\uparrow\downarrow$ ) cada uno de los niveles  $\epsilon_n(\mathbf{k})$  de menor a mayor energía, hasta ubicar todos los electrones

$N_e = n_c N$  donde  $n_c$  es el número de electrones por celda

Ej.: 1D

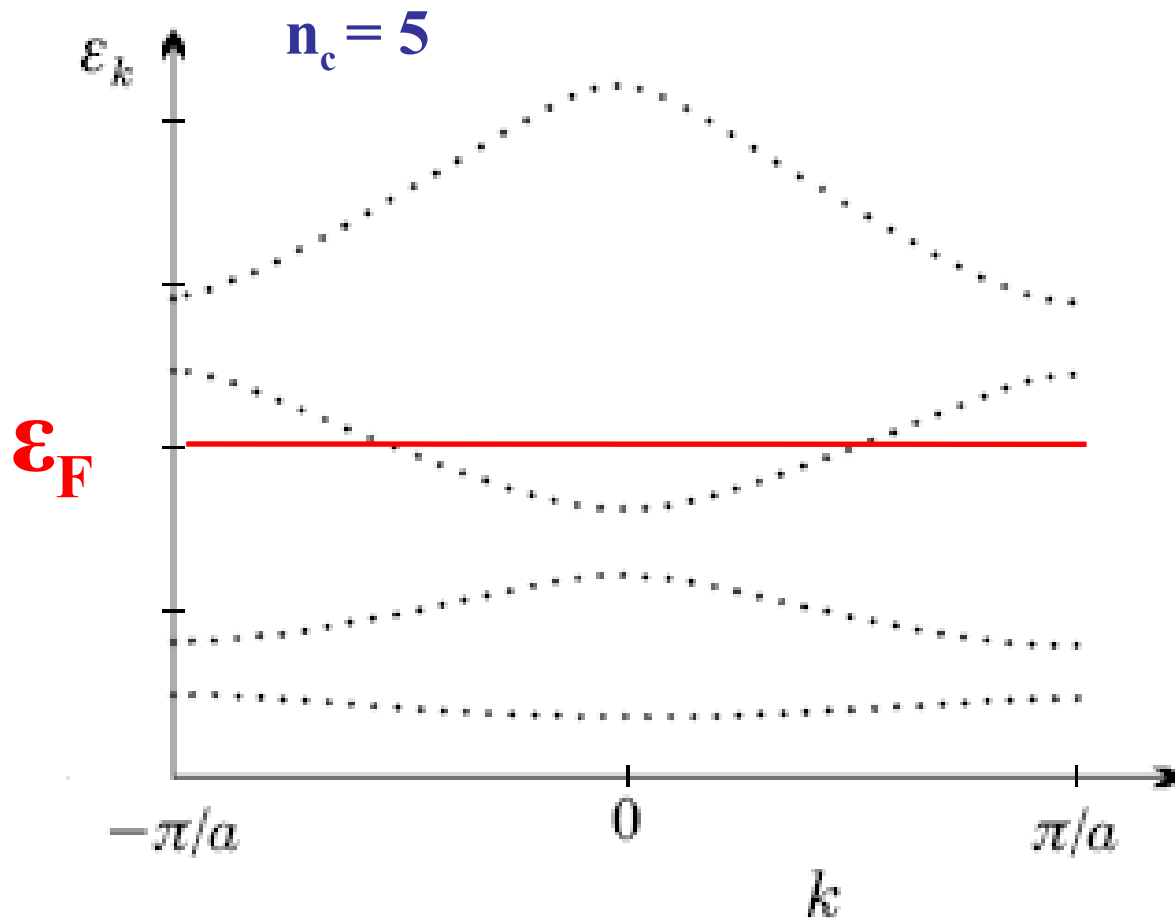
$n_c = 2, 4, 6, \dots$



**Aislador o  
semiconductor**

$$n_c = 1, 3, 5, \dots$$

**Metal**



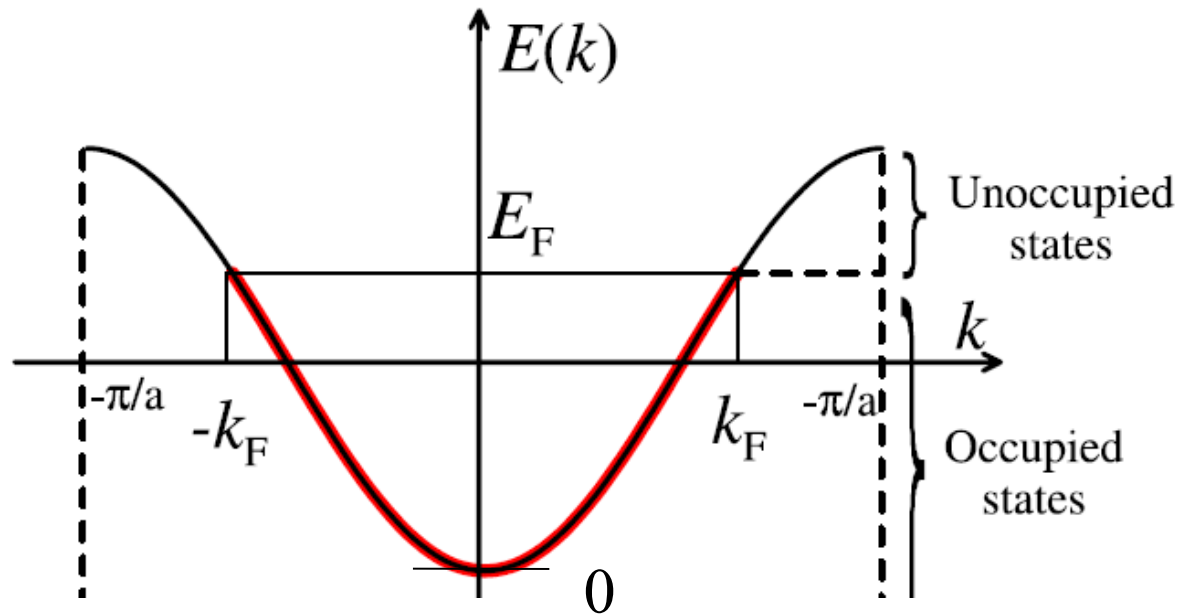
$$\epsilon_n(\mathbf{k}) = \epsilon_F.$$

Superficie de Fermi

Puede ocurrir que el nivel de Fermi cruce varias bandas



Una superficie para cada banda



Energía total del estado fundamental

$$E_0 = \sum_{|\mathbf{k}| \leq k_F} \sum_{\sigma} E(k) = 2 \sum_{|\mathbf{k}| \leq k_F} E(k)$$

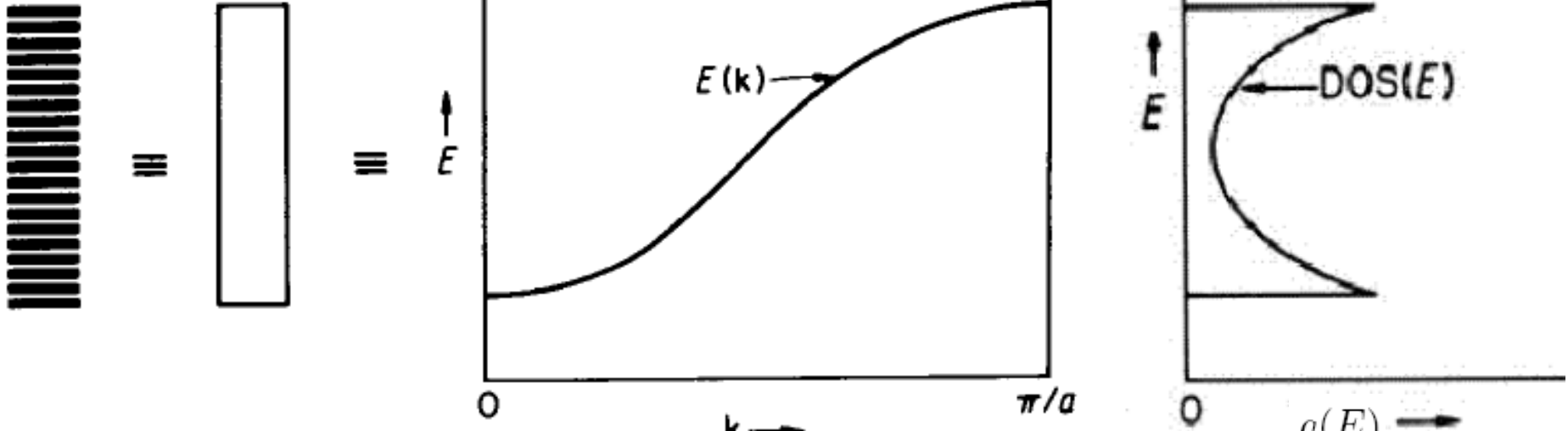
$$2 \sum_{\mathbf{k}} \rightarrow \int d^3k \rightarrow \int d\varepsilon \quad \Longrightarrow \quad \text{DOS: } g(\mathbf{k}) \quad g(\varepsilon)$$

$$g(\mathbf{k}) = \frac{2}{(2\pi)^3} \quad g(\varepsilon) ?$$

Depende de la relación de dispersión de la banda

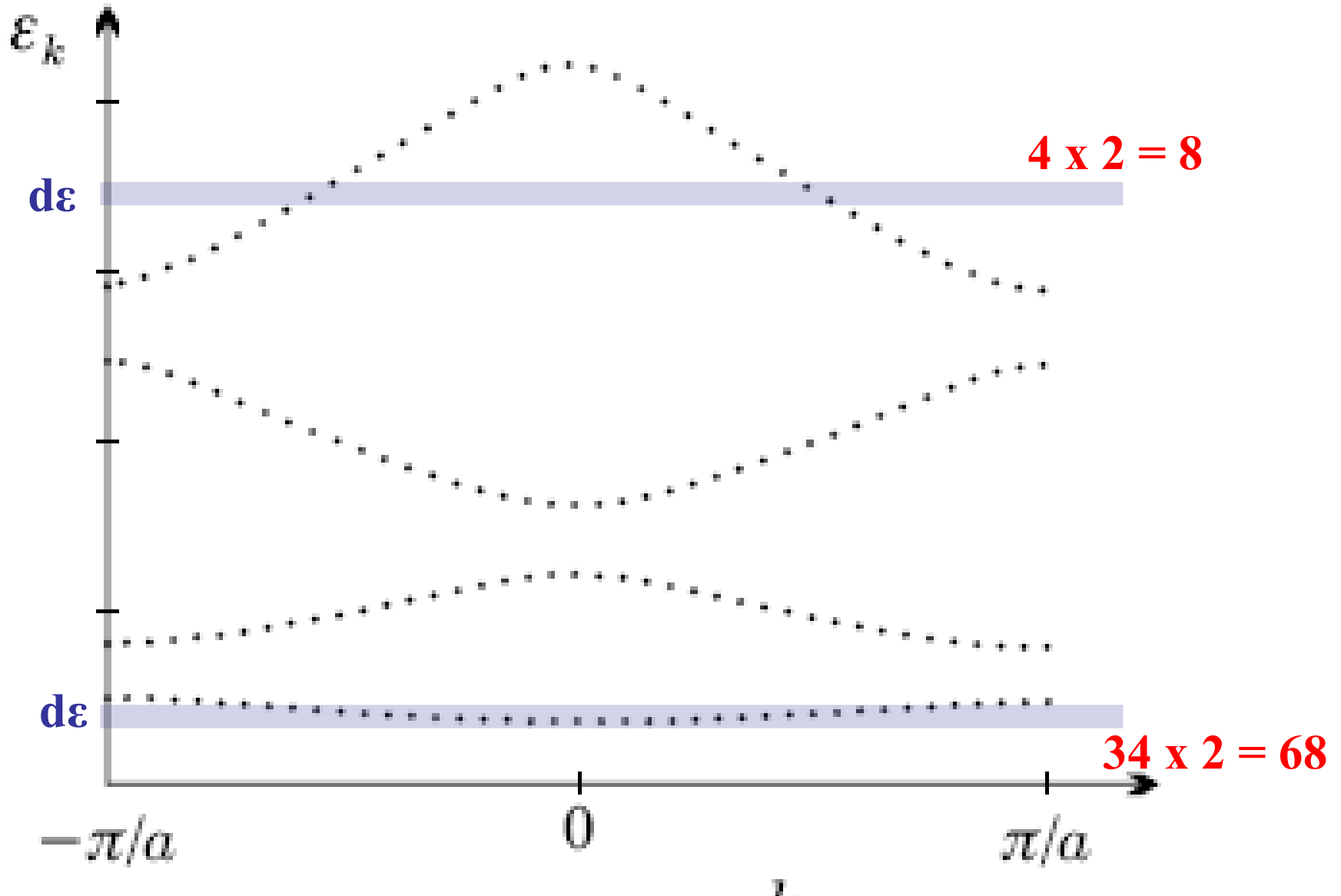
$g(\varepsilon) d\varepsilon =$  número de estados electrónicos (por unidad de volumen) comprendidos entre  $\varepsilon$  y  $\varepsilon + d\varepsilon$

$$g(E) = \sum_k \delta(E - E(k))$$

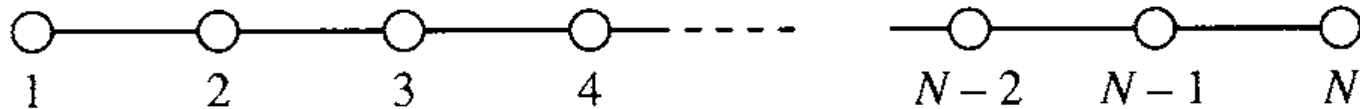




# DOS es proporcional a la inversa de $dE/dk$

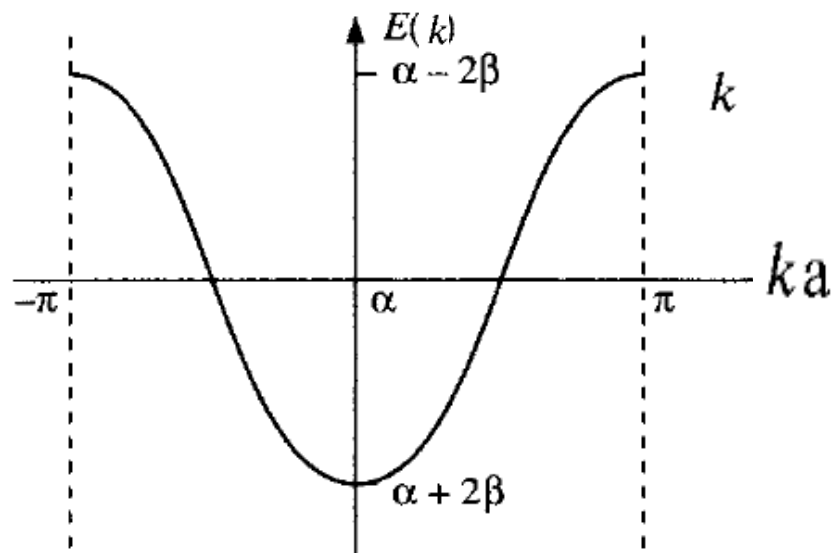
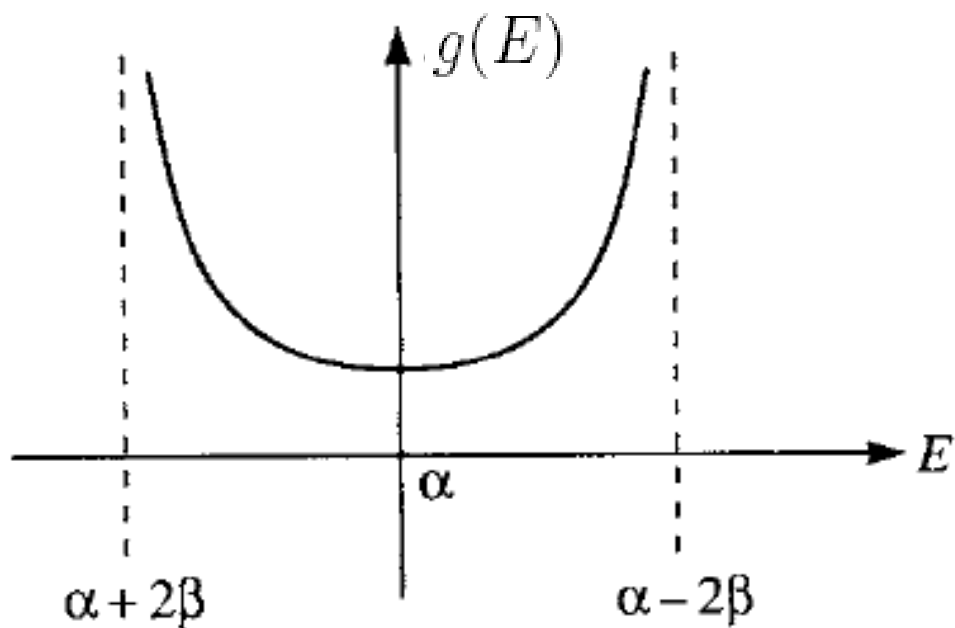


# 1D



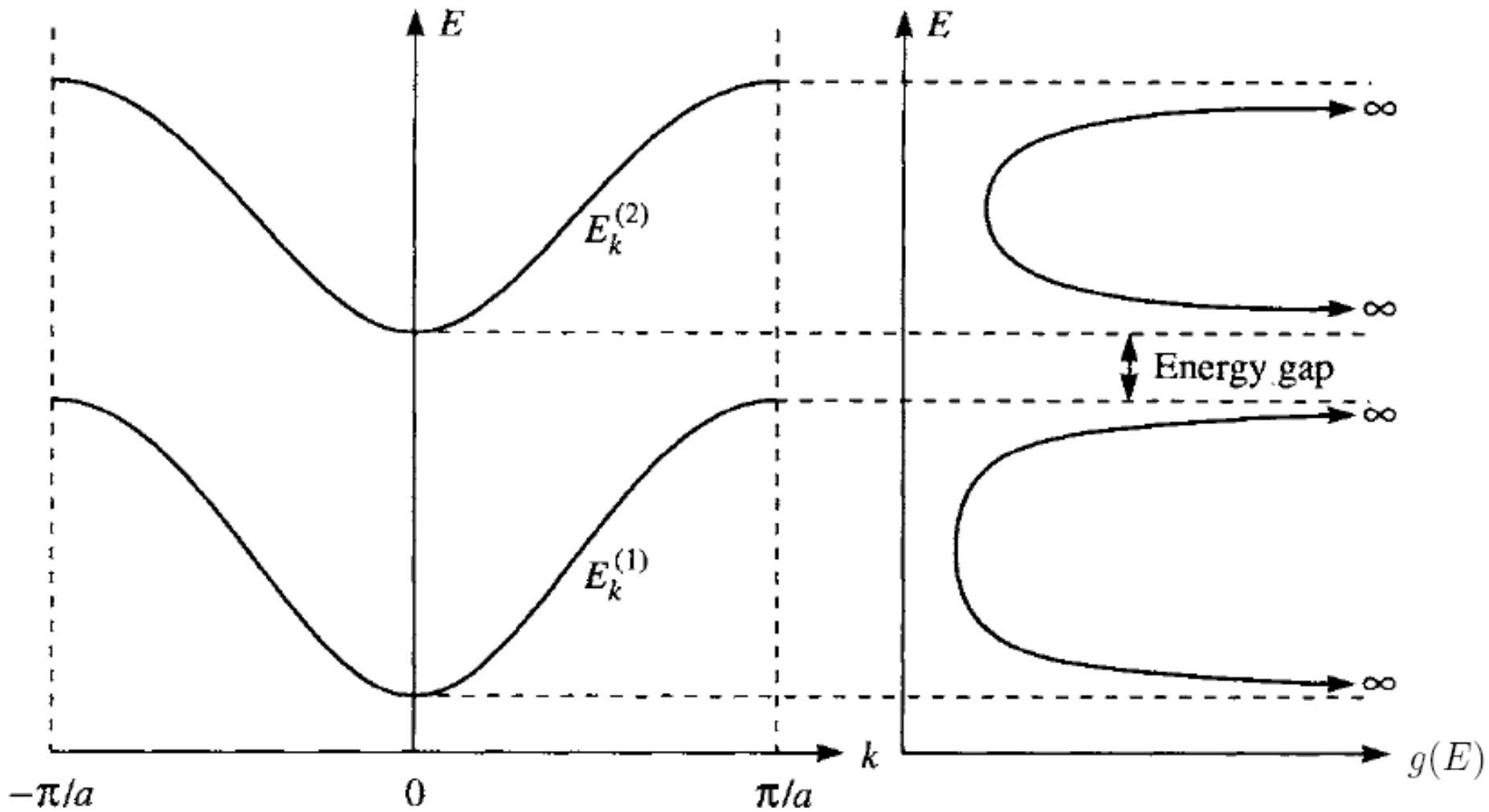
$$\langle p|H|p\rangle = \alpha \quad \langle p|H|j\rangle = \beta \quad \text{'hopping'}$$

$$E = \alpha + 2\beta \cos ka$$



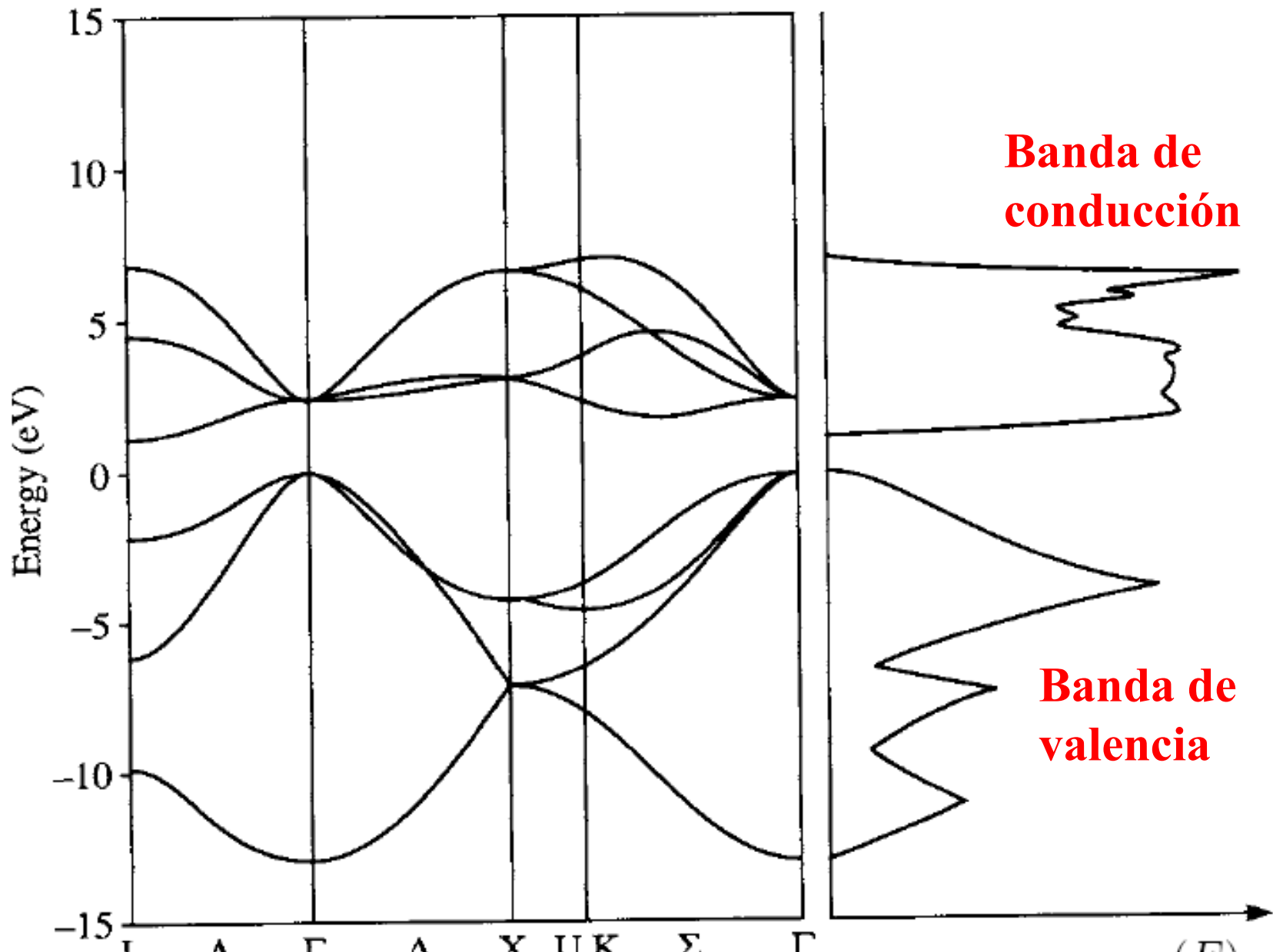
# 1D

# 2 bandas



3D

Si



# Electrones en un potencial periódico débil

$U(\mathbf{r})$  lo tratamos como una perturbación  $\longrightarrow$  Modelo de electrones casi libres

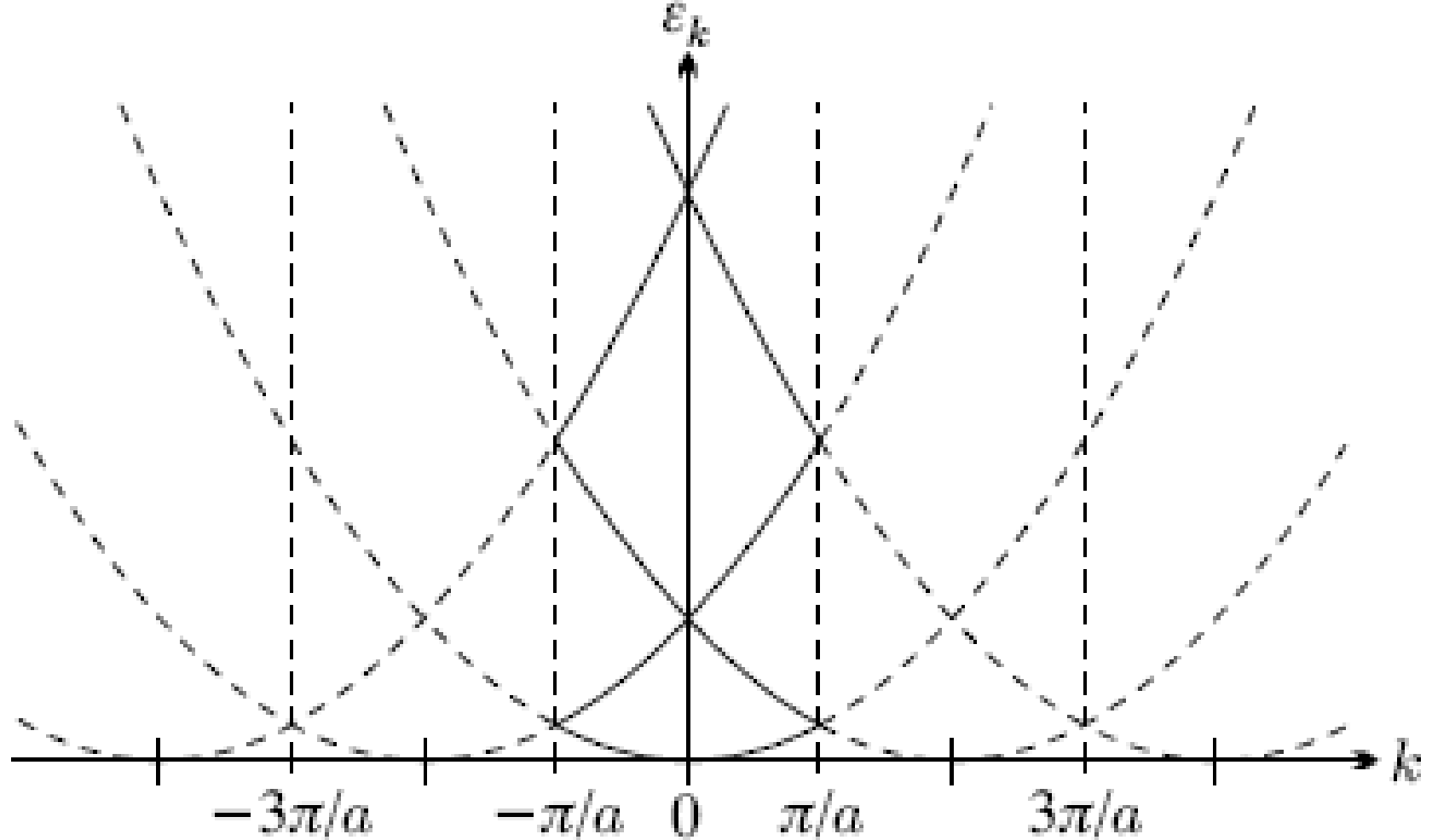
Empty Lattice Approximation (orden cero)

$U(\mathbf{r}) = 0 \longrightarrow e^-$  libres  $\epsilon_{\mathbf{k}}^{(0)} = \frac{\hbar^2}{2m_e} k^2$

**Pero: hay que imponer la condición de periodicidad (se tiene que cumplir el Teorema de Bloch)**

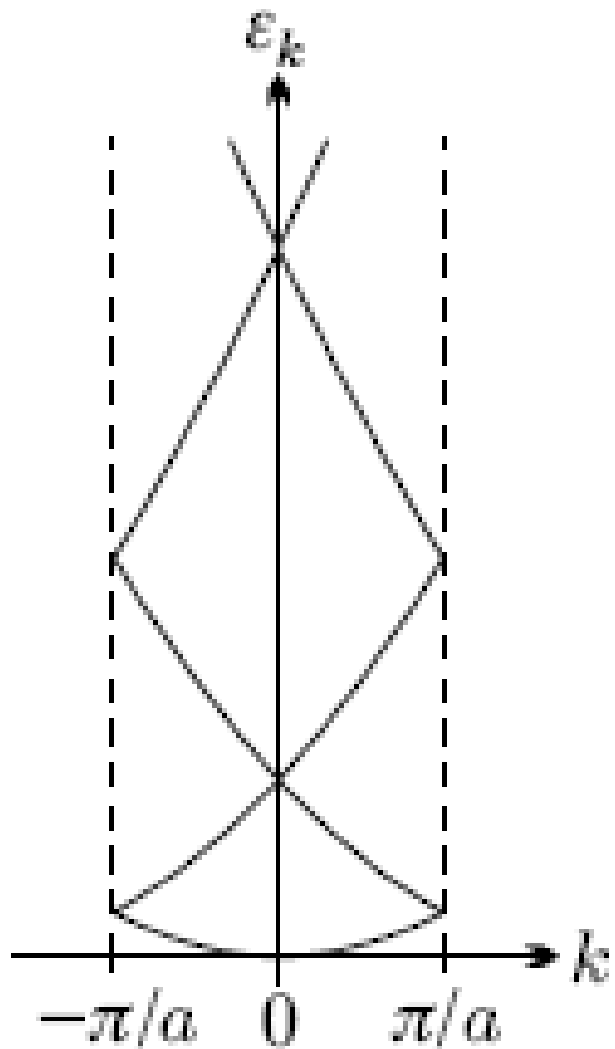
$$\begin{aligned}\psi_{n, \mathbf{k} + \mathbf{K}}(\mathbf{r}) &= \psi_{n\mathbf{k}}(\mathbf{r}), \\ \epsilon_{n, \mathbf{k} + \mathbf{K}} &= \epsilon_{n\mathbf{k}}.\end{aligned}$$

# Pongo una parábola en cada punto de la RR

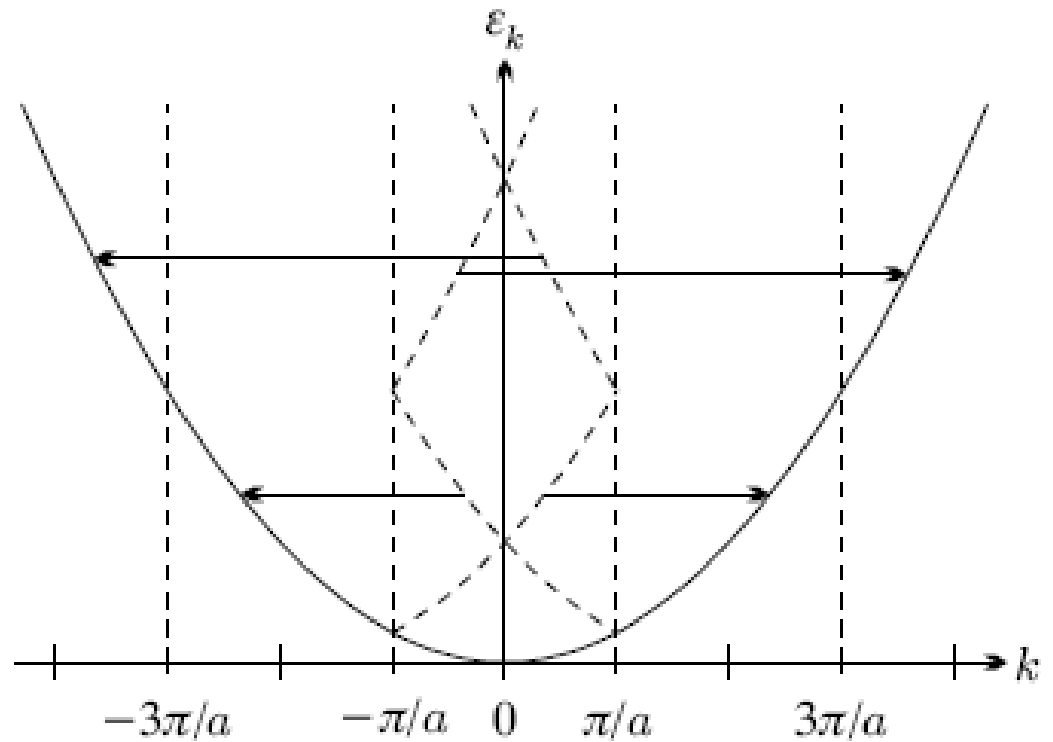


Esquema de  
zona repetida

$$\mathcal{E} = \mathcal{E}_{\mathbf{k}-\mathbf{K}}^0, \quad \psi_{\mathbf{k}} \propto e^{i(\mathbf{k}-\mathbf{K}) \cdot \mathbf{r}}.$$



**Esquema de  
zona reducida**



**Esquema de  
zona extendida**

Usando teoría de perturbaciones se puede mostrar que :

## -Niveles no degenerados

$$\varepsilon = \varepsilon_{\mathbf{k}-\mathbf{K}_1}^0 + \sum_{\mathbf{K}} \frac{|U_{\mathbf{K}-\mathbf{K}_1}|^2}{\varepsilon_{\mathbf{k}-\mathbf{K}_1}^0 - \varepsilon_{\mathbf{k}-\mathbf{K}}^0} + O(U^3).$$

## -Degeneración orden m $\varepsilon_{\mathbf{k}-\mathbf{K}_1}^0 = \dots = \varepsilon_{\mathbf{k}-\mathbf{K}_m}^0$

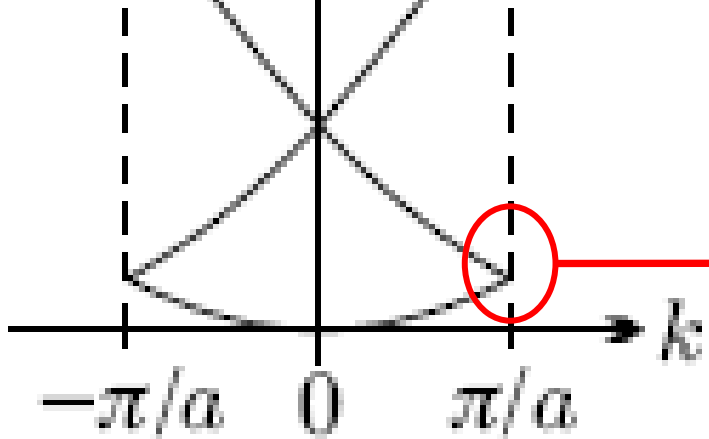
$$(\varepsilon - \varepsilon_{\mathbf{k}-\mathbf{K}_i}^0)c_{\mathbf{k}-\mathbf{K}_i} = \sum_{j=1}^m U_{\mathbf{K}_j-\mathbf{K}_i} c_{\mathbf{k}-\mathbf{K}_j}, \quad i = 1, \dots, m,$$

La corrección a la energía de los niveles **no degenerados** es de **segundo orden** en  $U_{\mathbf{K}}$

Para los niveles **degenerados** la corrección es de **primer orden**

**Sólo corregiremos los niveles degenerados**



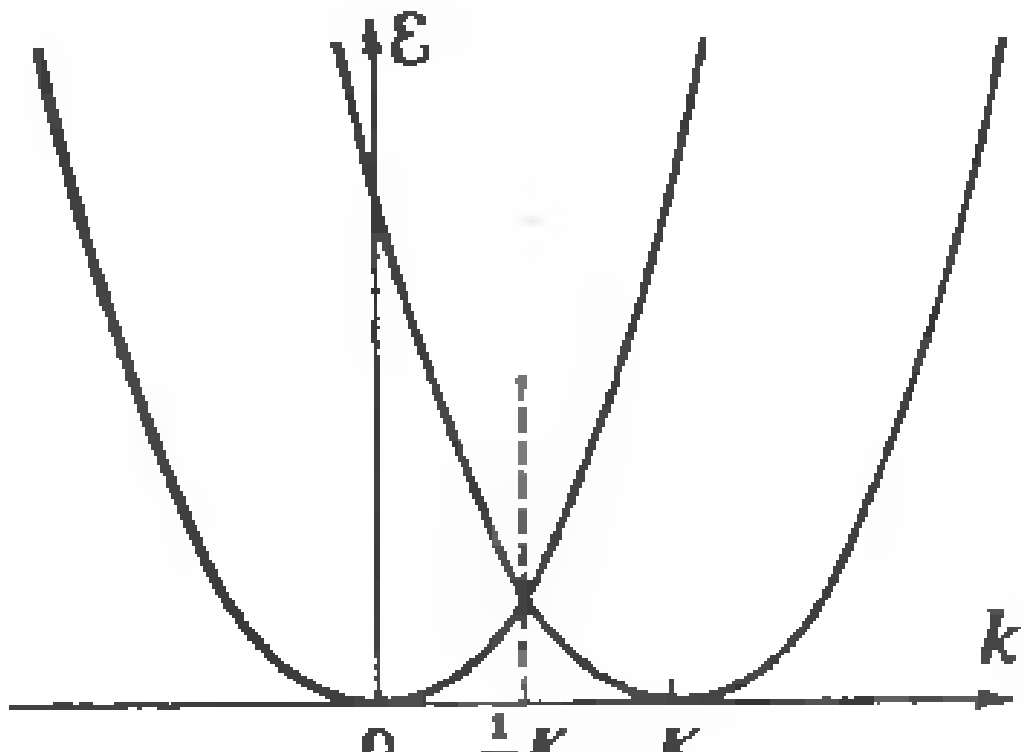


$$(\mathcal{E} - \mathcal{E}_{\mathbf{k}-\mathbf{K}_i}^0) c_{\mathbf{k}-\mathbf{K}_i} = \sum_{j=1}^m U_{\mathbf{K}_j-\mathbf{K}_i} c_{\mathbf{k}-\mathbf{K}_j}$$

**2 niveles degenerados**

$$(\mathcal{E} - \mathcal{E}_{\mathbf{k}-\mathbf{K}_1}^0) c_{\mathbf{k}-\mathbf{K}_1} = U_{\mathbf{K}_2-\mathbf{K}_1} c_{\mathbf{k}-\mathbf{K}_2}$$

$$(\mathcal{E} - \mathcal{E}_{\mathbf{k}-\mathbf{K}_2}^0) c_{\mathbf{k}-\mathbf{K}_2} = U_{\mathbf{K}_1-\mathbf{K}_2} c_{\mathbf{k}-\mathbf{K}_1}$$



**$\mathbf{K}_1=0$**

**$\mathbf{K}_2=2\pi/a$**

**$k=\pi/a$**

Llamando  $\mathbf{q} = \mathbf{k} - \mathbf{K}_1$  y  $\mathbf{K} = \mathbf{K}_2 - \mathbf{K}_1$

$$\begin{aligned}(\varepsilon - \varepsilon_{\mathbf{q}}^0)c_{\mathbf{q}} &= U_{\mathbf{K}}c_{\mathbf{q}-\mathbf{K}}, \\(\varepsilon - \varepsilon_{\mathbf{q}-\mathbf{K}}^0)c_{\mathbf{q}-\mathbf{K}} &= U_{-\mathbf{K}}c_{\mathbf{q}} = U_{\mathbf{K}}^*c_{\mathbf{q}}.\end{aligned}$$

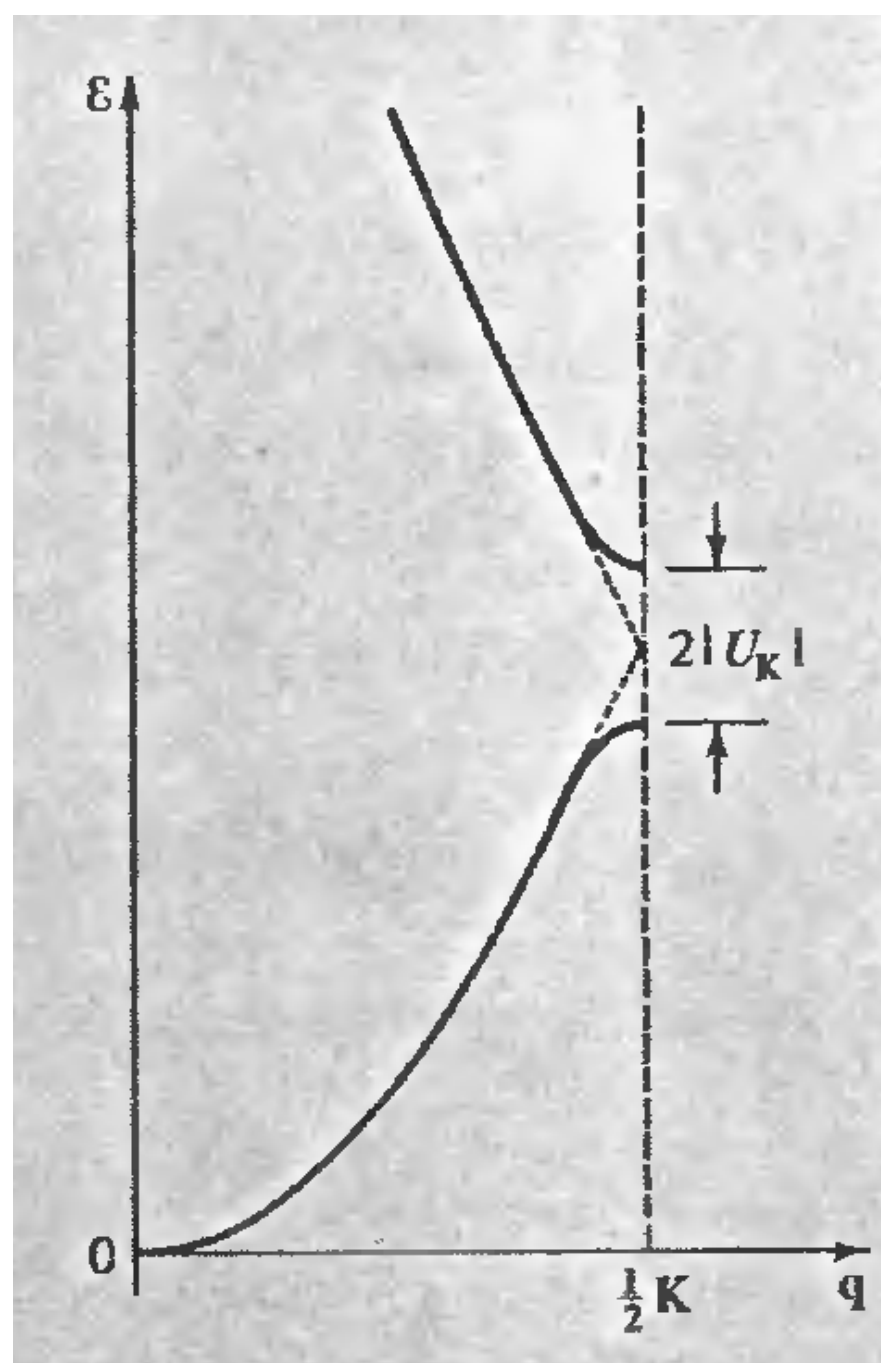
$$\begin{vmatrix} \varepsilon - \varepsilon_{\mathbf{q}}^0 & -U_{\mathbf{K}} \\ -U_{\mathbf{K}}^* & \varepsilon - \varepsilon_{\mathbf{q}-\mathbf{K}}^0 \end{vmatrix} = 0. \implies (\varepsilon - \varepsilon_{\mathbf{q}}^0)(\varepsilon - \varepsilon_{\mathbf{q}-\mathbf{K}}^0) = |U_{\mathbf{K}}|^2.$$

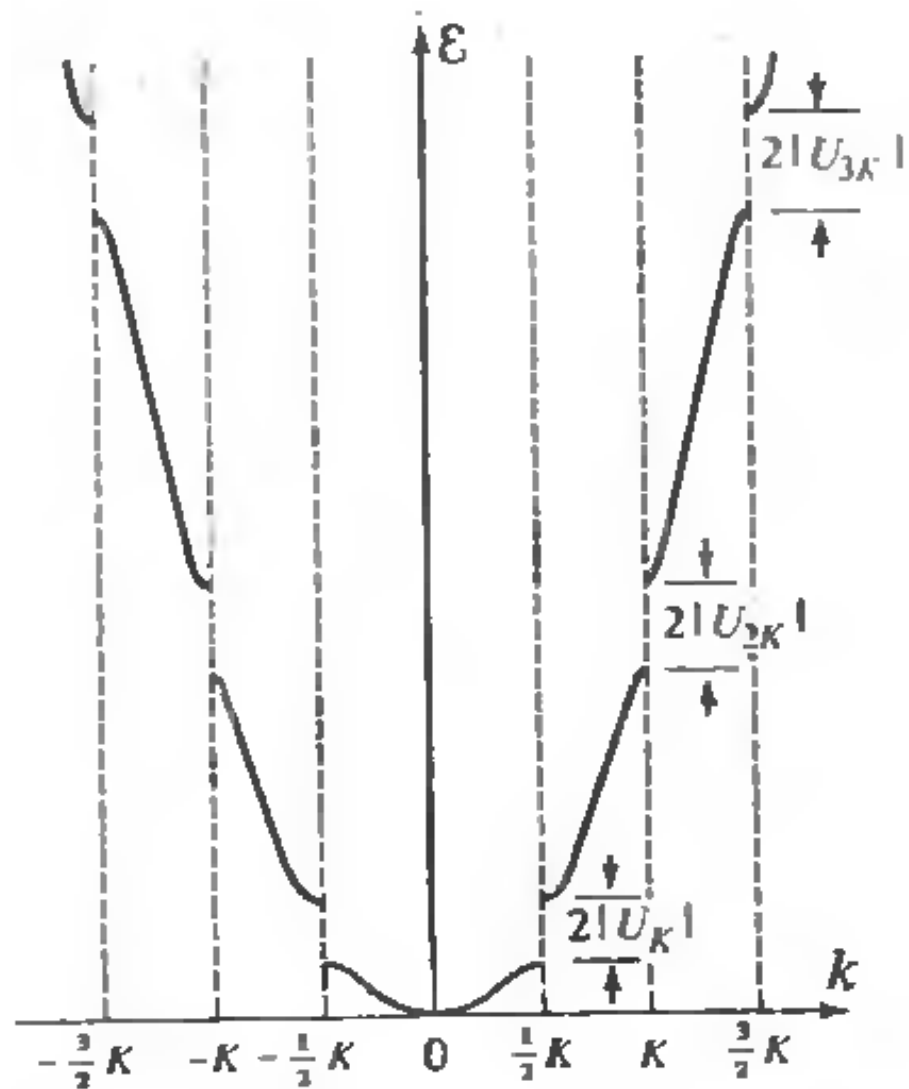
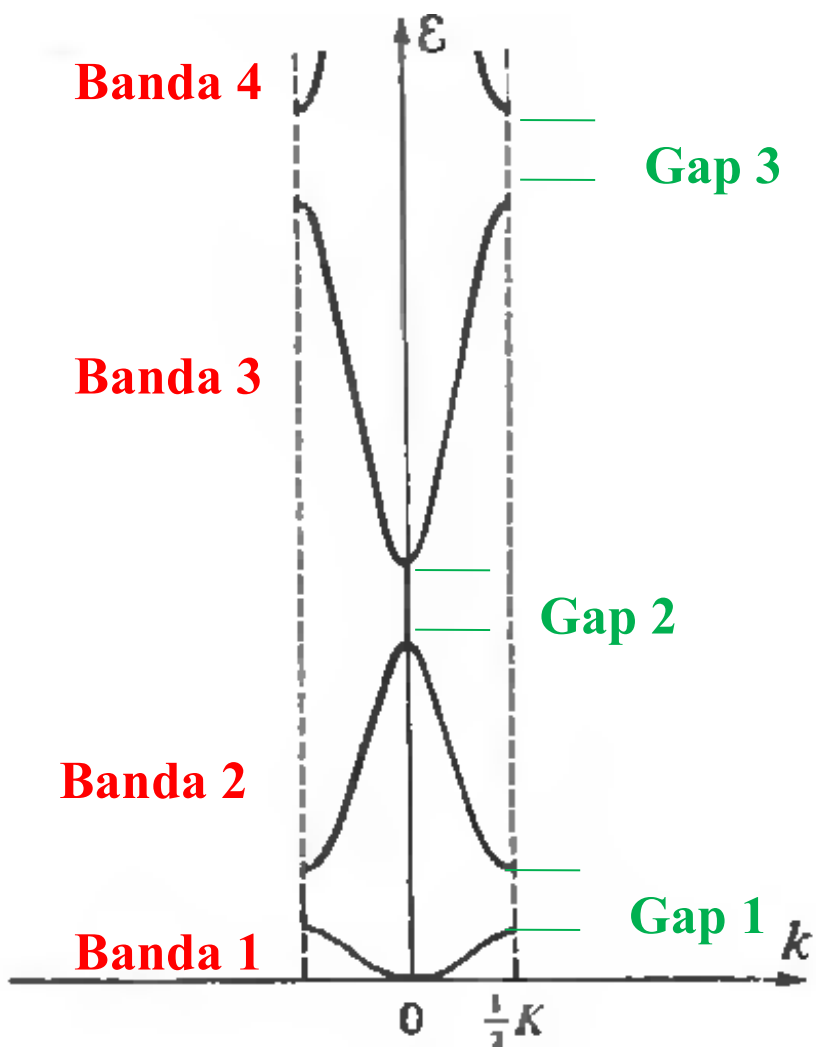
$$\varepsilon = \frac{1}{2}(\varepsilon_{\mathbf{q}}^0 + \varepsilon_{\mathbf{q}-\mathbf{K}}^0) \pm \left[ \left( \frac{\varepsilon_{\mathbf{q}}^0 - \varepsilon_{\mathbf{q}-\mathbf{K}}^0}{2} \right)^2 + |U_{\mathbf{K}}|^2 \right]^{1/2}$$

En el plano de Bragg  
( $q = \pi/a$ )

$$\varepsilon = \varepsilon_q^0 \pm |U_K|,$$

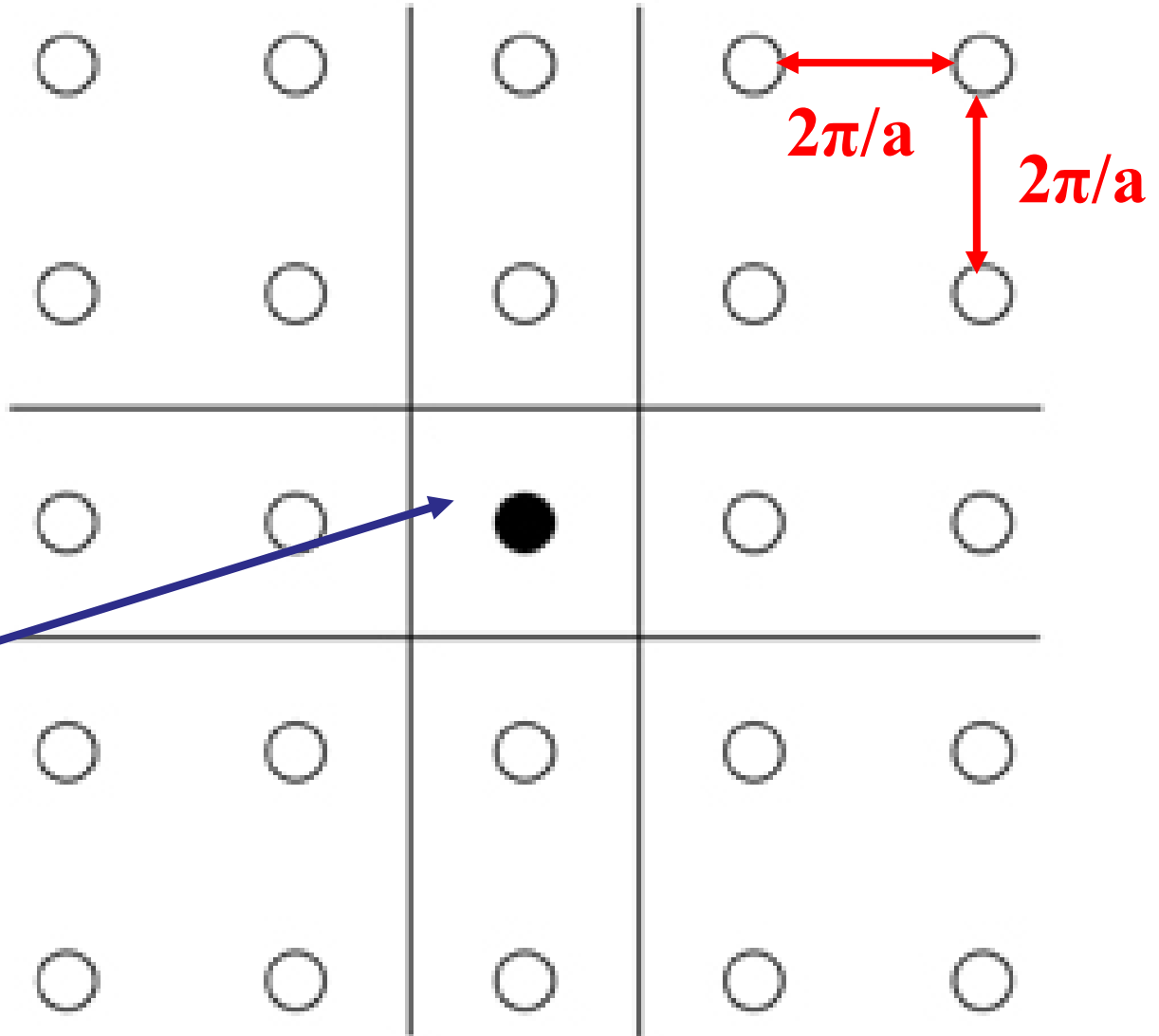
con  $K = 2\pi/a$



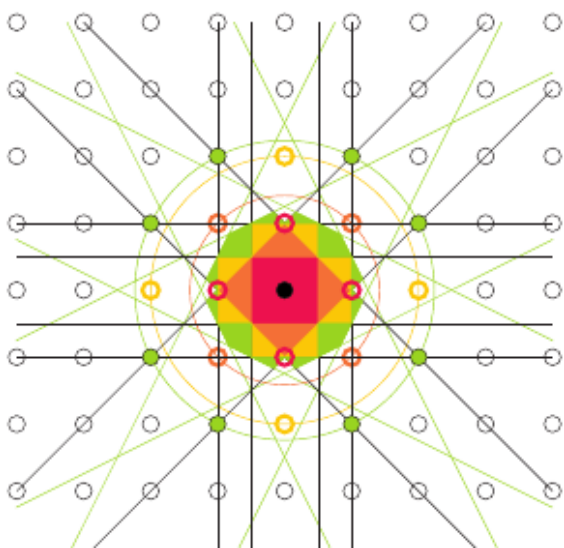
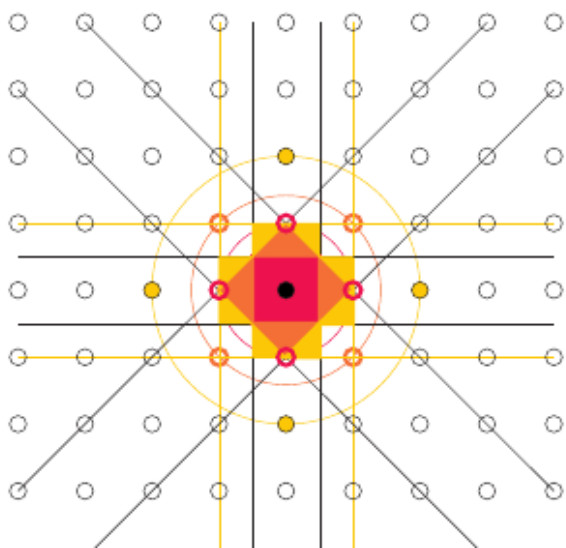
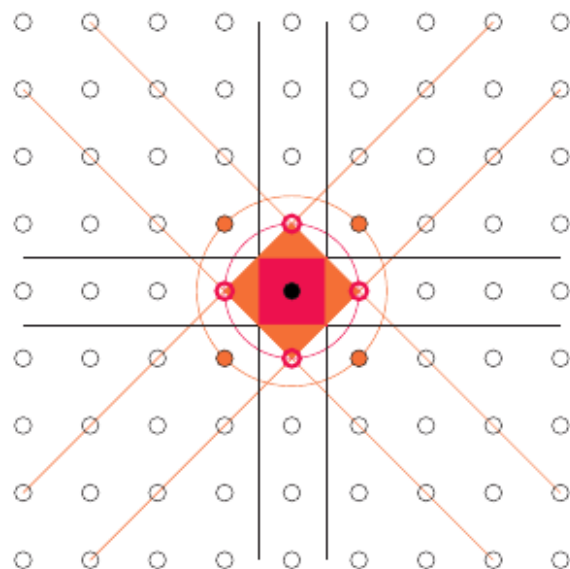
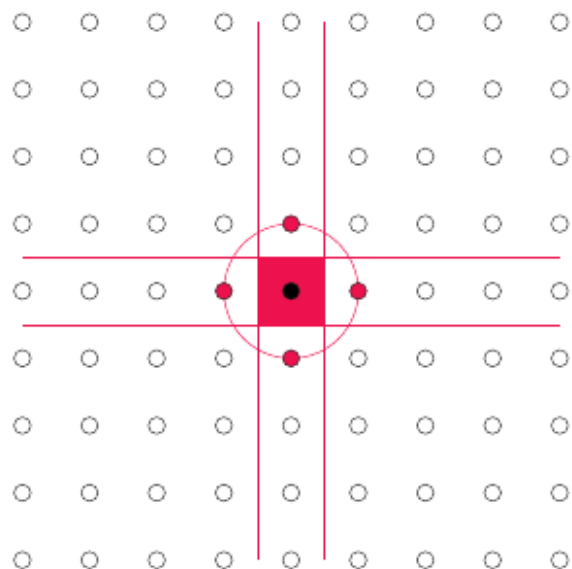


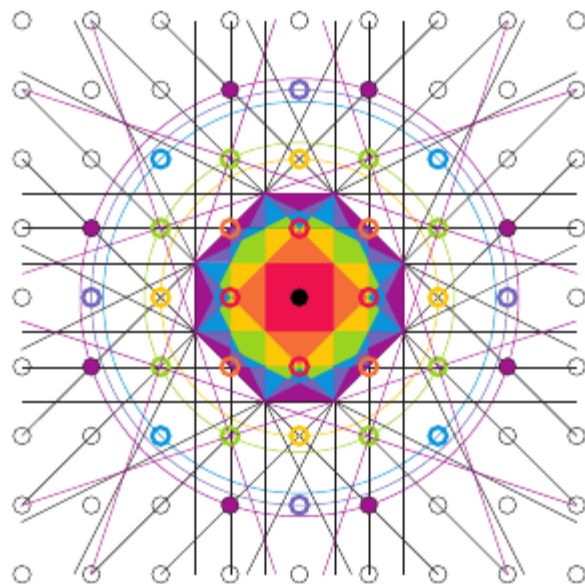
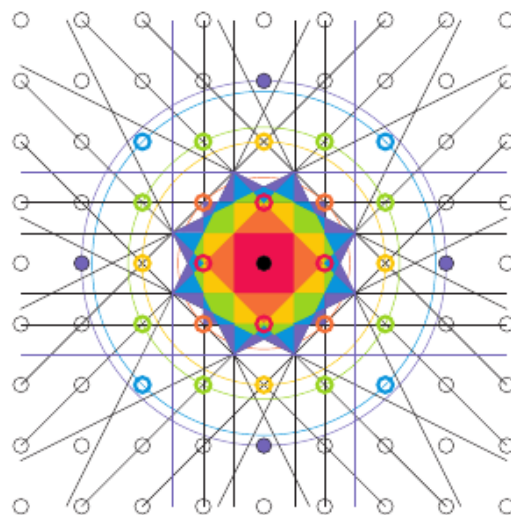
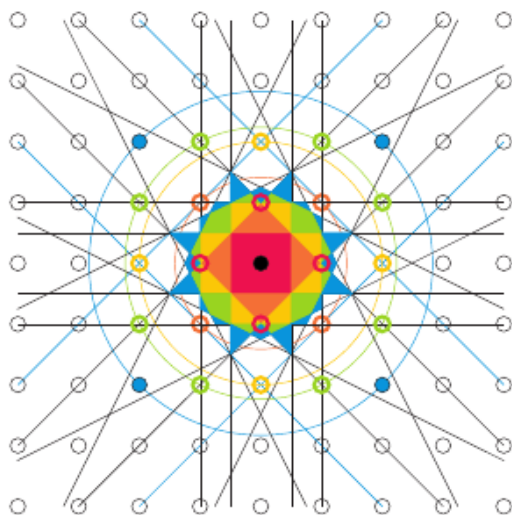
# Nearly free en una red cuadrada en 2D

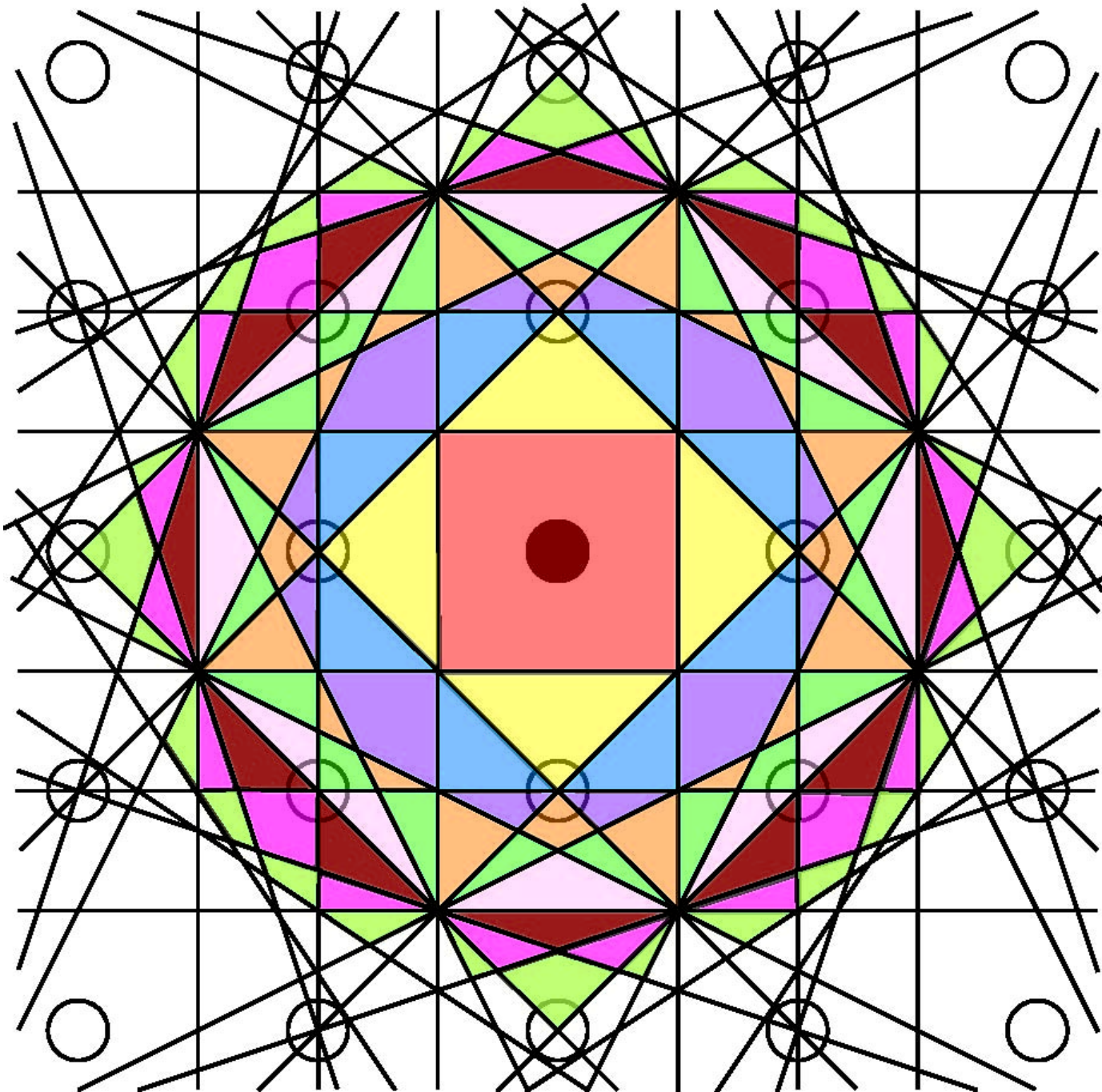
**Red  
reciproca**



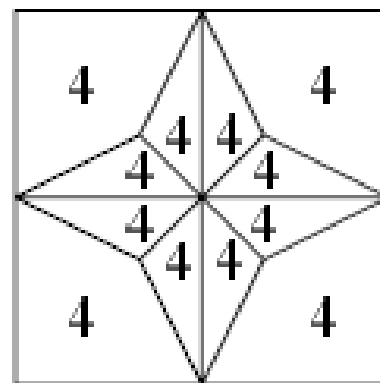
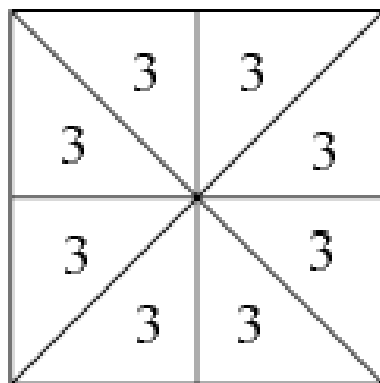
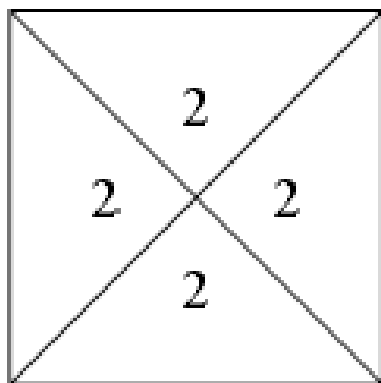
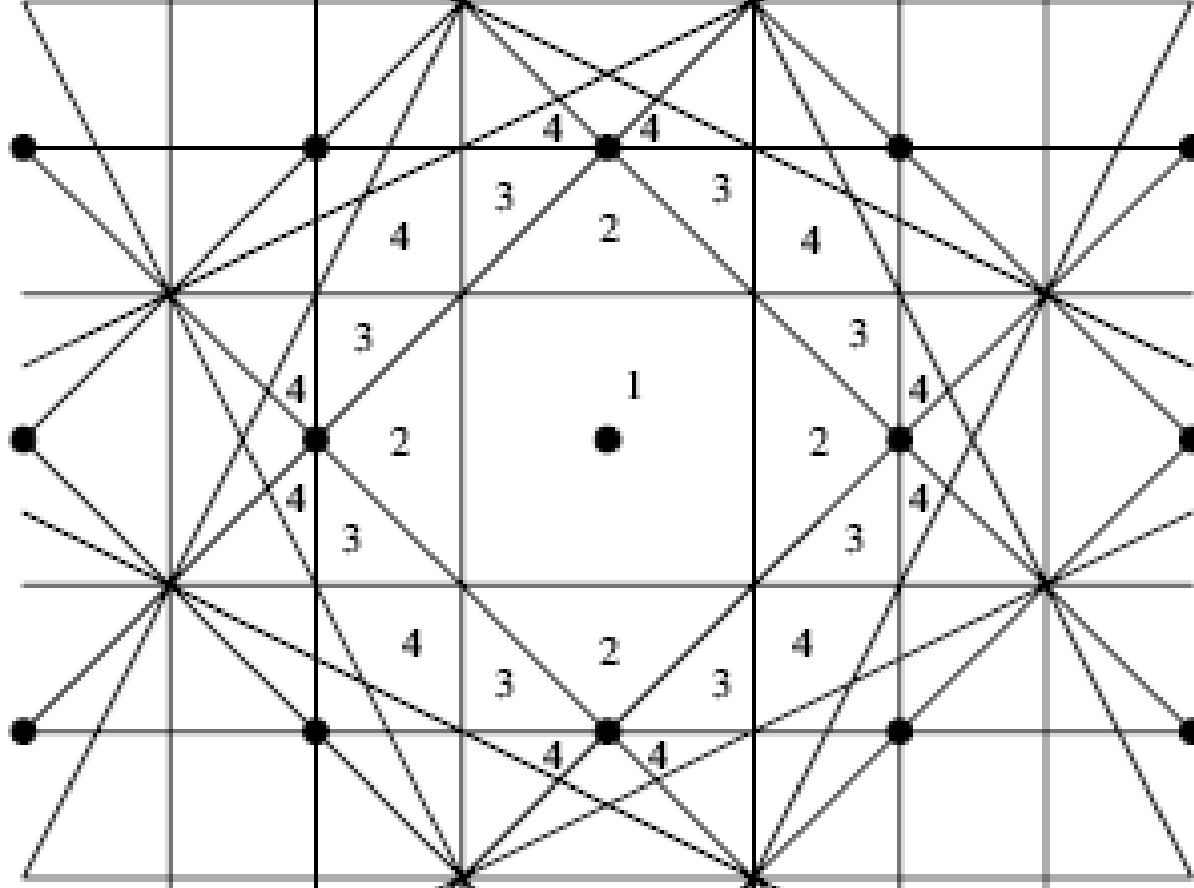
**1 Zona de  
Brillouin**









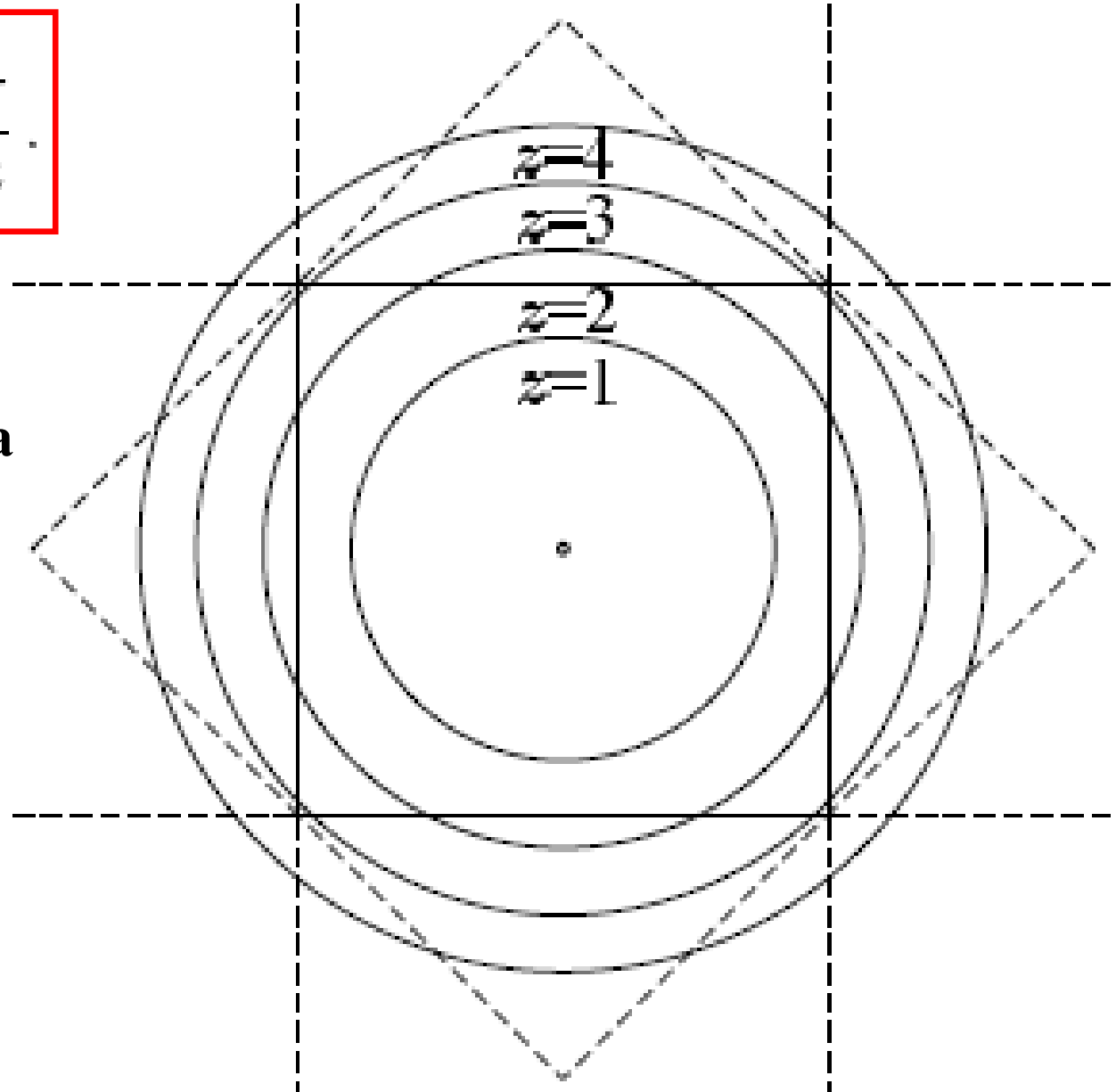


**Todas las zonas ocupan el mismo volumen**

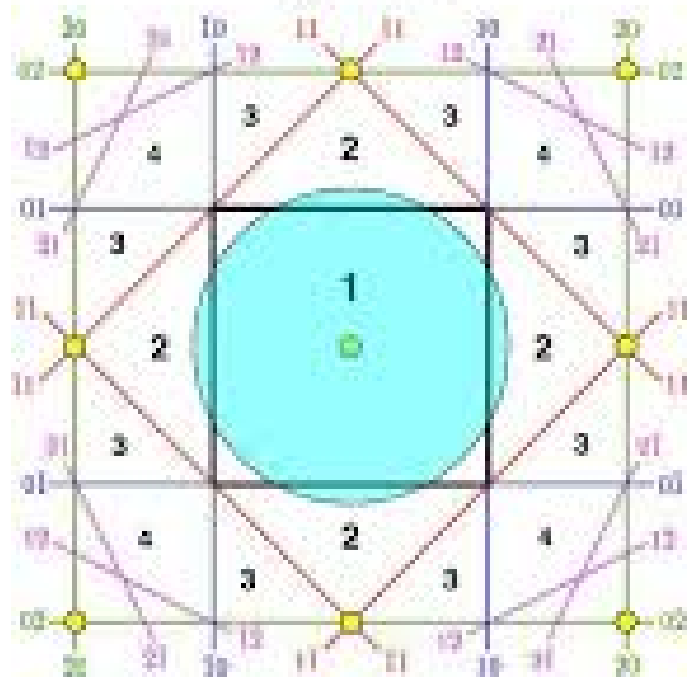
# Superficies de Fermi

$$k_F = \left( \frac{2z}{\pi} \right)^{1/2} \frac{\pi}{a}$$

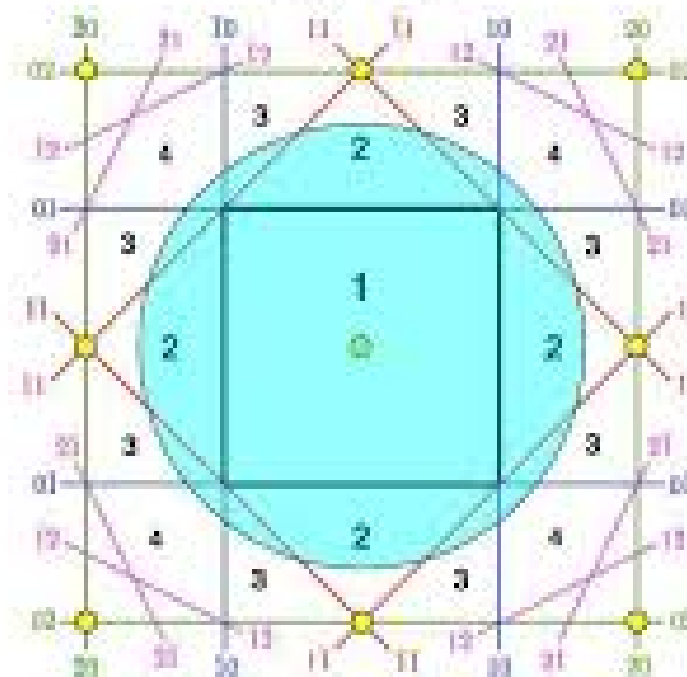
**z: número de  
electrones por celda**



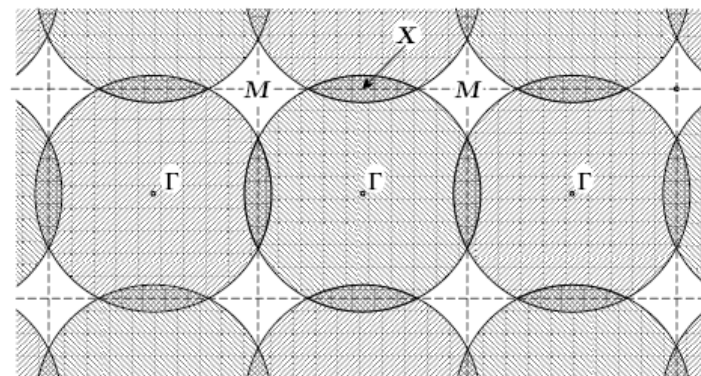
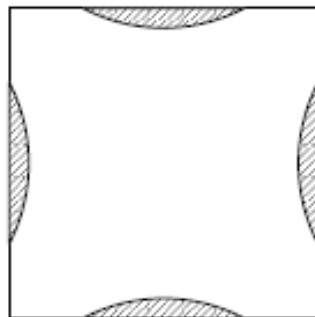
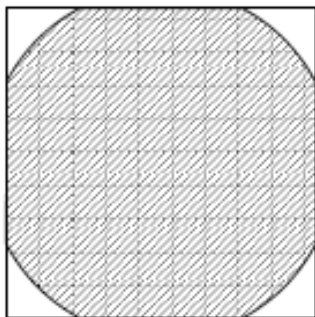
$Z = 2$



$Z = 4$



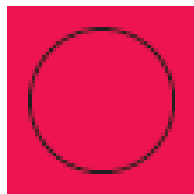
$z=2$



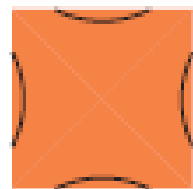
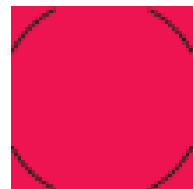
Esquema de zona reducida

Esquema de zona repetida

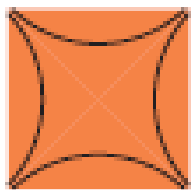
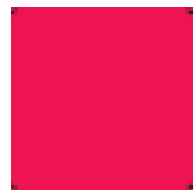
1e



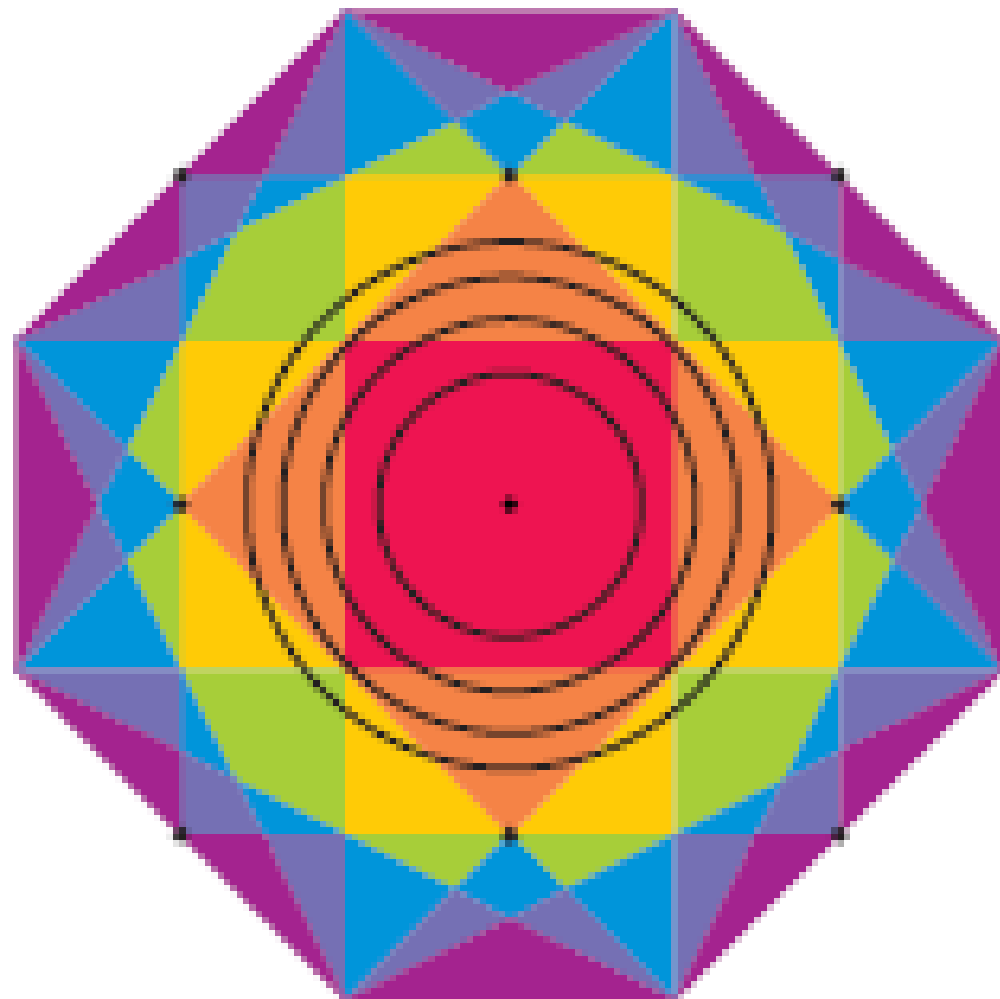
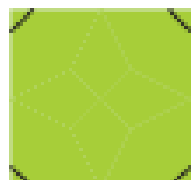
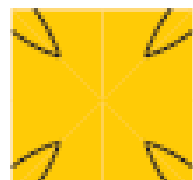
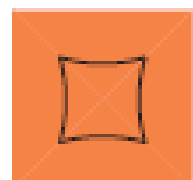
2e

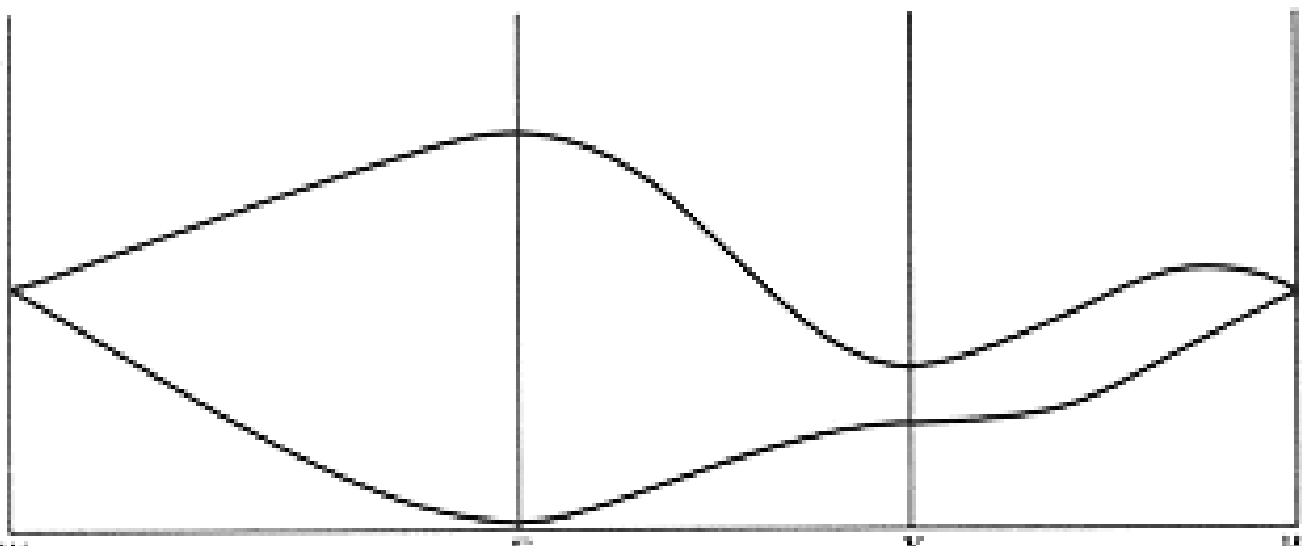
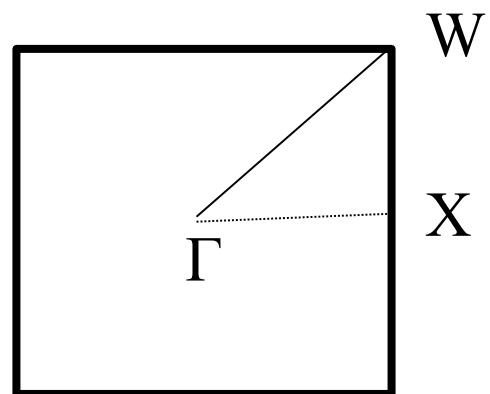
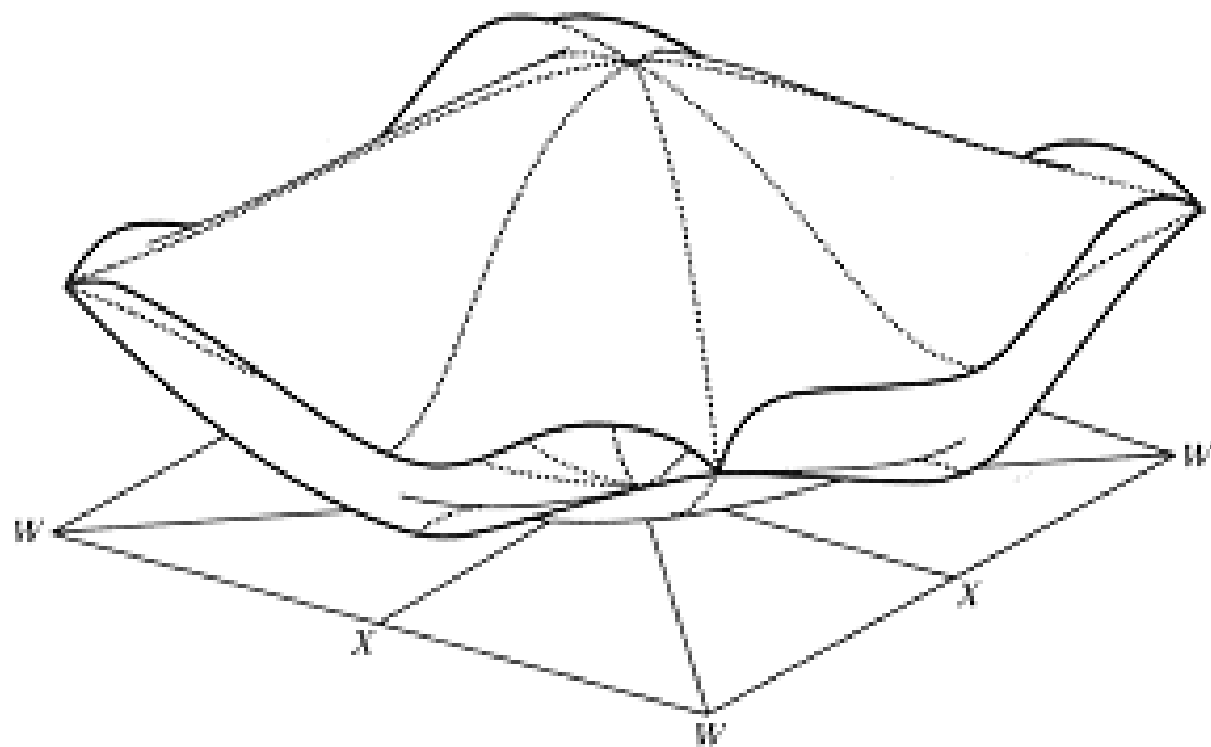


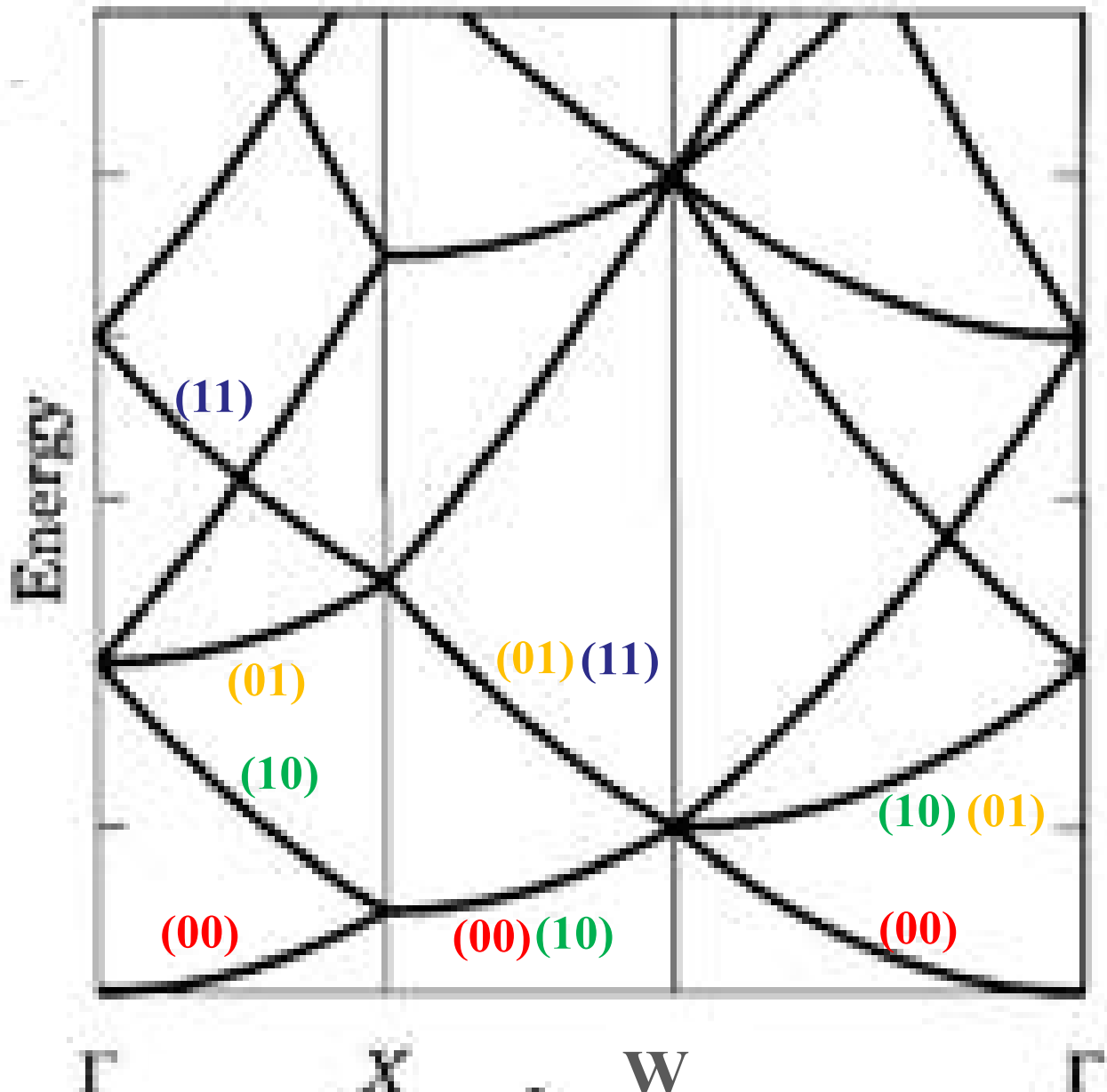
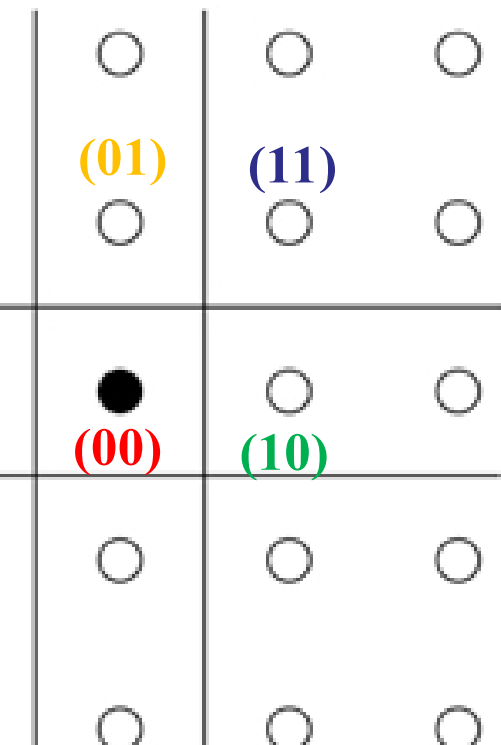
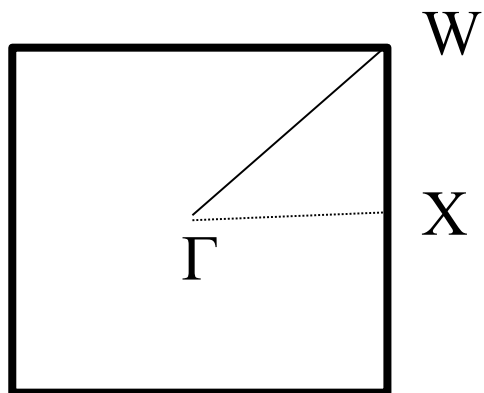
3e



4e

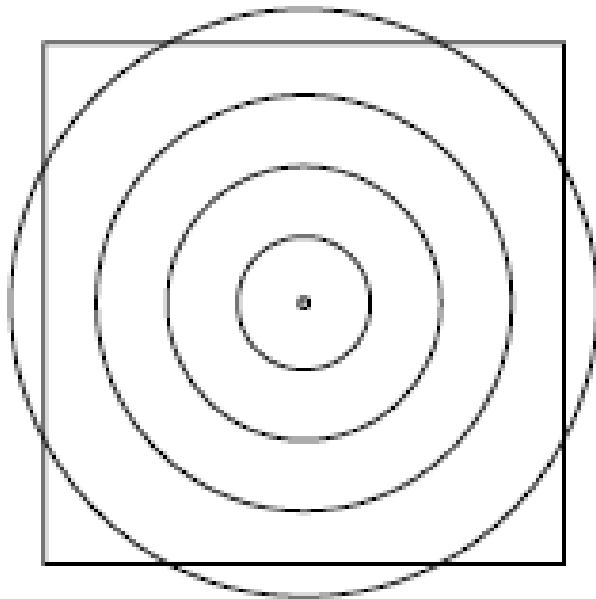




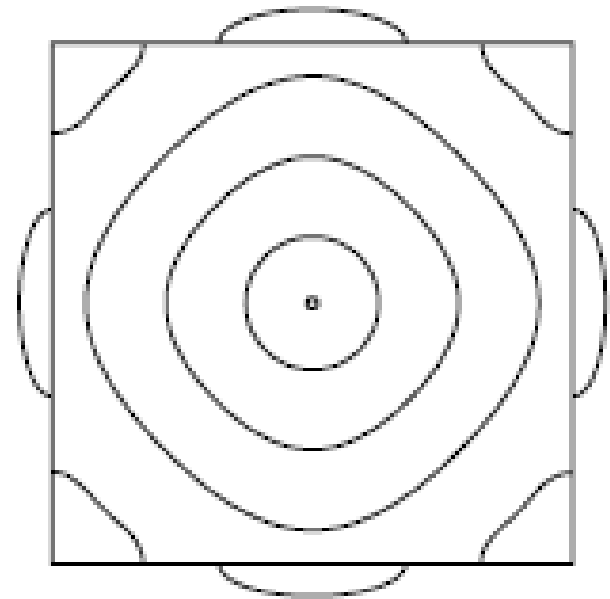


# Como se modifica la estructura de bandas de electrones libres un potencial periódico débil ?

Se abren gaps en los planos de Bragg y las bandas degeneradas se splitean



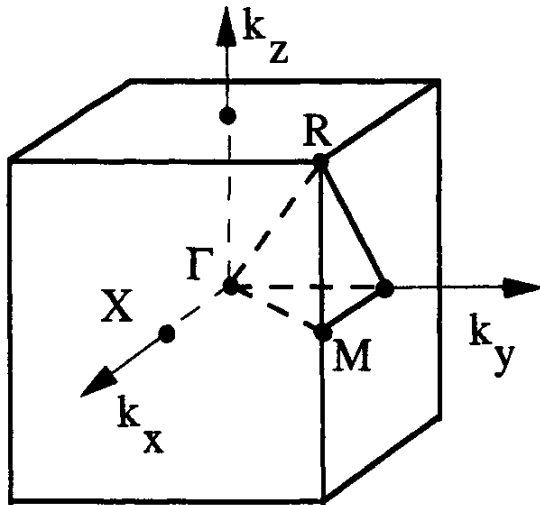
Empty lattice approx.



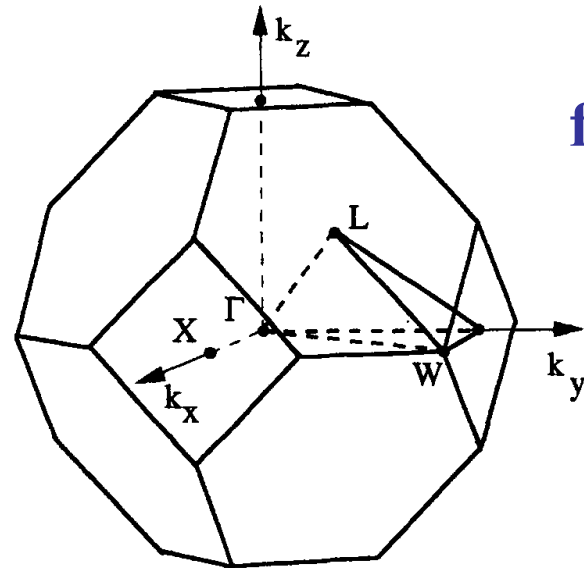
Nearly free electron approx.

# Redes en 3D

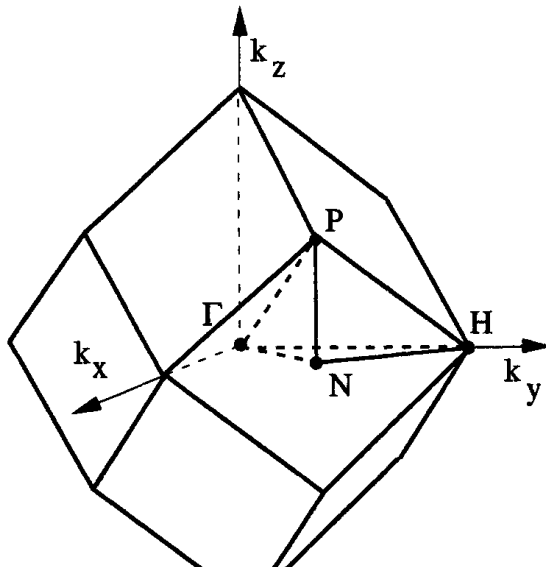
cubica  
simple



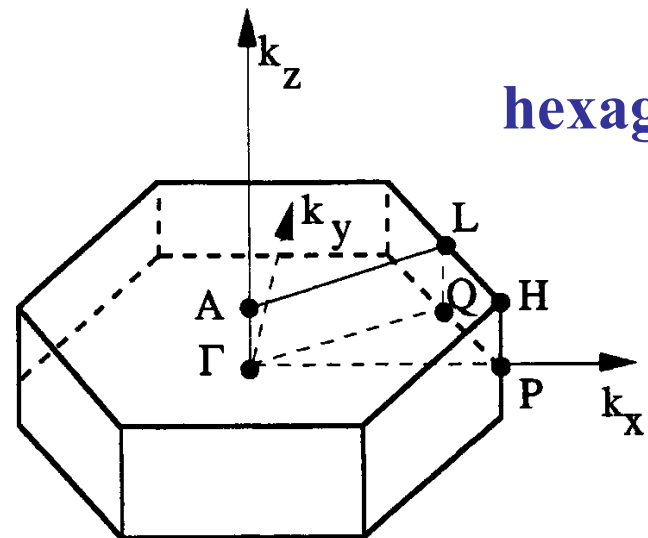
fcc



bcc



hexagonal

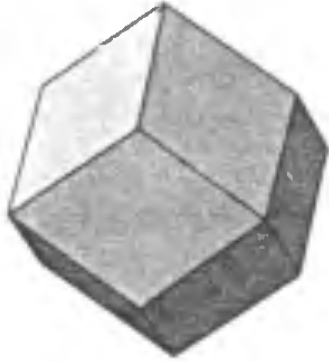




**bcc**

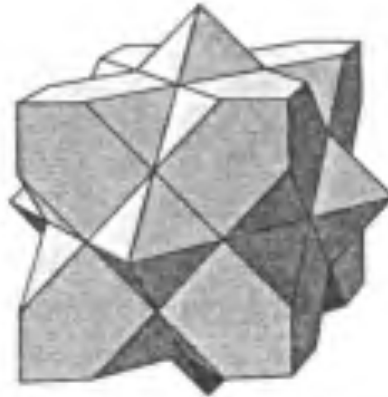
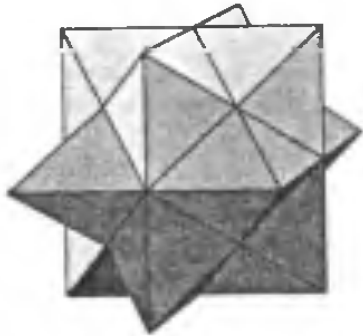
**fcc**

**I**



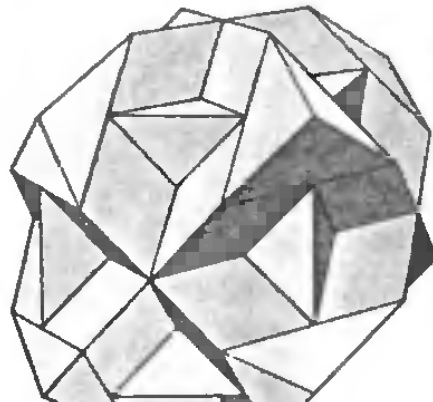
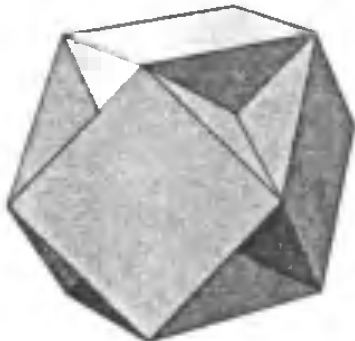
**1 Zona Brillouin**

**II**



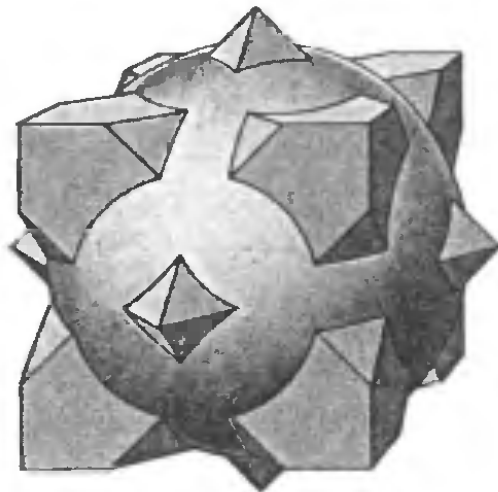
**2 Zona Brillouin**

**III**

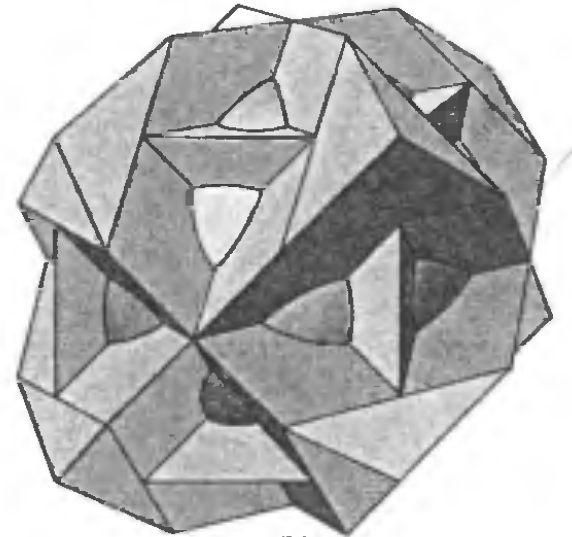


**3 Zona Brillouin**

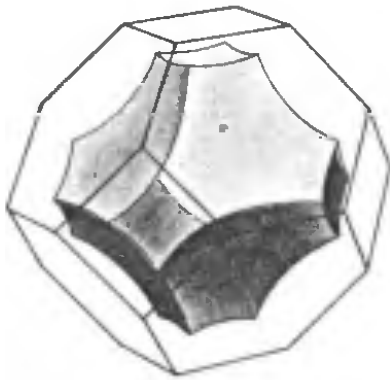
# Superficie de Fermi de electrón libre para una estructura fcc ( $z=4$ )



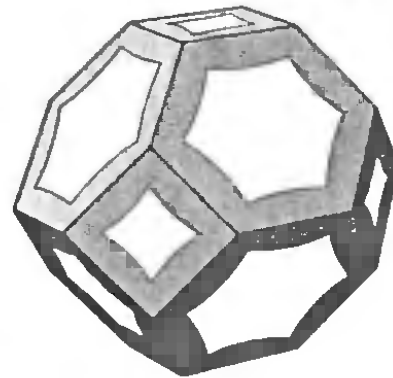
(a)



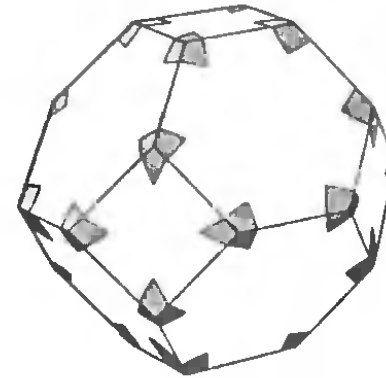
(b)



(c)



(d)



(e)

Band 1

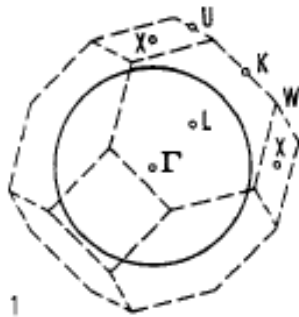
Band 2

Band 3

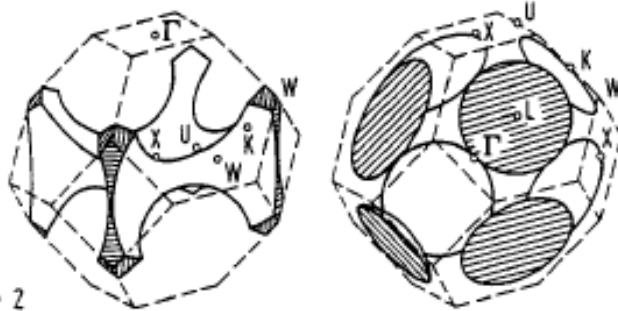
Band 4

fcc

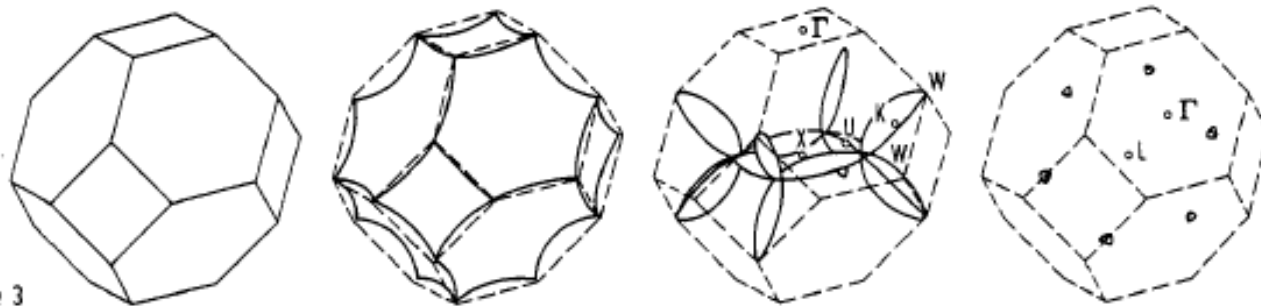
Valence 1



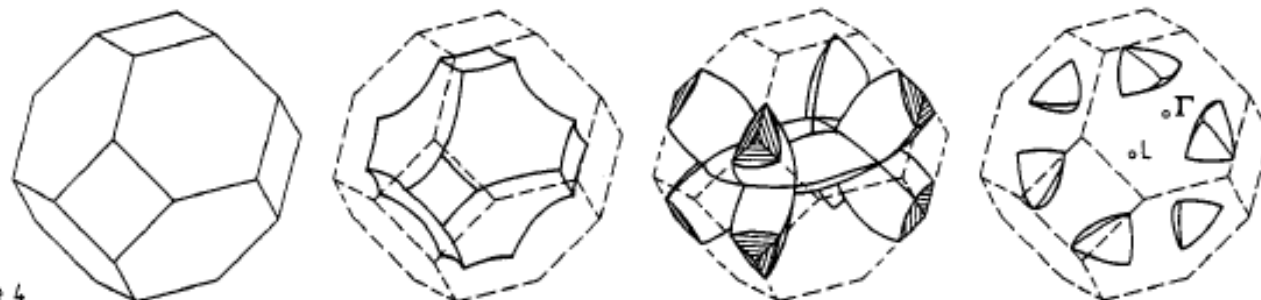
Valence 2

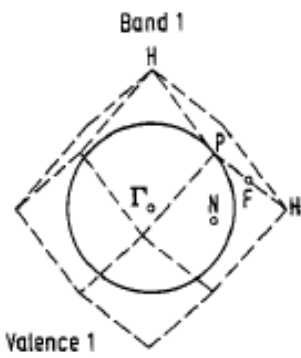


Valence 3



Valence 4



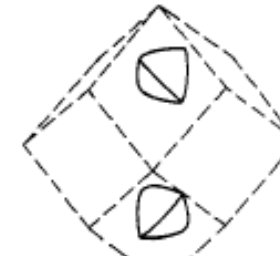
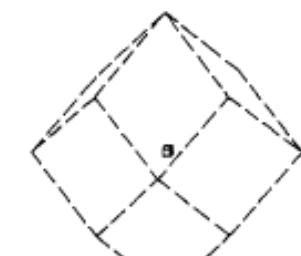
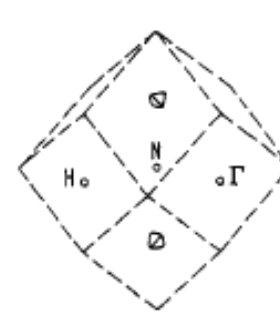
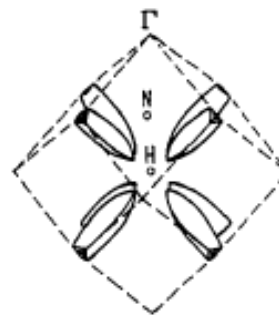
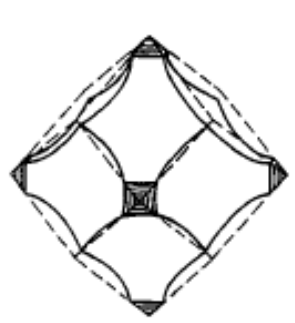
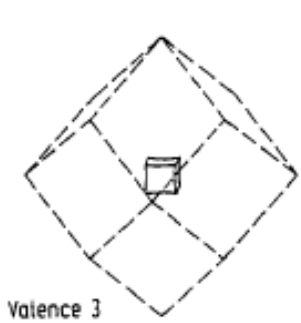
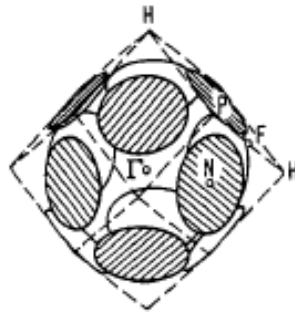
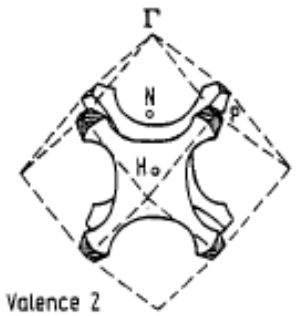


Band 2

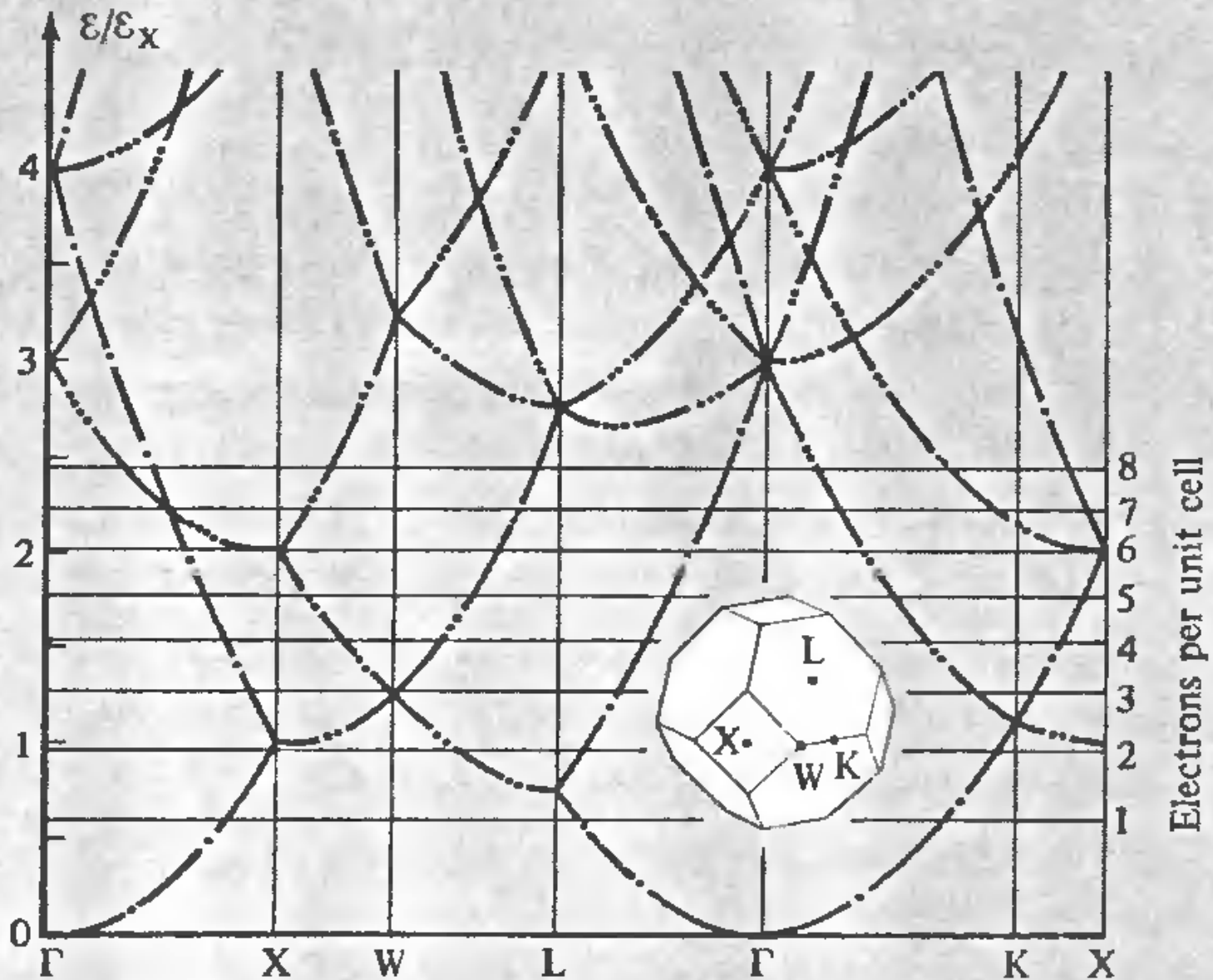
Band 3

Band 4

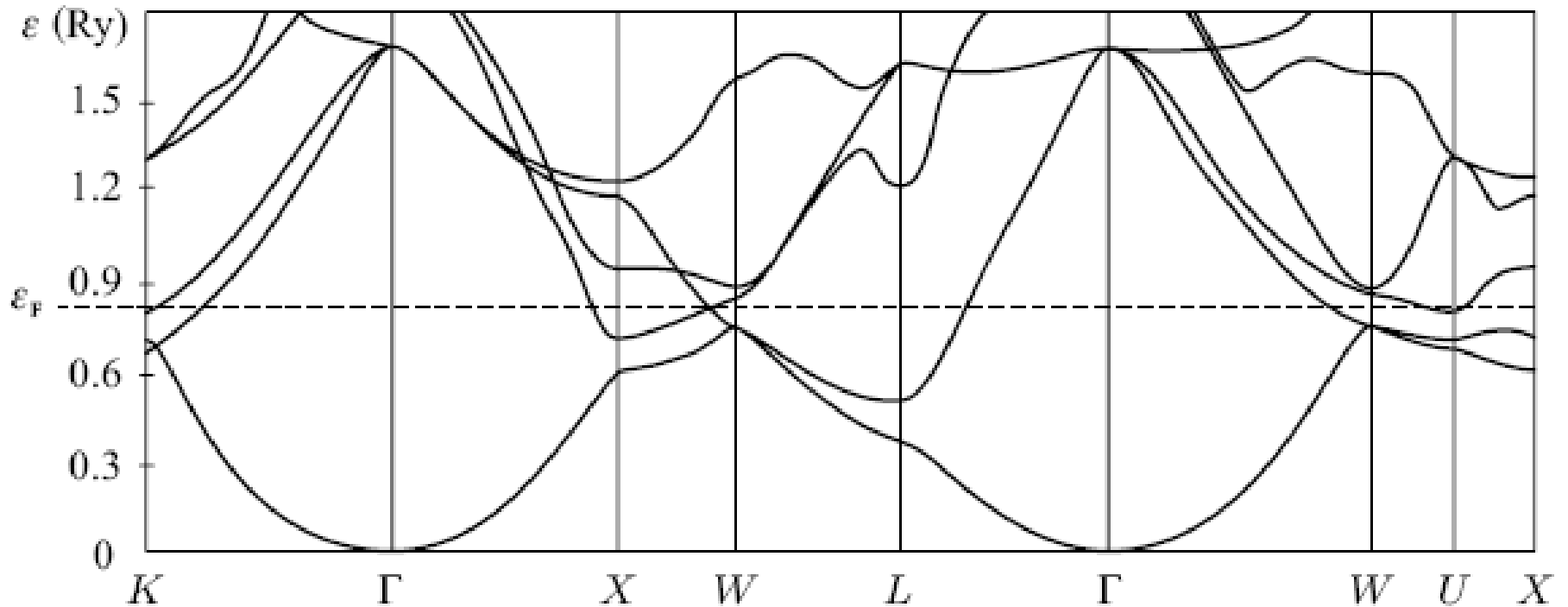
bcc



# Bandas de energía de electrón libre para una red fcc

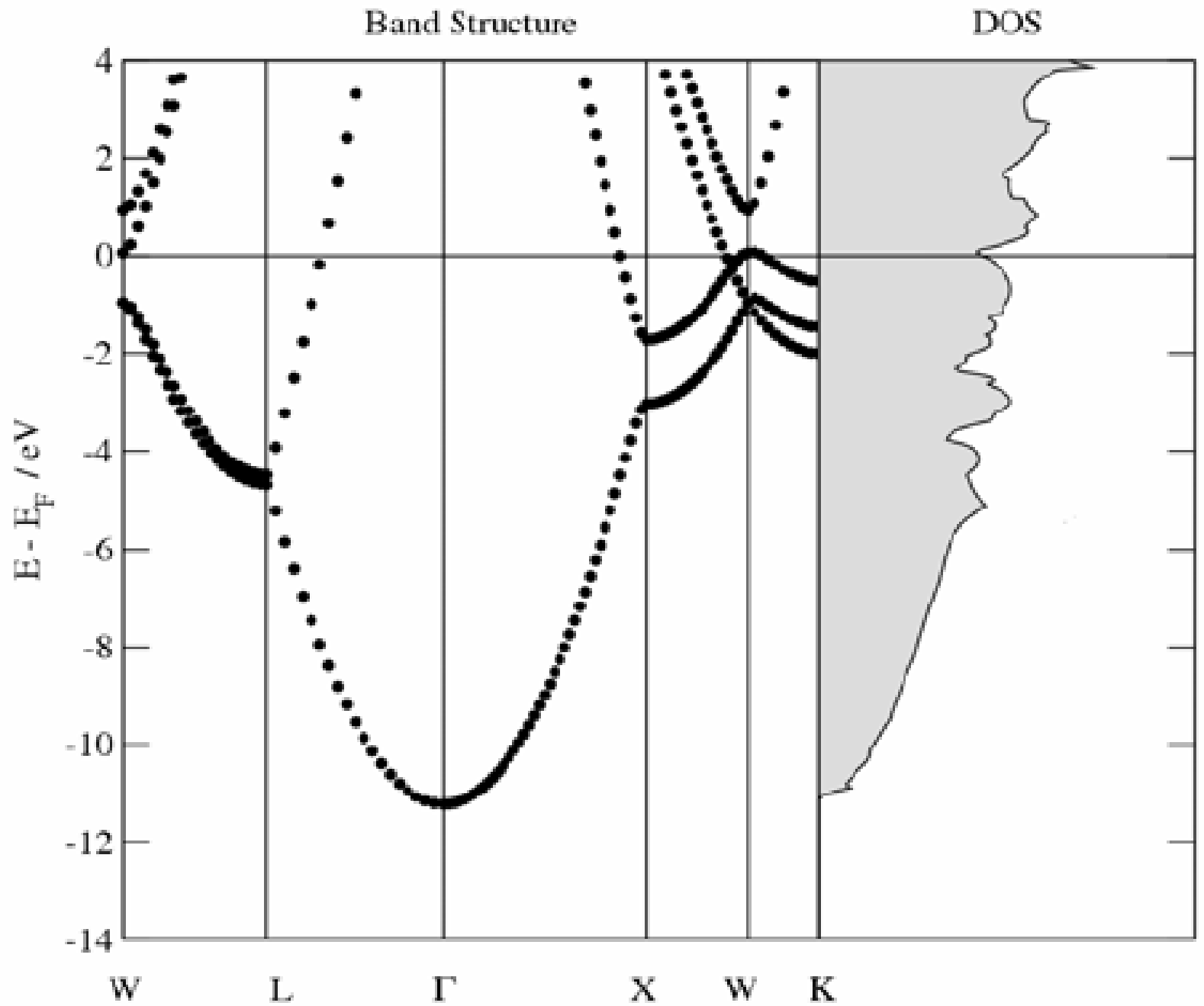


# Estructura de bandas del Aluminio

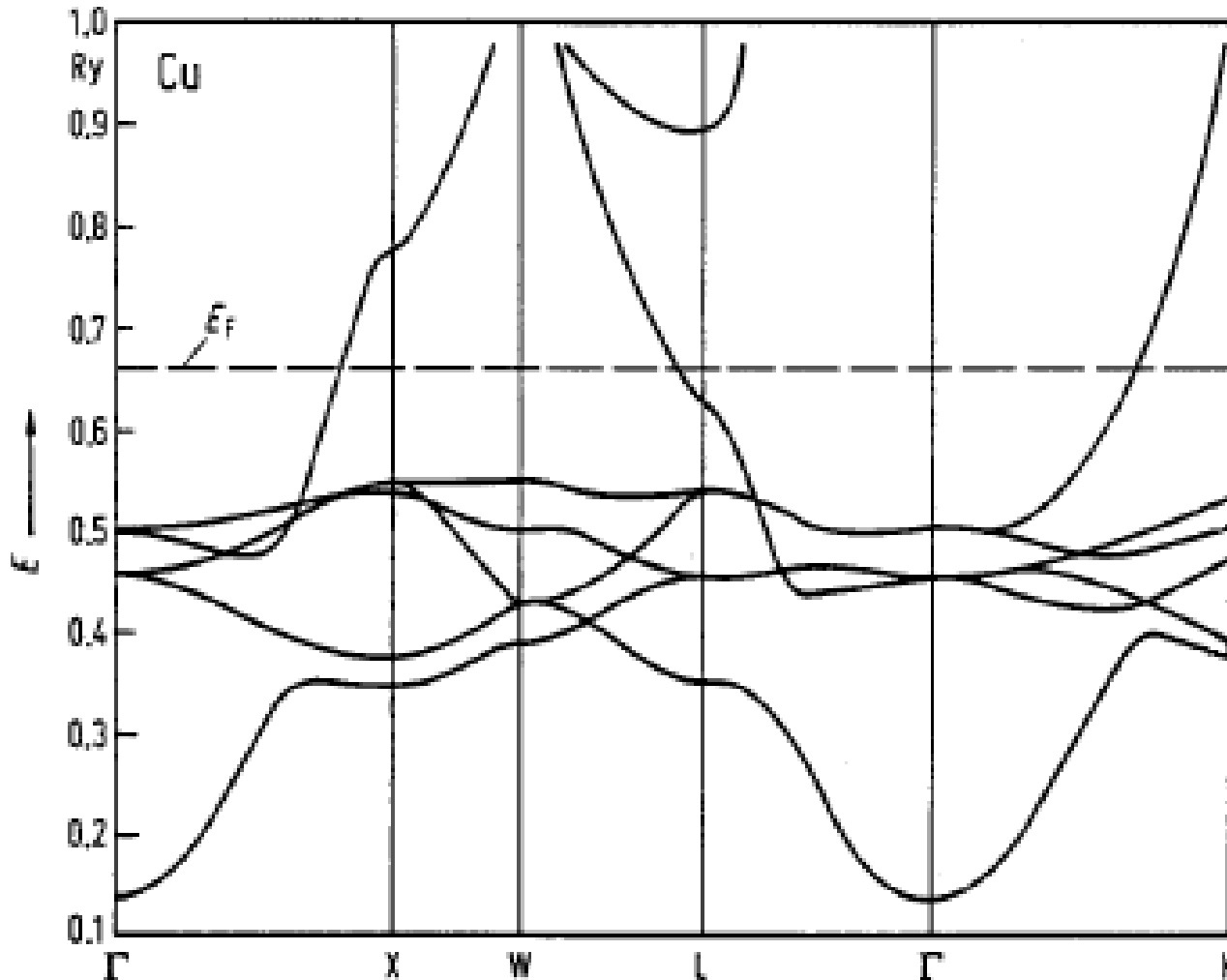


Se pueden describir con la aproximación electrones casi-libres

AI



# Estructura de bandas del Cobre



} Bandas chatas  
provenientes de  
los orbitales 3d  
**No se pueden  
obtener con NFE**



# Método Tight-Binding

Escribir la función de onda de Bloch como una combinación lineal de orbitales atómicos (LCAO).

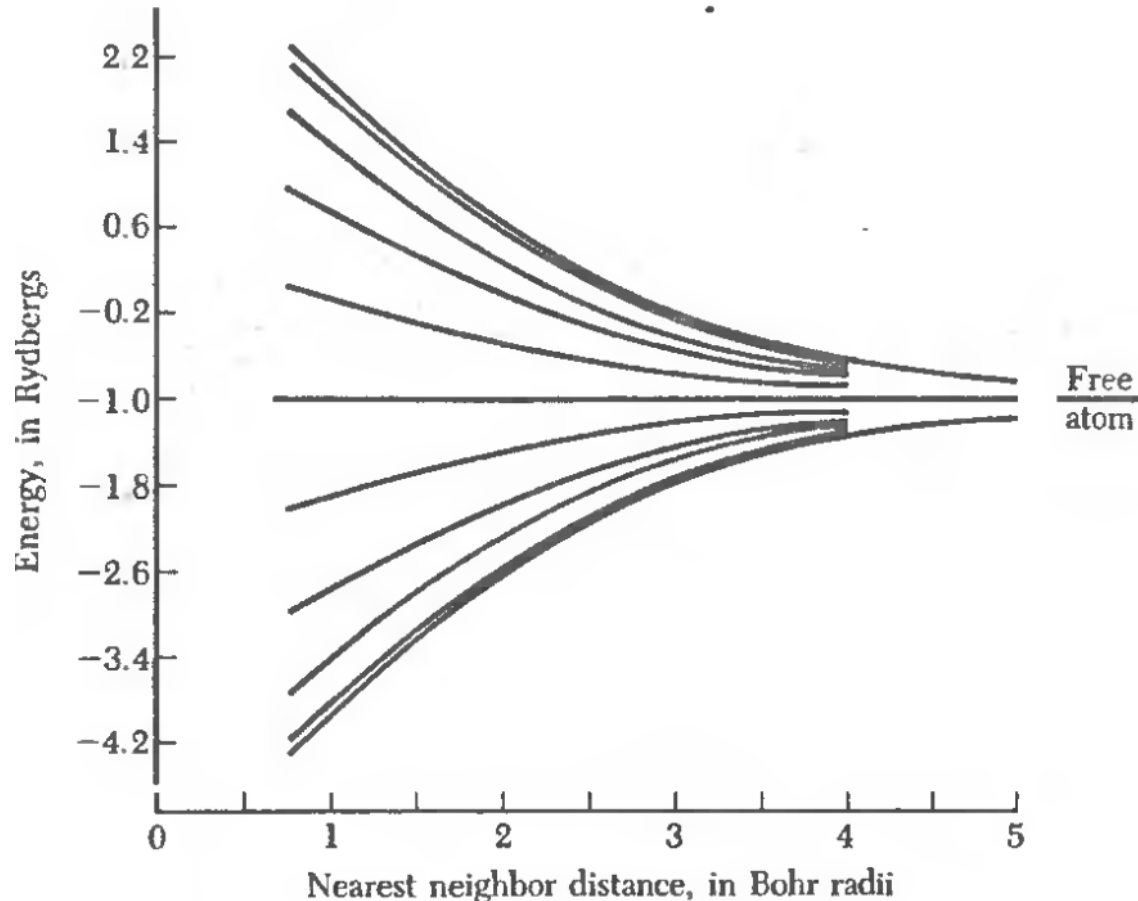


Figure 17 The 1s band of a ring of 20 hydrogen atoms; the one-electron energy calculated in the tight-binding approximation with the nearest-neighbor overlap integral of Eq. (9)

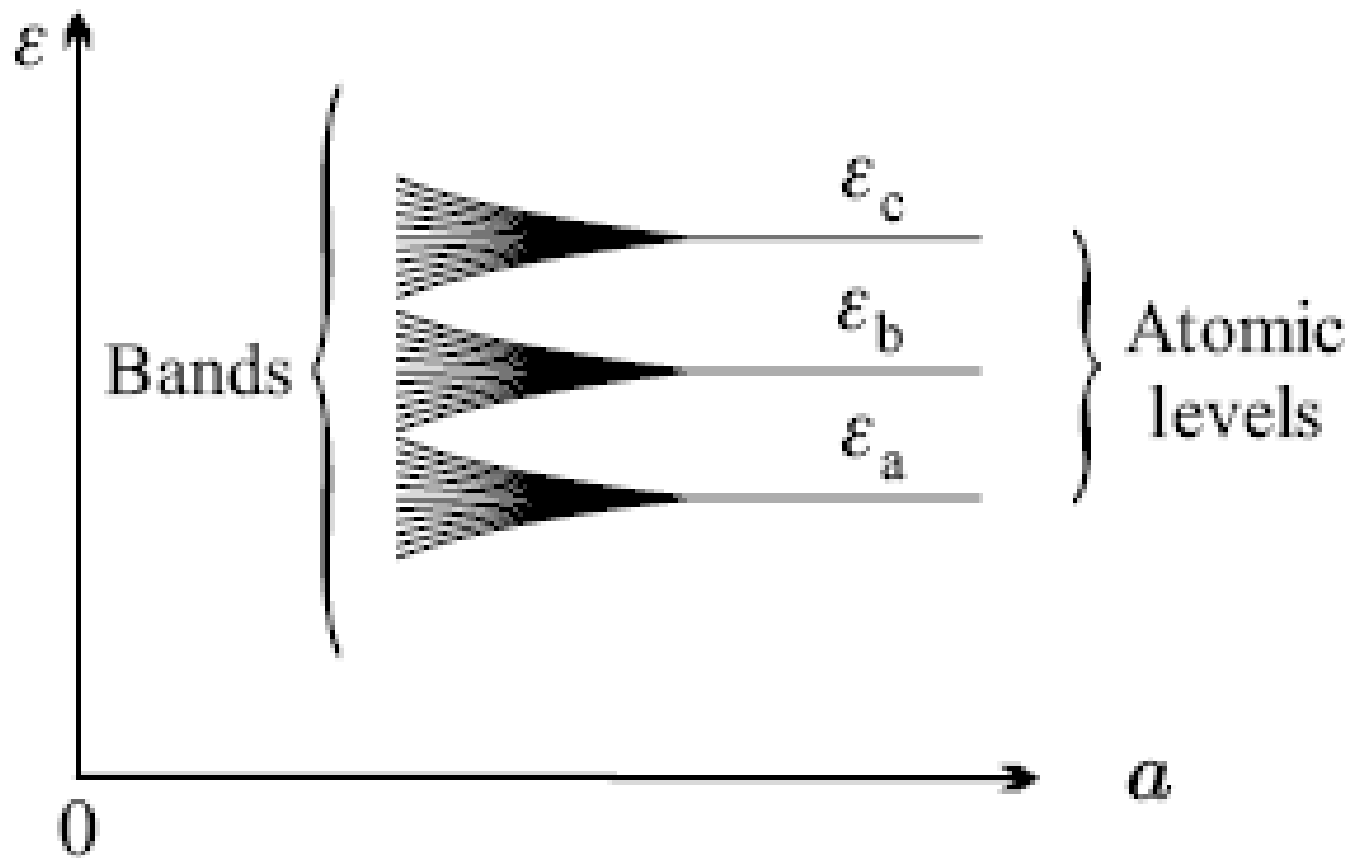
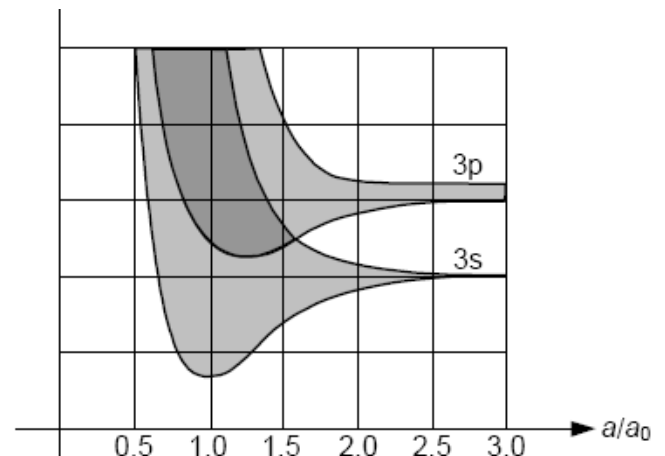


Fig. 3.7. Sketch of variation (with distance between atoms) of bandwidths of Na. Each energy unit represents 2 eV. The equilibrium lattice spacing is  $a_0$ . Higher bands such as the 4s and 3d are left out



# LCAO en cristales

$$\psi_k \approx \Phi_k = \sum_n \mathbf{a}_n \varphi_i(\mathbf{r} - \mathbf{r}_n) = \sum_n e^{i\mathbf{k} \cdot \mathbf{r}_n} \varphi_i(\mathbf{r} - \mathbf{r}_n)$$

$a_n = \exp(i\mathbf{k} \cdot \mathbf{r}_n)$  para que sea una función de onda de Bloch

$$\Phi_{k+G} = \sum_n e^{i\mathbf{k} \cdot \mathbf{r}_n} e^{i\mathbf{G} \cdot \mathbf{r}_n} \varphi_i(\mathbf{r} - \mathbf{r}_n) = \Phi_k$$

$$\langle \Phi_k | \Phi_k \rangle = \sum_{n,m} e^{i\mathbf{k} \cdot (\mathbf{r}_n - \mathbf{r}_m)} \int \varphi_i^*(\mathbf{r} - \mathbf{r}_m) \varphi_i(\mathbf{r} - \mathbf{r}_n) d\mathbf{r}$$

$$\langle \Phi_k | \Phi_k \rangle \simeq \sum_n \int \varphi_i^*(\mathbf{r} - \mathbf{r}_n) \varphi_i(\mathbf{r} - \mathbf{r}_n) d\mathbf{r} = N$$

$$\psi(k, r) = \frac{1}{\sqrt{N}} \sum_j e^{ik \cdot R_j} \varphi_i(r - R_j)$$

$\varphi_i(r - R_j)$  orbital atómico  $i$  centrado en el sitio  $R_j$

$$\begin{aligned} \psi(k, r + R_n) &= \frac{1}{\sqrt{N}} \sum_j e^{ik \cdot R_j} \varphi_i(r + R_n - R_j) \\ &= e^{ik \cdot R_n} \frac{1}{\sqrt{N}} \sum_j e^{ik \cdot (R_j - R_n)} \varphi_i(r - (R_j - R_n)) \\ &= e^{ik \cdot R_n} \psi(k, r). \quad \text{cumple teorema de Bloch} \end{aligned}$$

Trabajaremos en notación  
de brakets

$$\psi(k, r) \longrightarrow |\Psi_k\rangle$$

$$\varphi_i(r - R_j) \longrightarrow |i, R_j\rangle$$

Para un cristal monoatómico con un orbital por sitio

$$| \Psi_{\mathbf{k}} \rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j} e^{i(\bar{\mathbf{k}} \cdot \bar{\mathbf{R}}_j)} | \mathbf{R}_j \rangle$$

Quiero resolver:  $H | \Psi_{\mathbf{k}} \rangle = E(\mathbf{k}) | \Psi_{\mathbf{k}} \rangle$

Proyecto la ecuación de Schrödinger sobre  $\langle \mathbf{R}_0 |$

***Tight-Binding:***

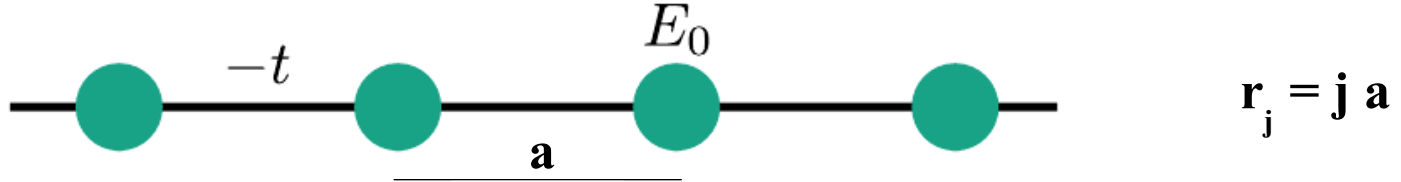
$$\langle \mathbf{R}_0 | \mathbf{R}_j \rangle = \delta_{0j}$$

$$\langle \mathbf{R}_0 | H | \mathbf{R}_j \rangle =$$

$$\left\{ \begin{array}{ll} \mathbf{E}_0 & j = 0 \\ -t & j \text{ primer vecino de } 0 \\ 0 & \text{los otros casos} \end{array} \right.$$

$$E(\mathbf{k}) = E_0 + \sum_{j \text{ (pv)}} (-t) e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_0)}$$

## Ej1. Cadena monoatómica con un orbital por sitio



$$\varphi_k(x) = \frac{1}{\sqrt{N}} \sum_j e^{ikr_j} \varphi(x - x_j) \quad \Longrightarrow \quad |k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikr_j} |j\rangle$$

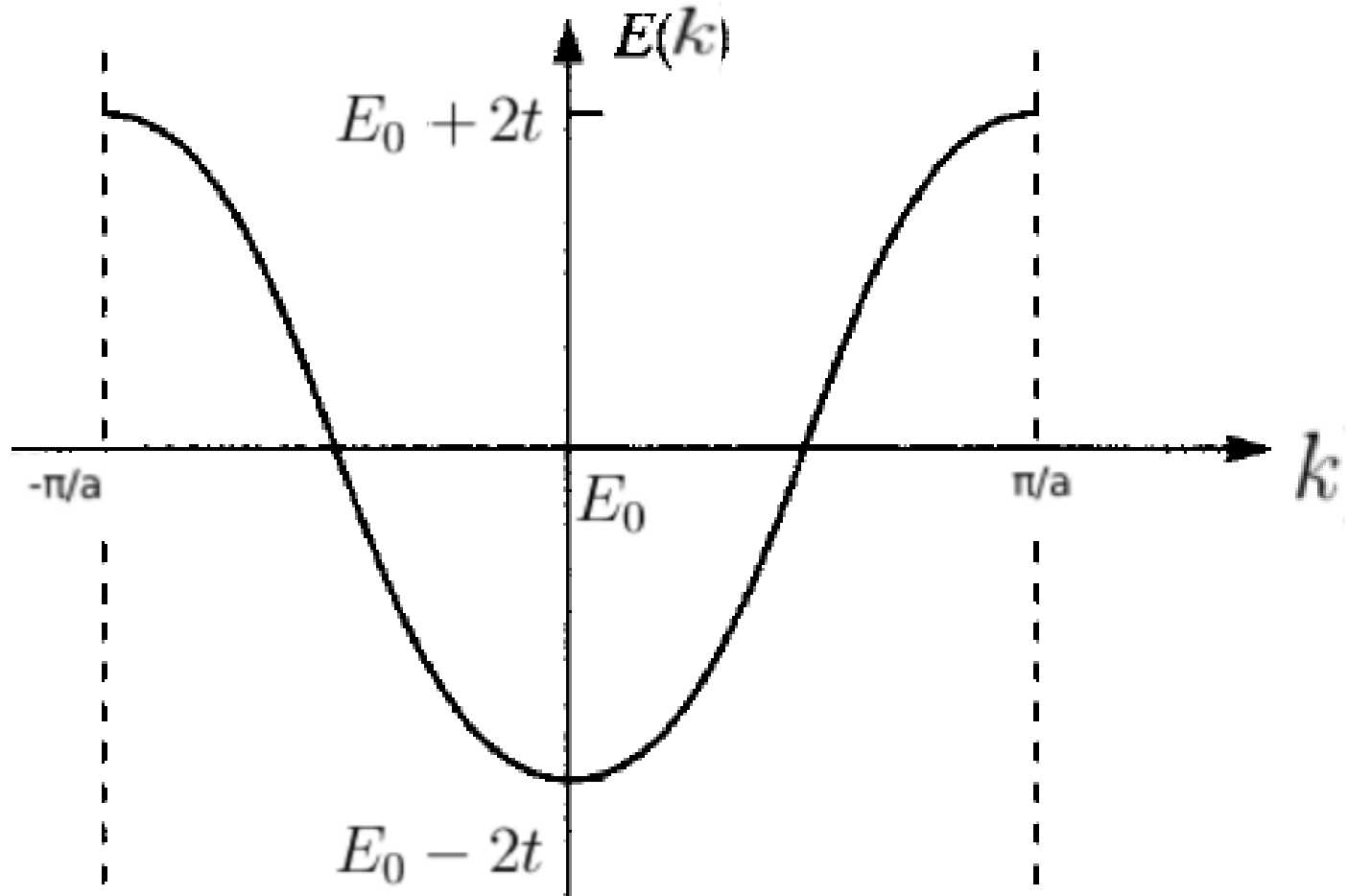
$$H|k\rangle = E|k\rangle \quad \text{Proyecto sobre un orbital arbitrario} \quad |j=0\rangle = |0\rangle$$

$$\langle 0|H|k\rangle = E\langle 0|k\rangle$$

$$\frac{1}{\sqrt{N}} \sum_j e^{ikr_j} \langle 0|H|j\rangle = \frac{E}{\sqrt{N}} \sum_j e^{ikr_j} \langle 0|j\rangle$$

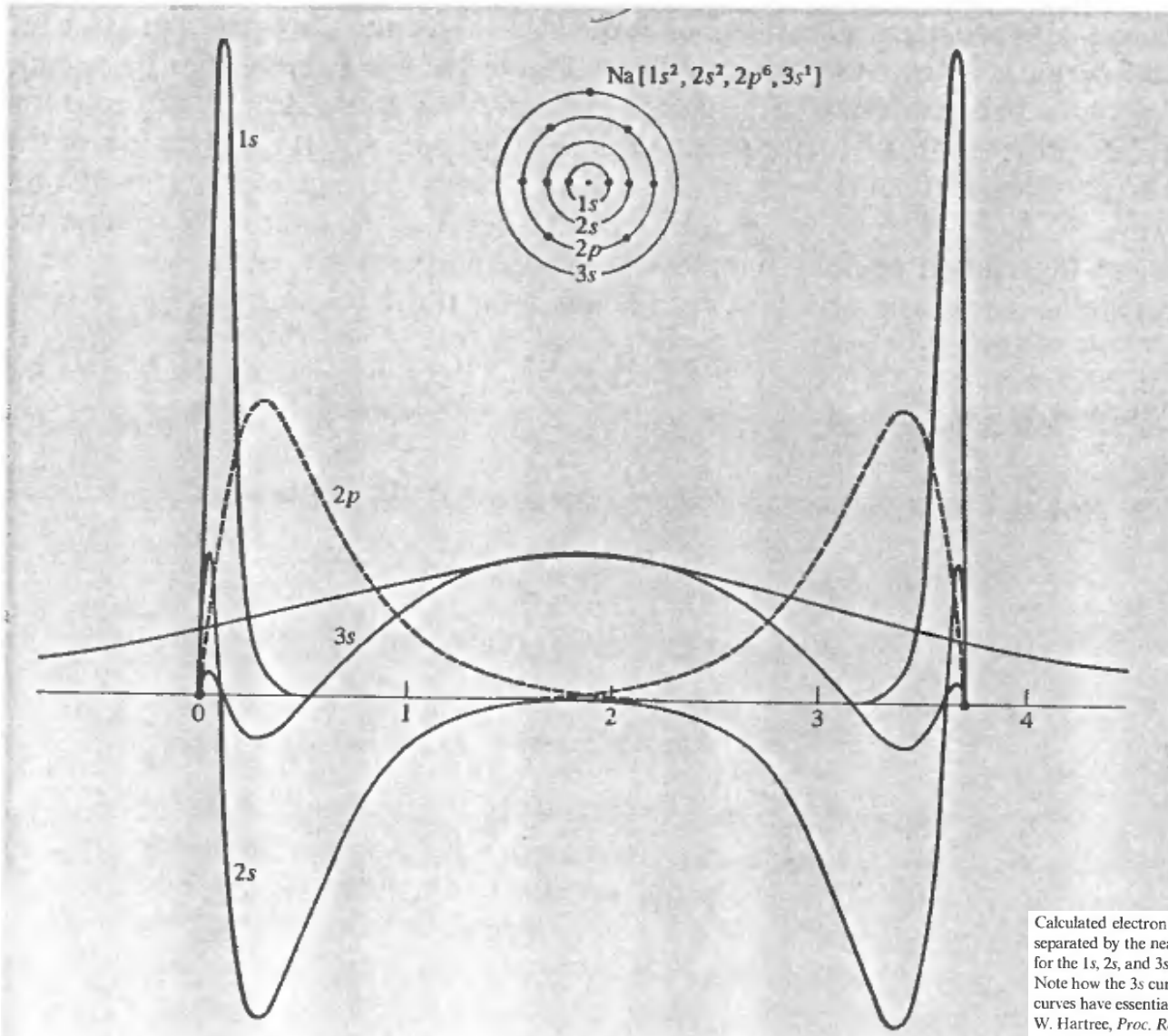
$$E = E_0 - t (e^{ika} + e^{-ika}) = E_0 - 2t \cos(ka)$$

$$E = E_0 - 2t \cos(ka)$$



El parámetro de hopping determina el ancho de la banda ( $4t$ ) !!

$$t(\mathbf{R}_l) = \int \varphi_i^*(\mathbf{r} - \mathbf{R}_l) \mathcal{H}(\mathbf{r}) \varphi_j(\mathbf{r}) d\mathbf{r}$$



Calculated electron wave functions for the levels of atomic sodium, plotted about two nuclei separated by the nearest-neighbor distance in metallic sodium, 3.7 Å. The solid curves are  $r\psi(r)$  for the 1s, 2s, and 3s levels. The dashed curve is  $r$  times the radial wave function for the 2p levels. Note how the 3s curves overlap extensively, the 2s and 2p curves overlap only a little, and the 1s curves have essentially no overlap. The curves are taken from calculations by D. R. Hartree and W. Hartree, *Proc. Roy. Soc. A193*, 299 (1948). The scale on the  $r$ -axis is in angstroms.



## Ej2. Cúbica simple con un orbital por sitio

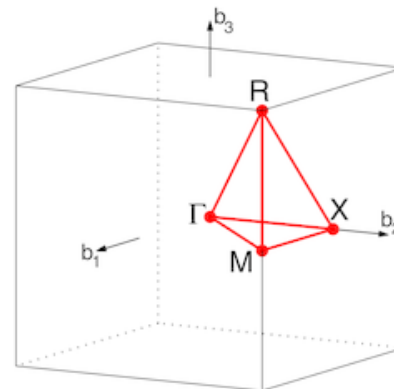
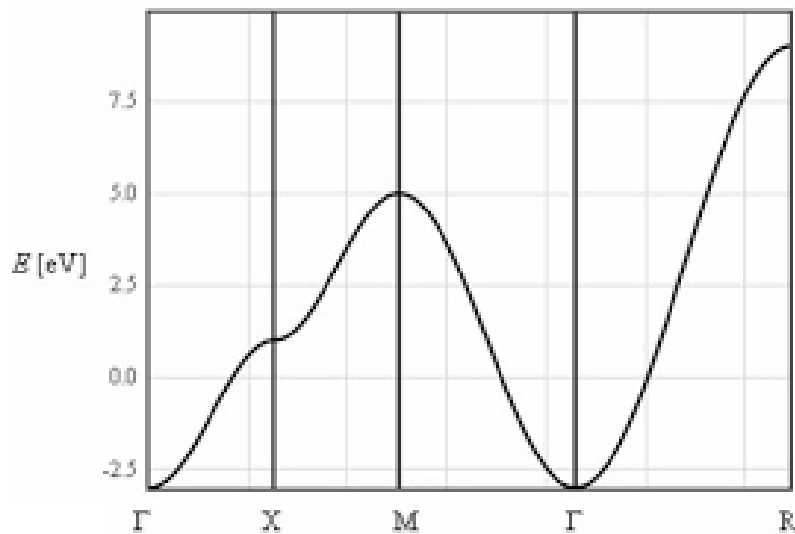
$$E(k) = \epsilon_0 - t \sum_m e^{i\mathbf{k} \cdot (\mathbf{r}_0 - \mathbf{r}_m)}$$

$\mathbf{r}_0$  átomo de referencia  
 $\mathbf{r}_m$  sus primeros vecinos

Para la red cúbica simple:

$$\mathbf{r}_0 - \mathbf{r}_m = (\pm a, 0, 0); (0, \pm a, 0); (0, 0, \pm a)$$

$$E(k) = \epsilon_0 - 2t(\cos k_x a + \cos k_y a + \cos k_z a)$$



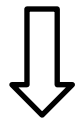
**Para  $m$  orbitales por celda, la función de onda tight binding se escribe:**

$$|\Psi_{\mathbf{k}}\rangle = \sum_{\mathbf{R}_j} e^{i(\bar{\mathbf{k}} \cdot \bar{\mathbf{R}}_j)} \left( \sum_{\alpha} c_{\alpha} |\alpha, \mathbf{R}_j\rangle \right)$$

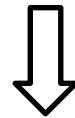
índice de celda  
(vectores de la red  
Bravais)

$(\alpha = 1, m)$  orbitales  
de los átomos del motivo

**Proyecto la ecuación de Schrödinger sobre los  $m$  orbitales  $\langle \mathbf{R}_0, \alpha |$  de una celda de referencia  $\mathbf{R}_0$**



**Sistema de  $m \times m$  para los coeficientes  $c_{\alpha}$**

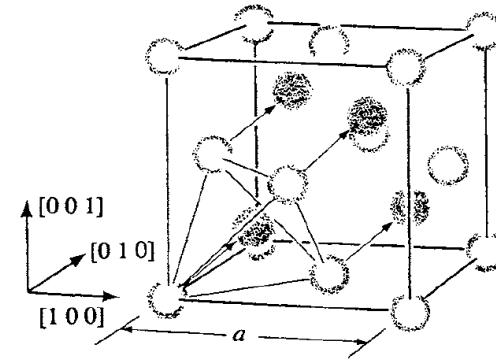


**$m$  bandas**

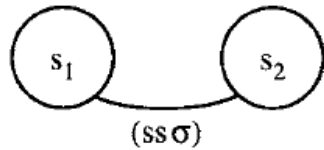
# Ej3. Si (orbitales s y p) en estructura de diamante

-fcc con 2 átomos por celda

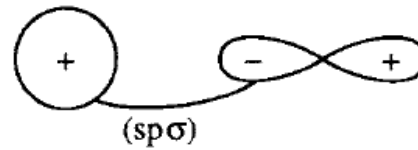
-Si:  $3s, 3p_x, 3p_y, 3p_z$



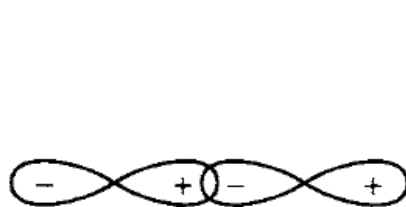
## Matriz 8x8



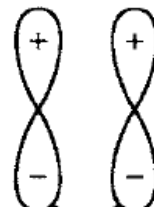
(a)



(b)

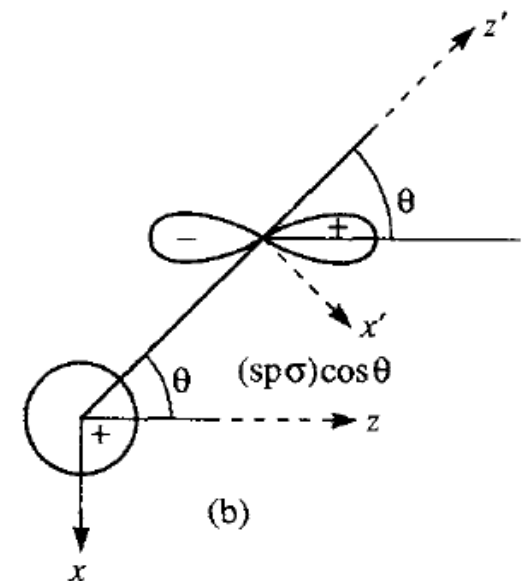


(c)



(d)

Dependencia angular !!



**Fig. 6.2** The four fundamental hopping integrals between s and p orbitals: (a) (ssσ), (b) (spσ), (c) (ppσ), and (d) (ppπ).

$$\varepsilon_s = -5.25 \text{ eV};$$

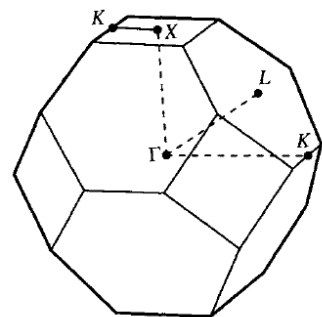
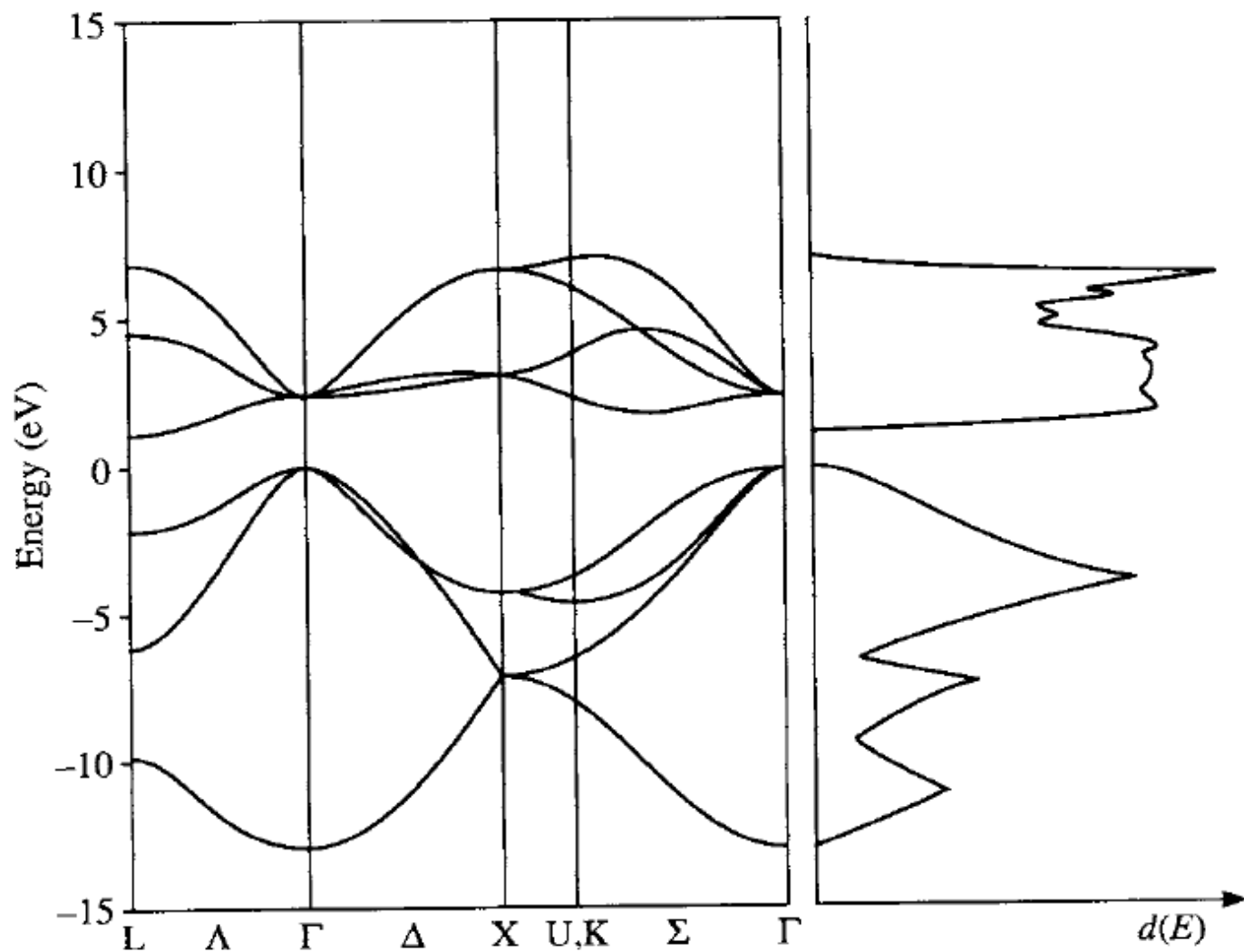
$$(ss\sigma) = -1.9375 \text{ eV};$$

$$(sp\sigma) = 1.745 \text{ eV};$$

$$\varepsilon_p = 1.20 \text{ eV}.$$

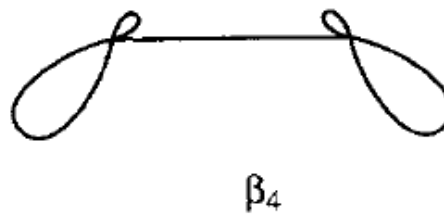
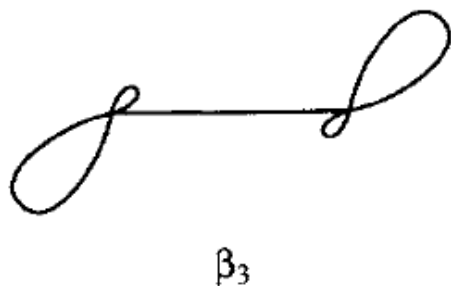
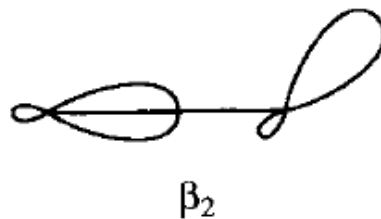
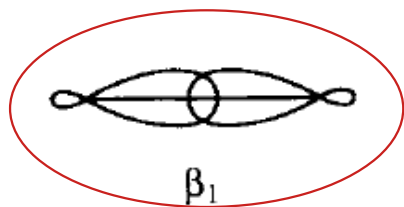
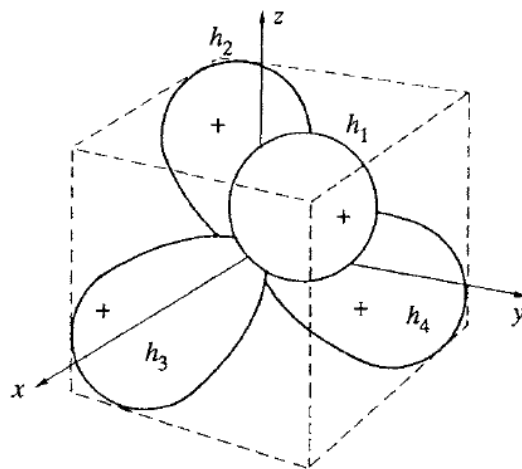
$$(pp\sigma) = 3.050 \text{ eV};$$

$$(pp\pi) = -1.075 \text{ eV}.$$



# Usando orbitales híbridos $sp_3$

$$\left. \begin{aligned} h_1 &= \frac{1}{2}(s + p_x + p_y + p_z) \\ h_2 &= \frac{1}{2}(s + p_x - p_y - p_z) \\ h_3 &= \frac{1}{2}(s - p_x + p_y - p_z) \\ h_4 &= \frac{1}{2}(s - p_x - p_y + p_z) \end{aligned} \right\}$$



$$\varepsilon_h = (\varepsilon_s + 3\varepsilon_p)/4.$$

$$\beta_1 = \frac{(ss\sigma) - 2(3^{1/2})(sp\sigma) - 3(pp\sigma)}{4}.$$

$$\Delta = (\varepsilon_s - \varepsilon_p)/4.$$

$$\beta_2, \beta_3, \text{ and } \beta_4 = 0$$

*Weaire-Thorpe model.*

# Estructura de bandas y superficie de Fermi de metales simples

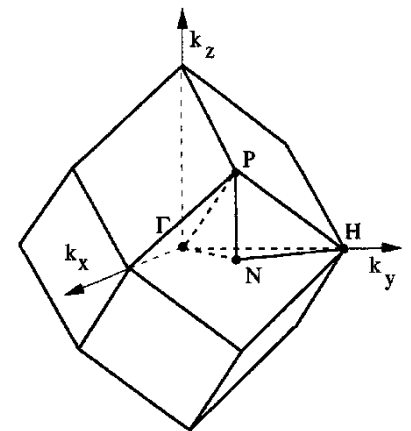
## Monovalentes

Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc			
Na	$[\text{Ne}] 3s^1$	bcc			
K	$[\text{Ar}] 4s^1$	bcc	Cu	$[\text{Ar}] 3d^{10} 4s^1$	fcc
Rb	$[\text{Kr}] 5s^1$	bcc	Ag	$[\text{Kr}] 4d^{10} 5s^1$	fcc
Cs	$[\text{Xe}] 6s^1$	bcc	Au	$[\text{Xe}] 4f^{14} 5d^{10} 6s^1$	fcc

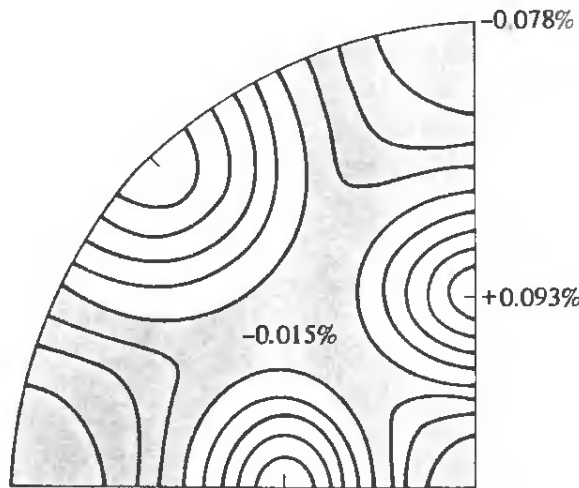
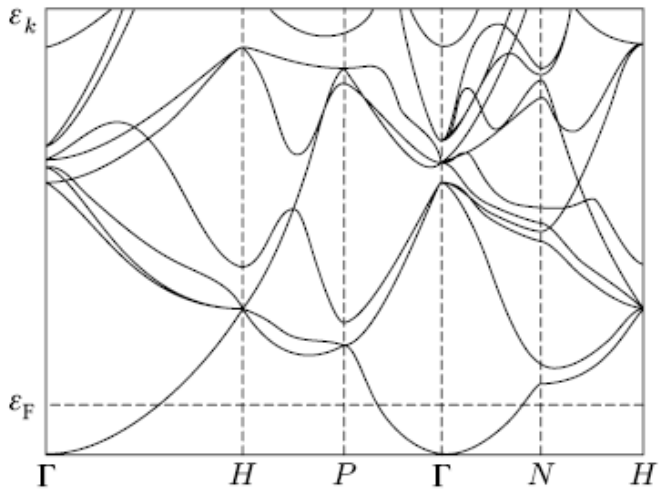
## Alcalinos:

$$k_F = 0.620(2\pi/a)$$

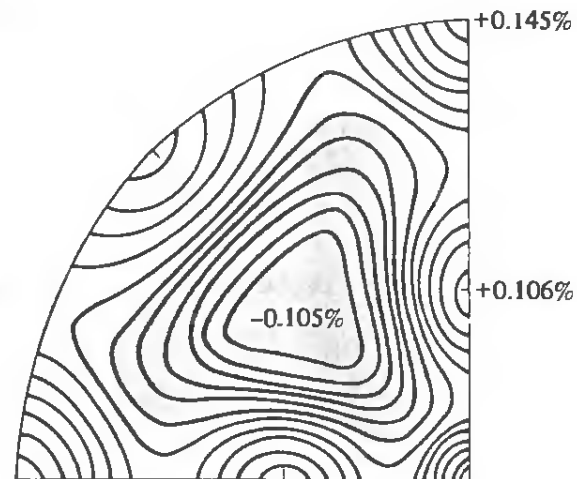
$$\overline{\Gamma N} = (2\pi/a) \sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = 0.707(2\pi/a)$$



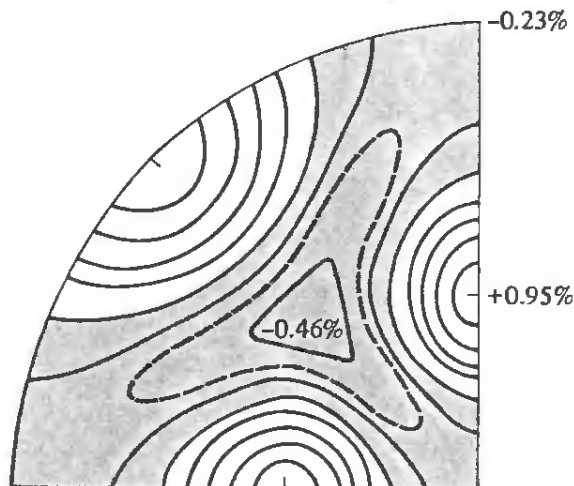
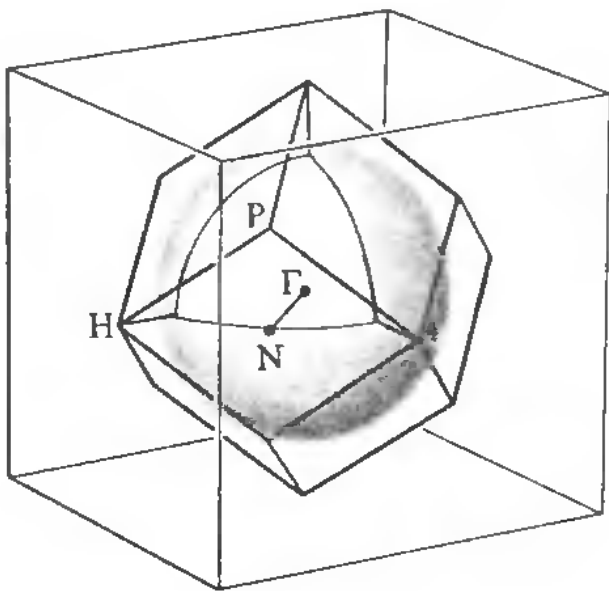
# Sodio



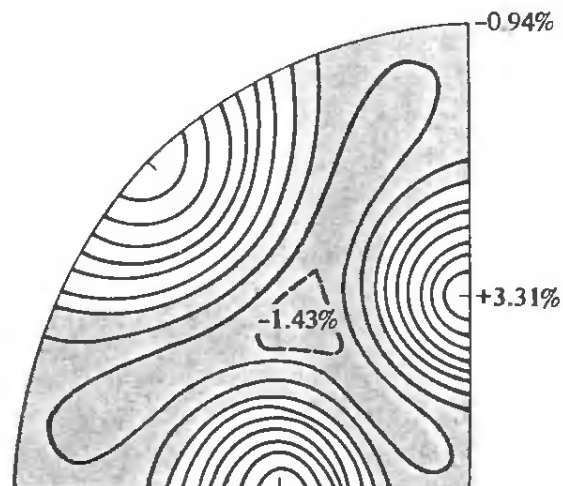
Sodium



Potassium



Rubidium

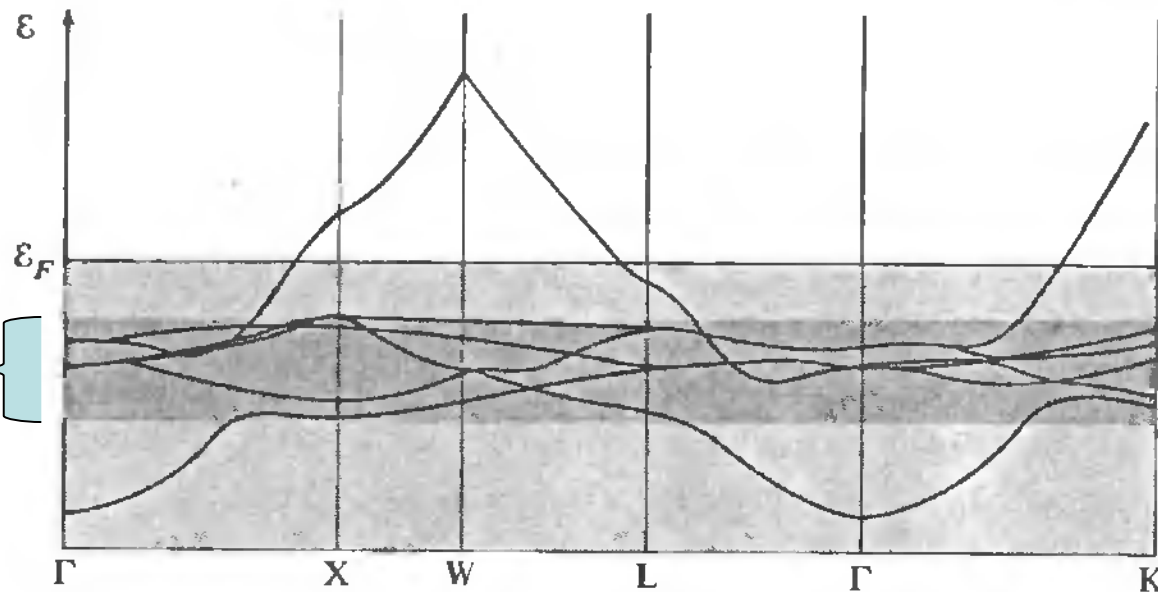


Cesium

Desviaciones de la superficie de Fermi medida respecto a una esfera perfecta

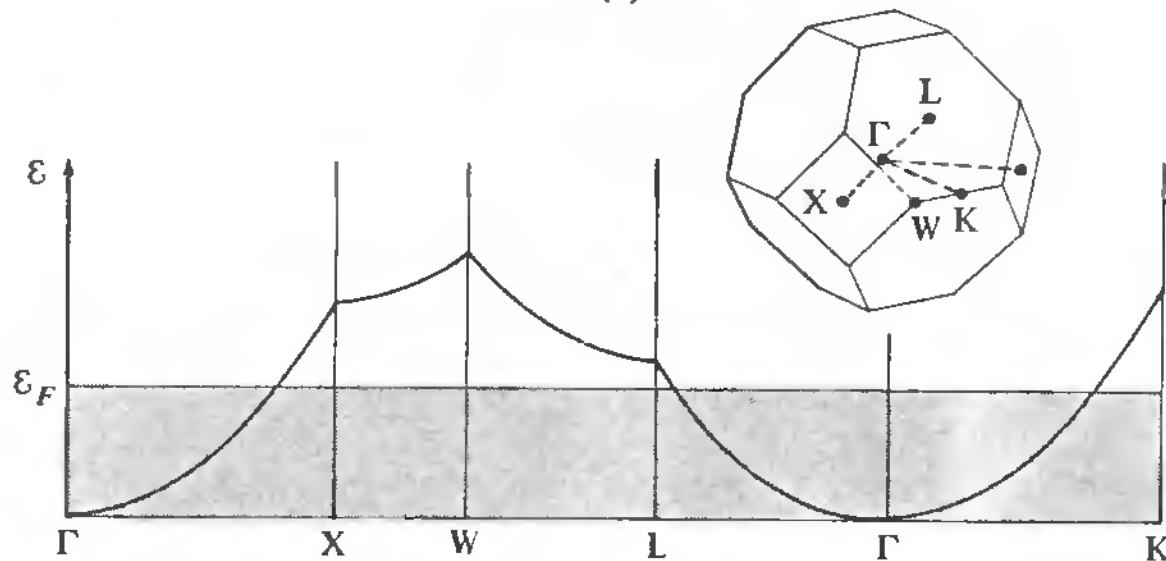
**Nobles:**

**Bandas d**



(a)

**Banda s**



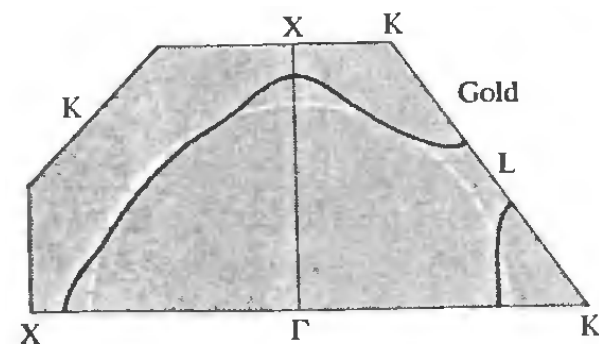
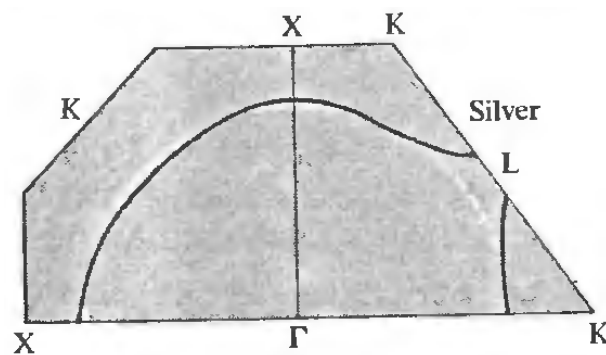
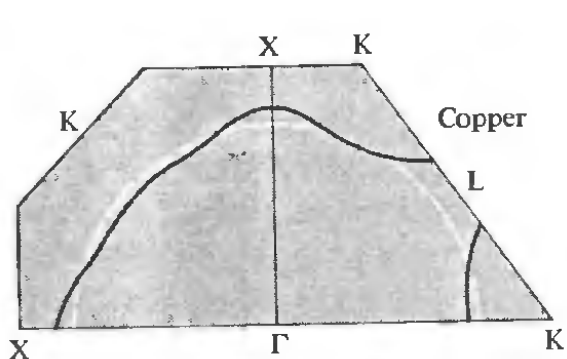
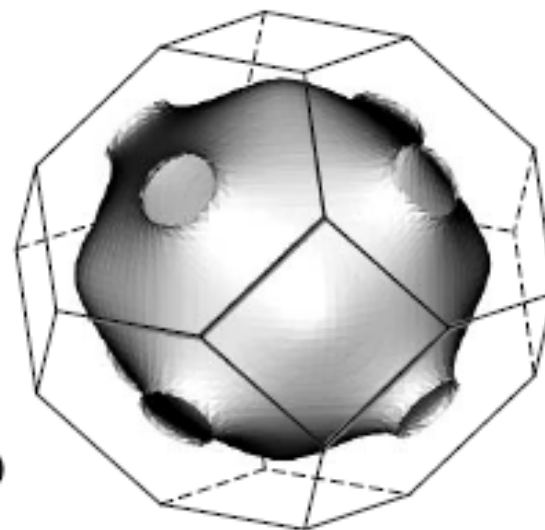
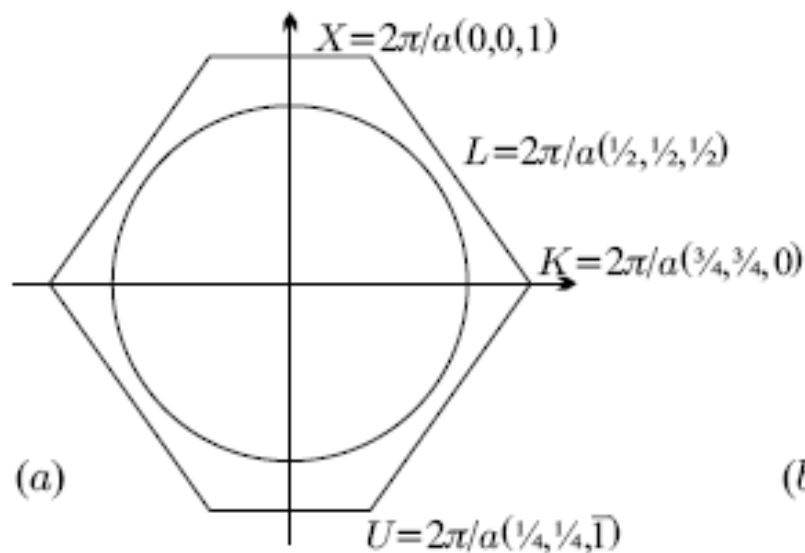
(b)

**Estructura de bandas del Cu**

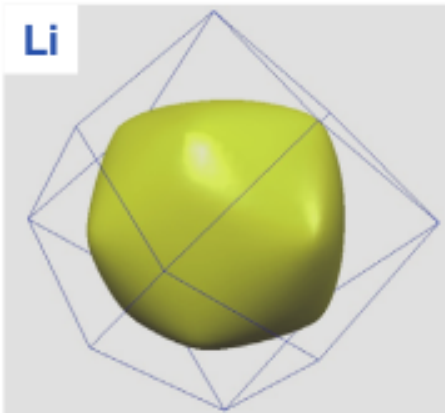


$$k_F = 0.782(2\pi/a)$$

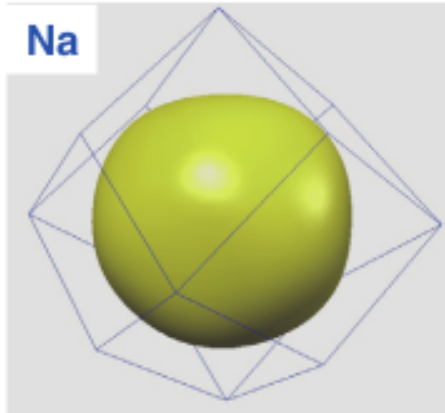
$$\Gamma-L = 0.866(2\pi/a)$$



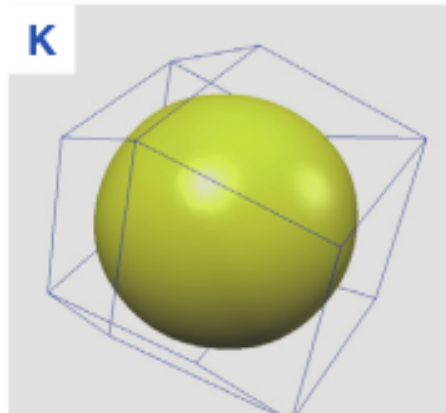
Li



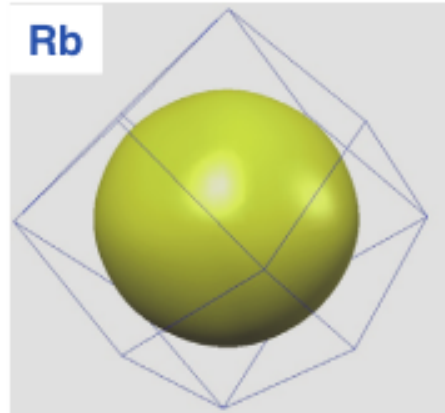
Na



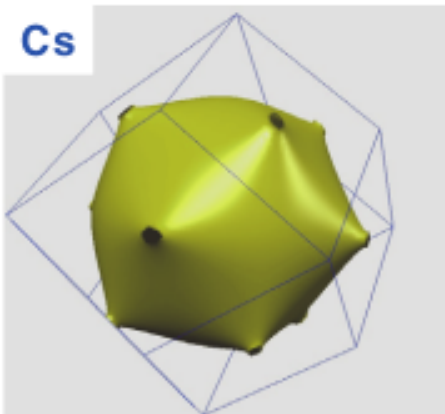
K



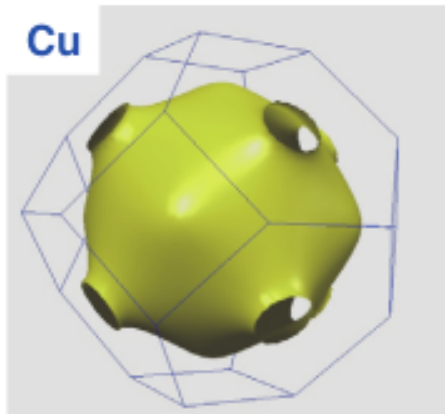
Rb



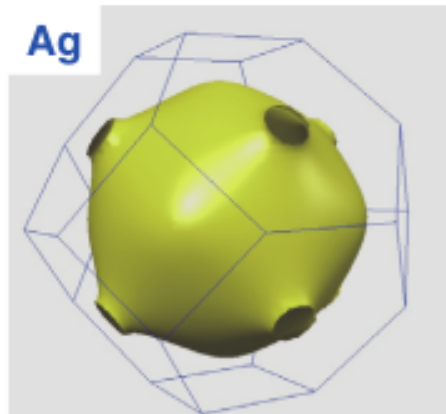
Cs



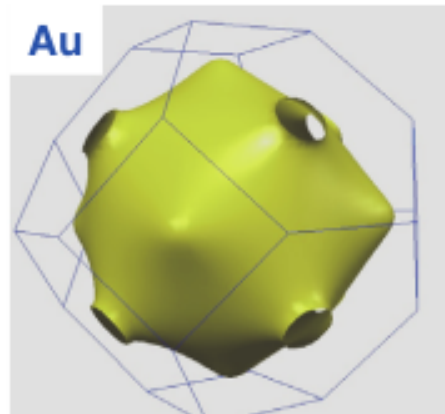
Cu



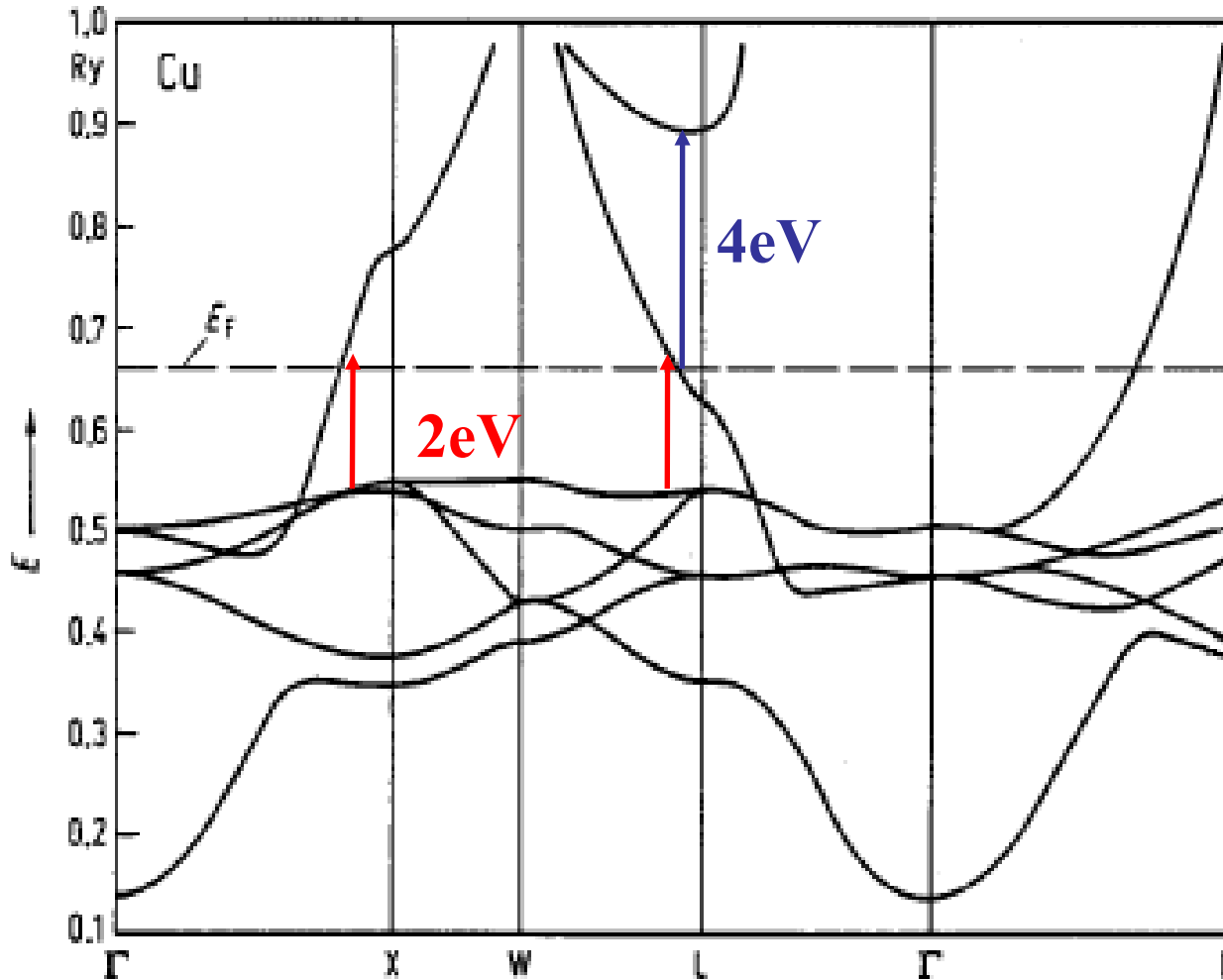
Ag



Au



# Estructura de bandas del Cobre



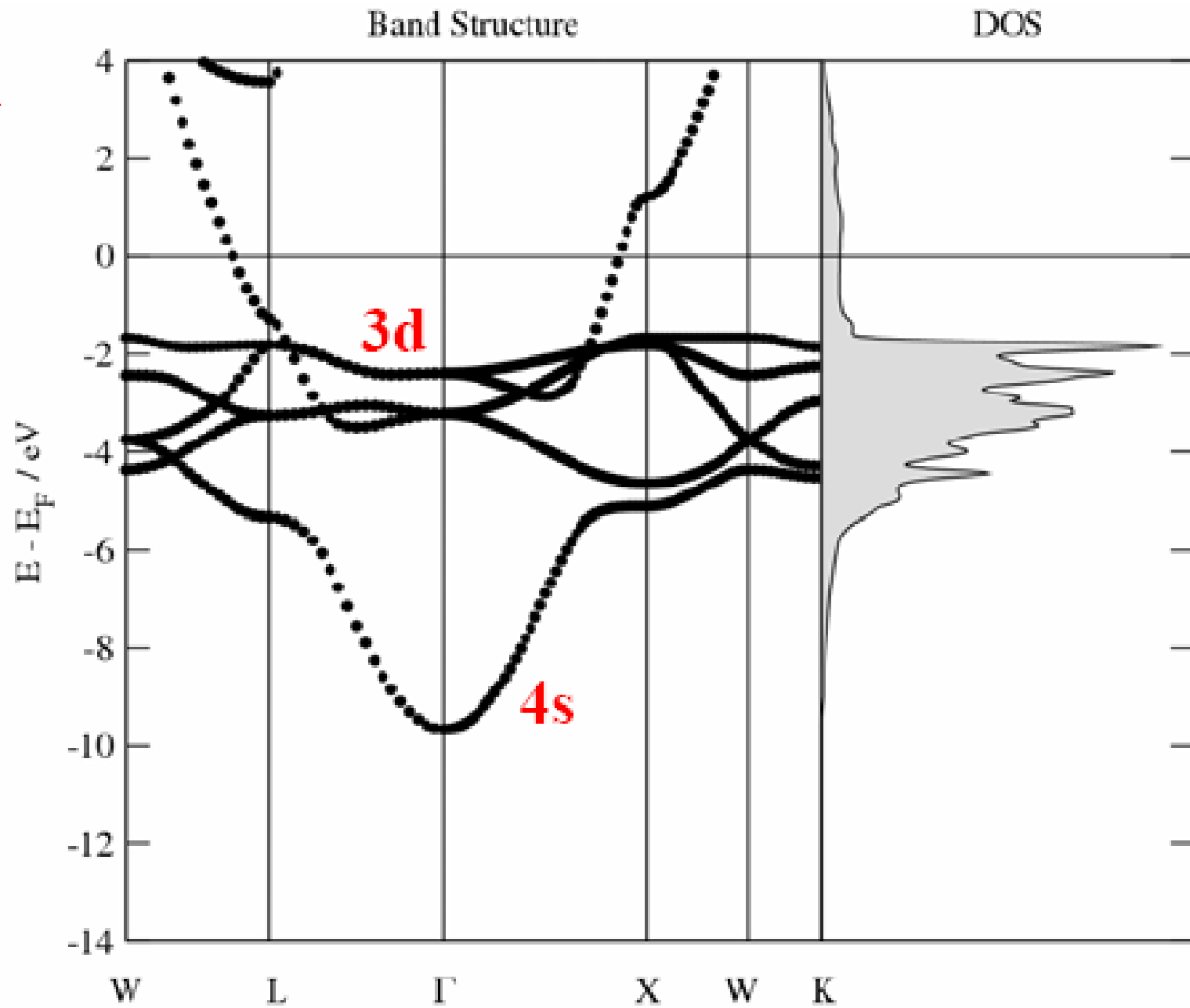
Bandas chatas  
provenientes de  
los orbitales 3d

$3d^{10} 4s^1$

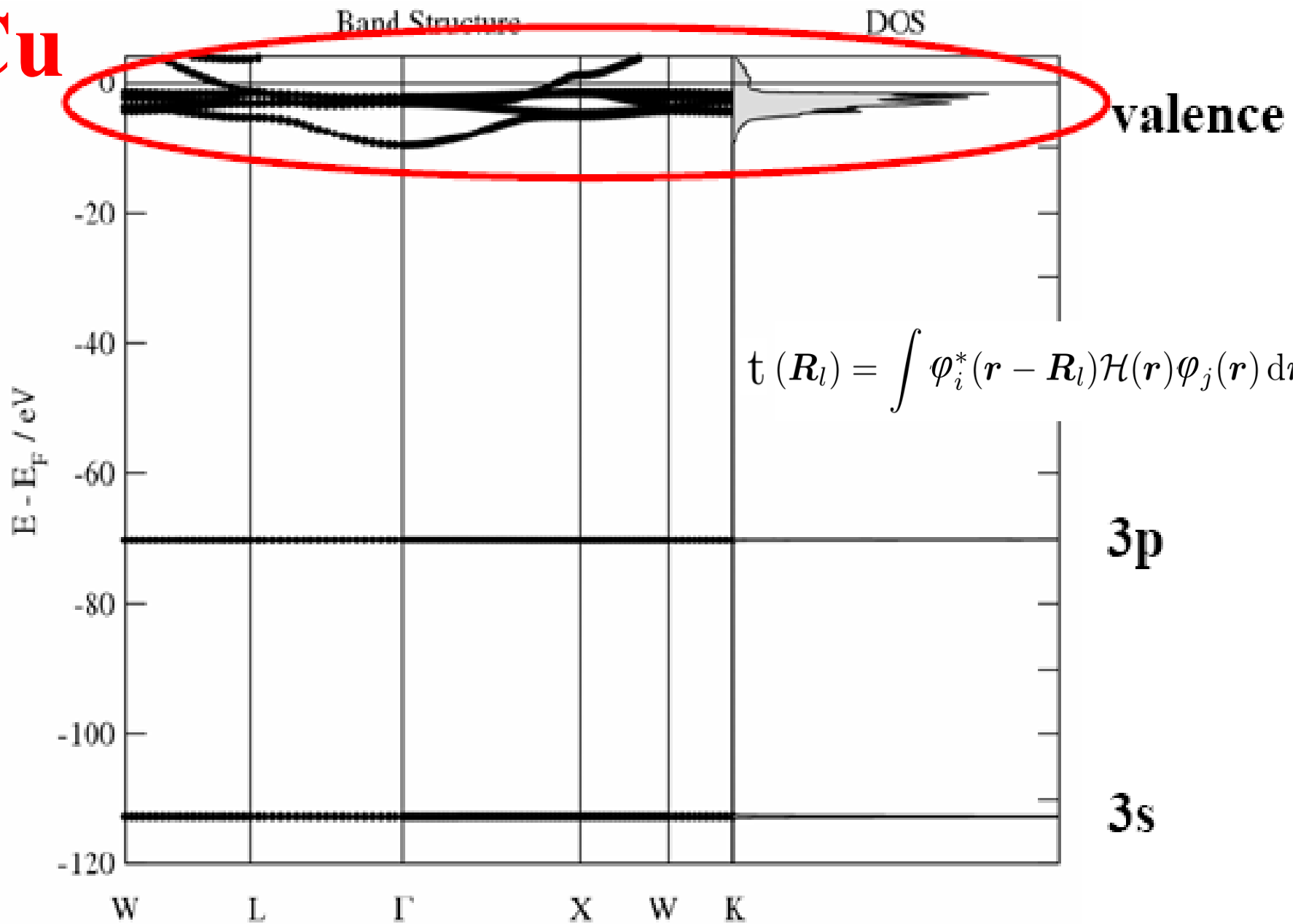
valence

Transiciones verticales  $K_{\perp} \ll \pi/a$

# Cu



# Cu



## Divalentes

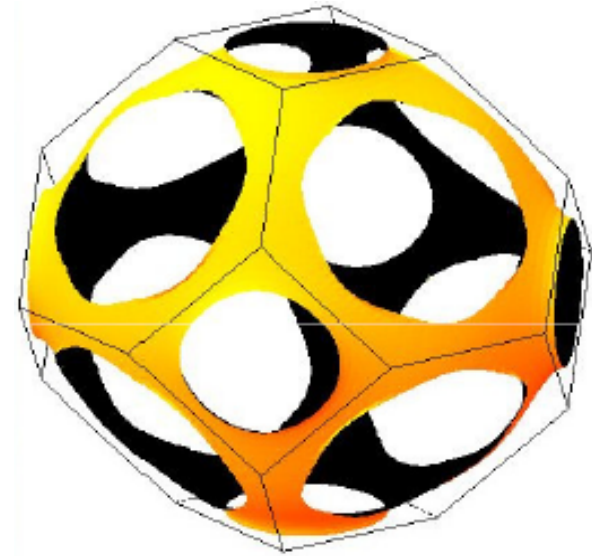
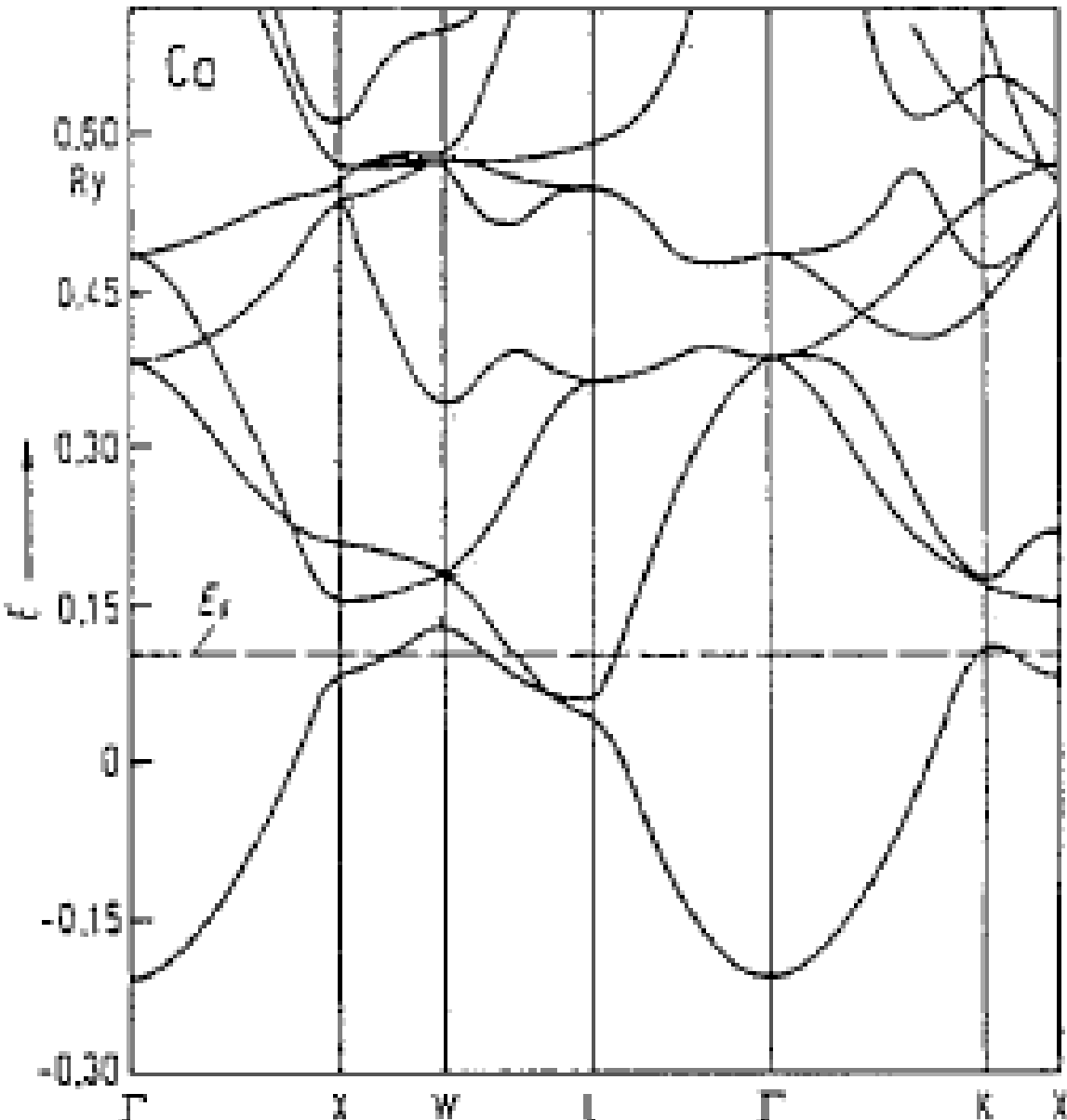
Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Be	$1s^2 2s^2$	hcp			
Mg	[Ne] $3s^2$	hcp			
Ca	[Ar] $4s^2$	fcc	Zn	[Ar] $3d^{10} 4s^2$	hcp
Sr	[Kr] $5s^2$	fcc	Cd	[Kr] $4d^{10} 5s^2$	hcp
Ba	[Xe] $6s^2$	bcc	Hg	[Xe] $4f^{14} 5d^{10} 6s^2$	rhombohedral

$$\text{bcc} \quad k_F = 0.782 (2\pi/a) > \overline{\Gamma N}$$

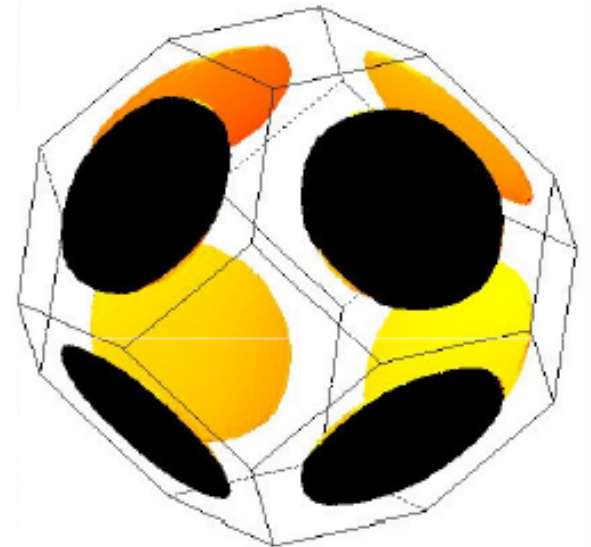
$$\text{fcc} \quad k_F = 0.985 (2\pi/a) > \overline{\Gamma L}$$

Las superficies de Fermi se extienden más allá de la 1ZB

# Ca (fcc)

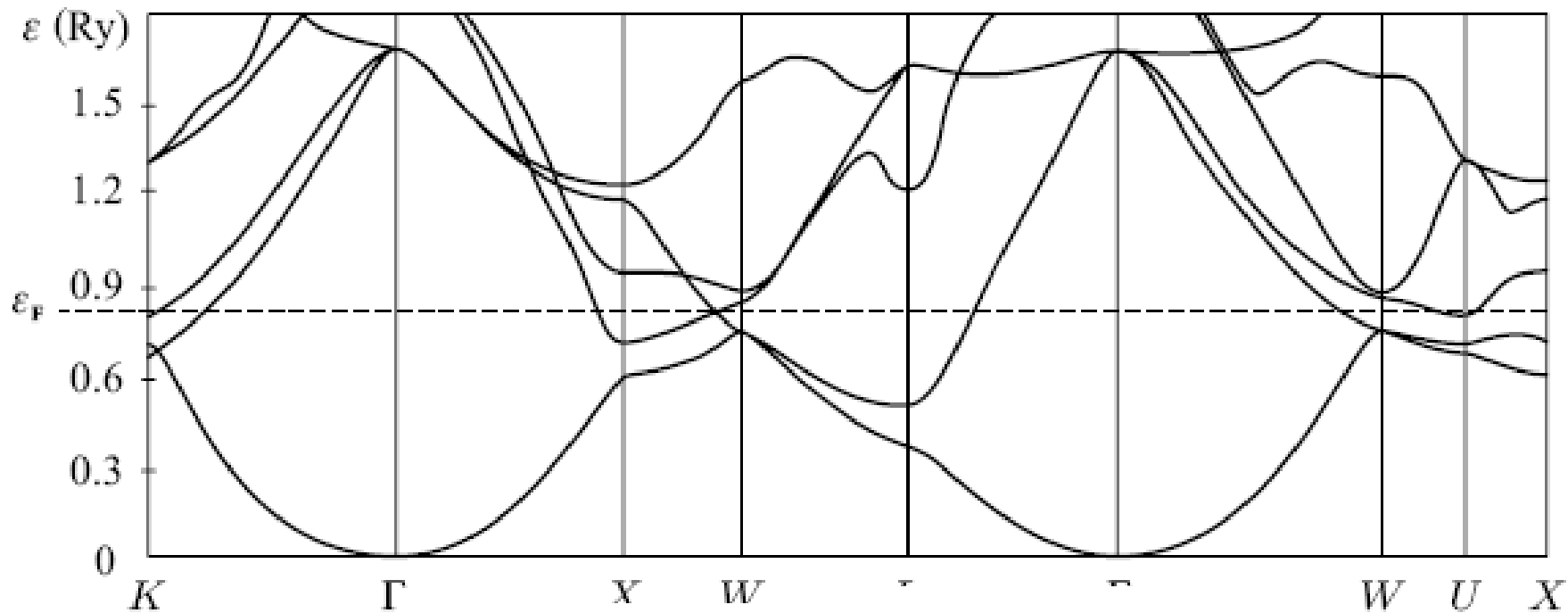


1<sup>st</sup> band

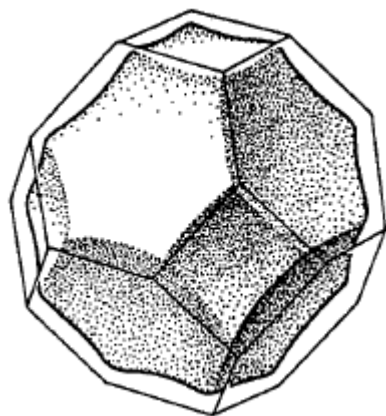


# Trivalentes

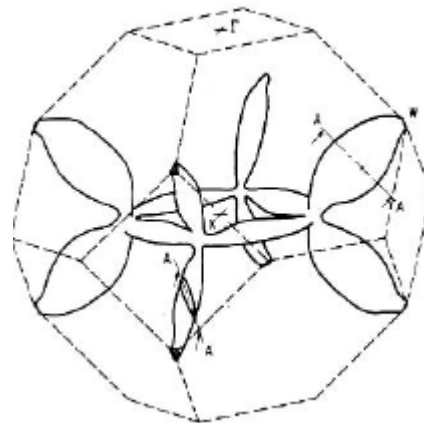
# Aluminio



$n=2$



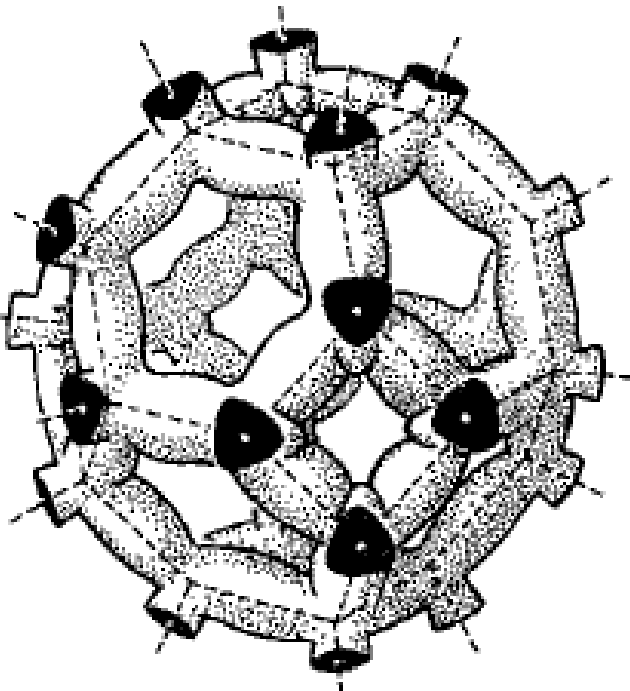
$n=3$



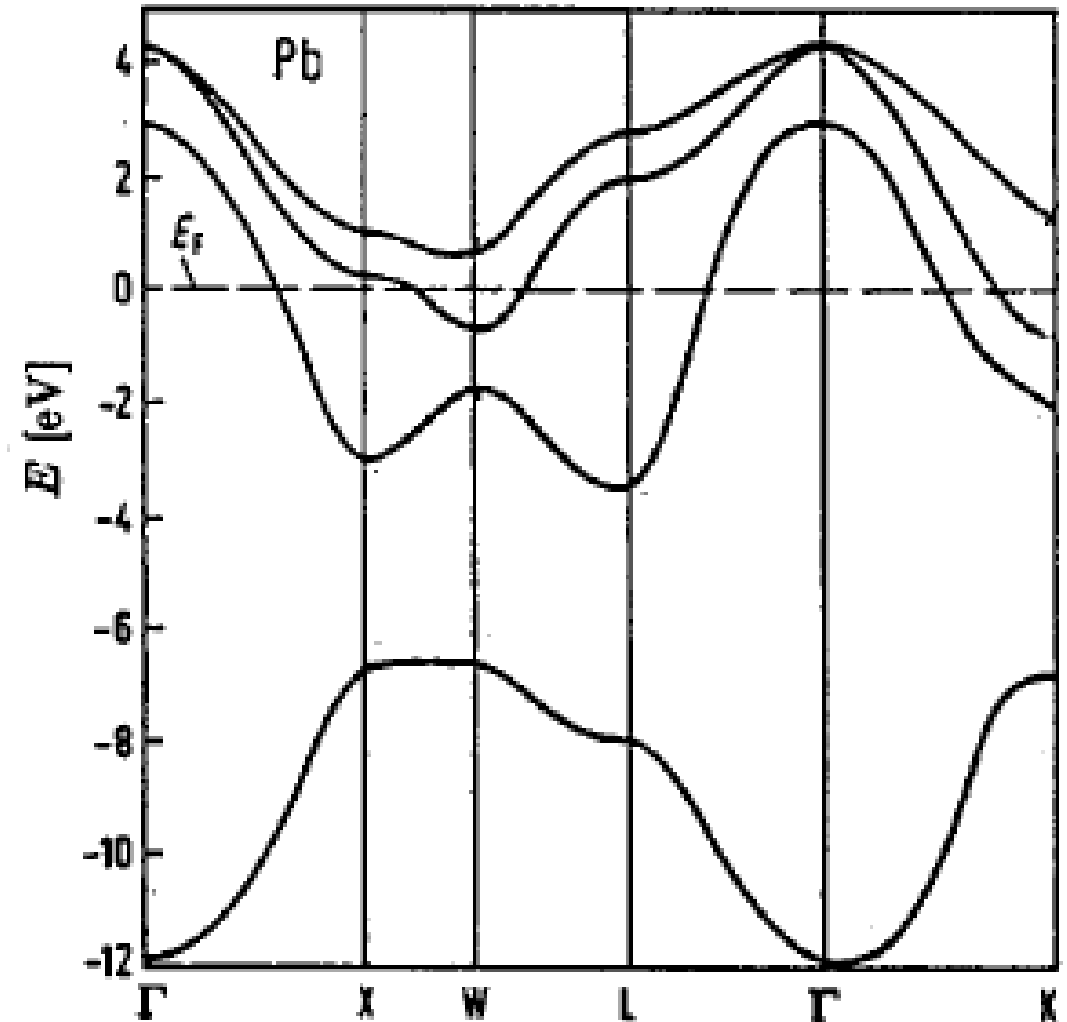


# Tetravalentes

Pb: [Xe] 4f<sup>14</sup> 5d<sup>10</sup> 6s<sup>2</sup> 6p<sup>2</sup>

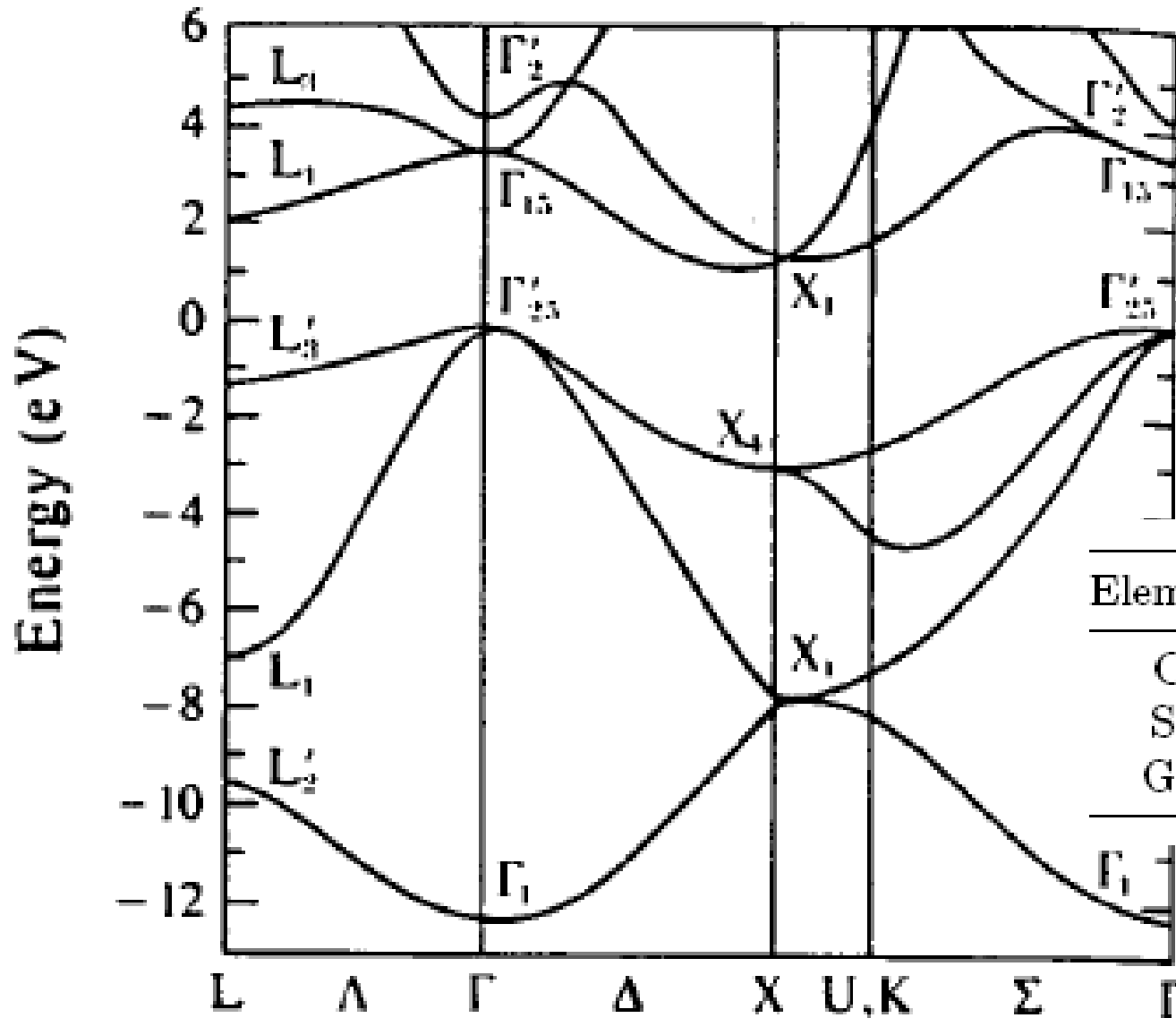


n=3



Si : [Ne] 3s<sup>2</sup> 3p<sup>2</sup>

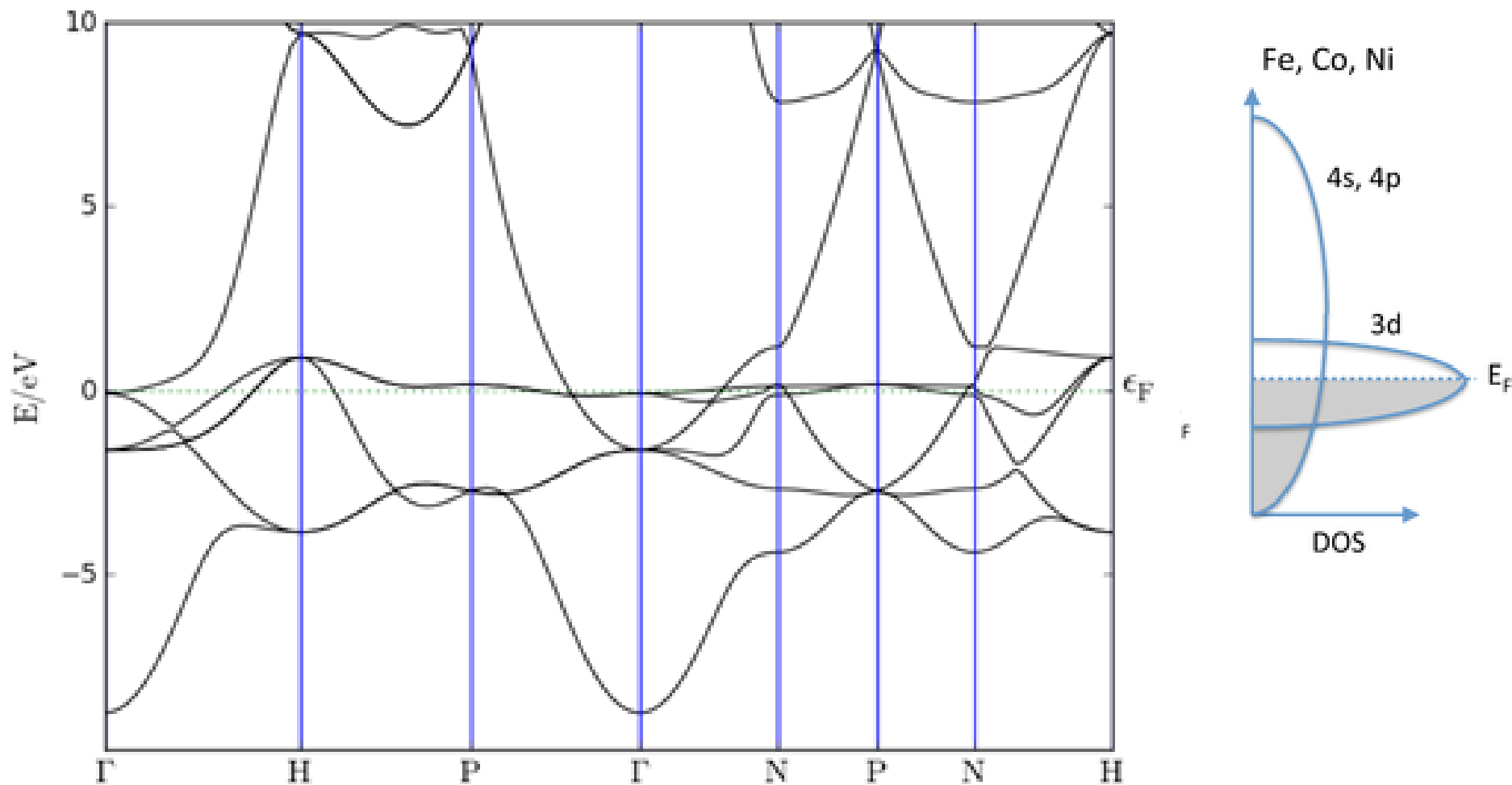
semiconductor

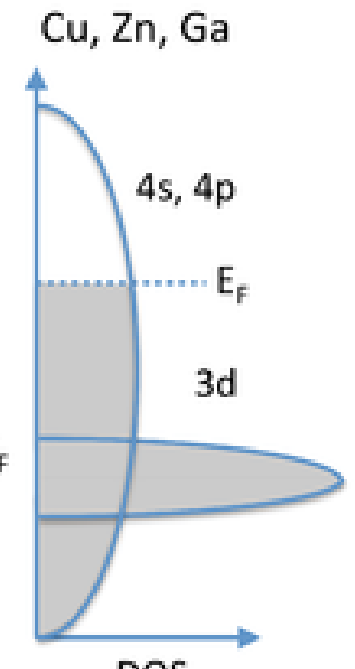
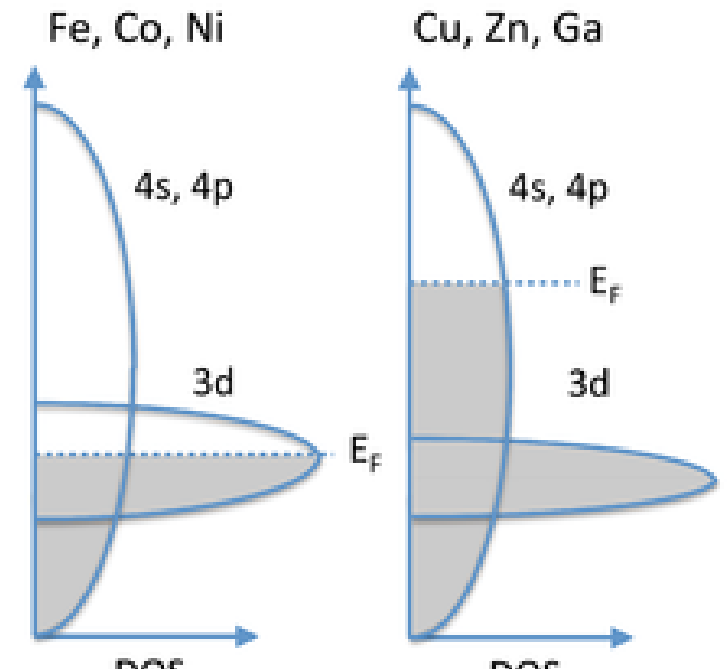
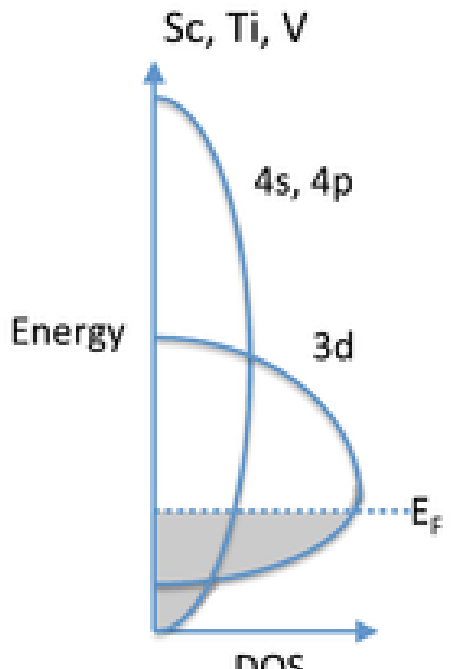
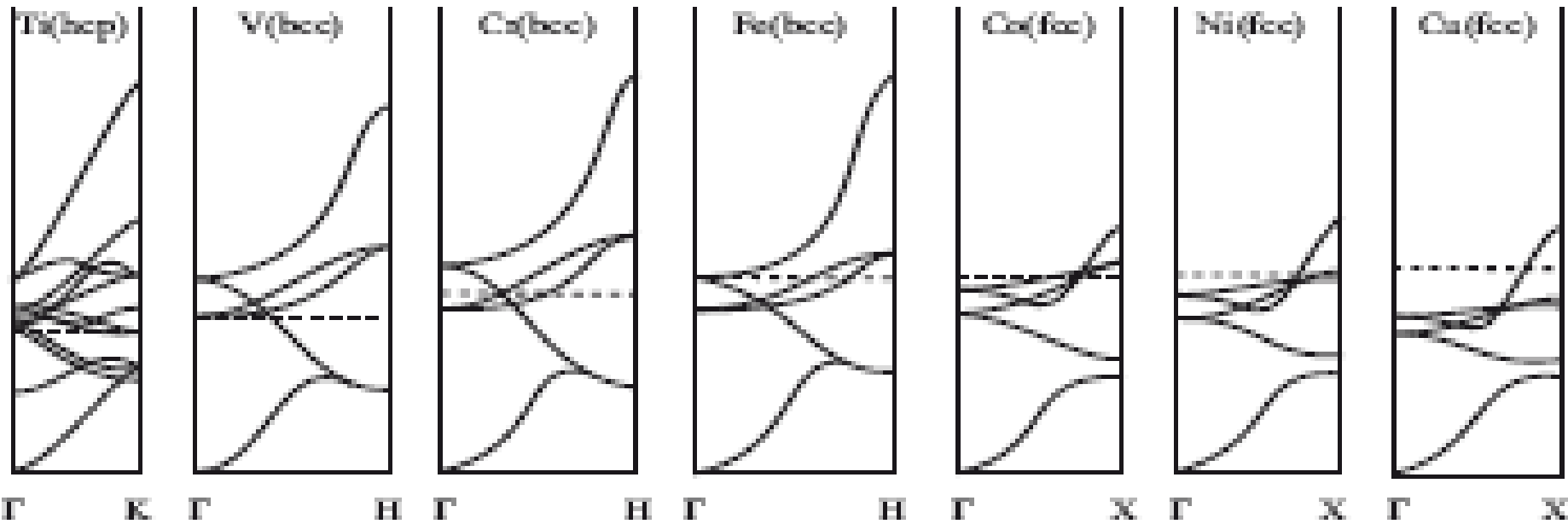


Element	$\epsilon_g(300\text{ K})$ (eV)
C	5.48
Si	1.110
Ge	0.664

# Metales de transición

**Fe: [Ar] 3d<sup>6</sup>4s<sup>2</sup>**



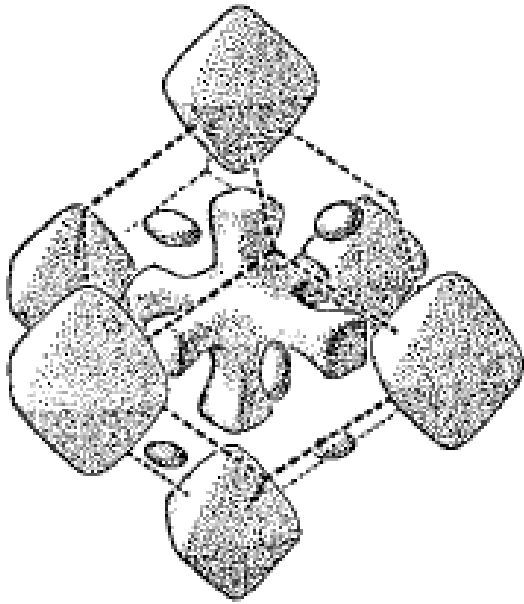


$$C_v = \gamma T$$

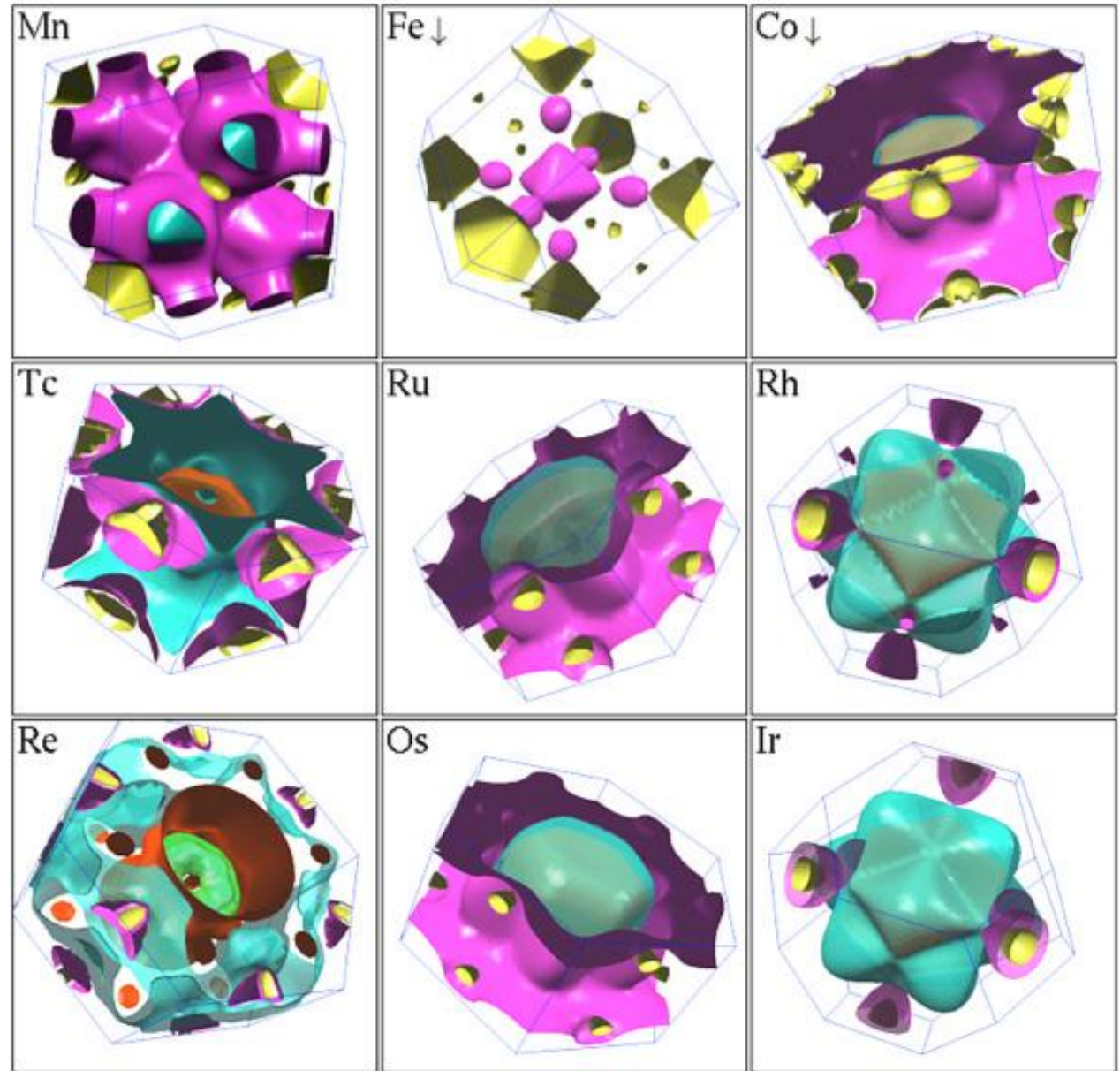
$$\gamma \sim g(E_F)$$

**Na**  
 $\gamma = 3.5 \cdot 10^{-4} \text{ cal/mol K}^2$

**Mn**  
 $\gamma = 40 \cdot 10^{-4} \text{ cal/mol K}^2$

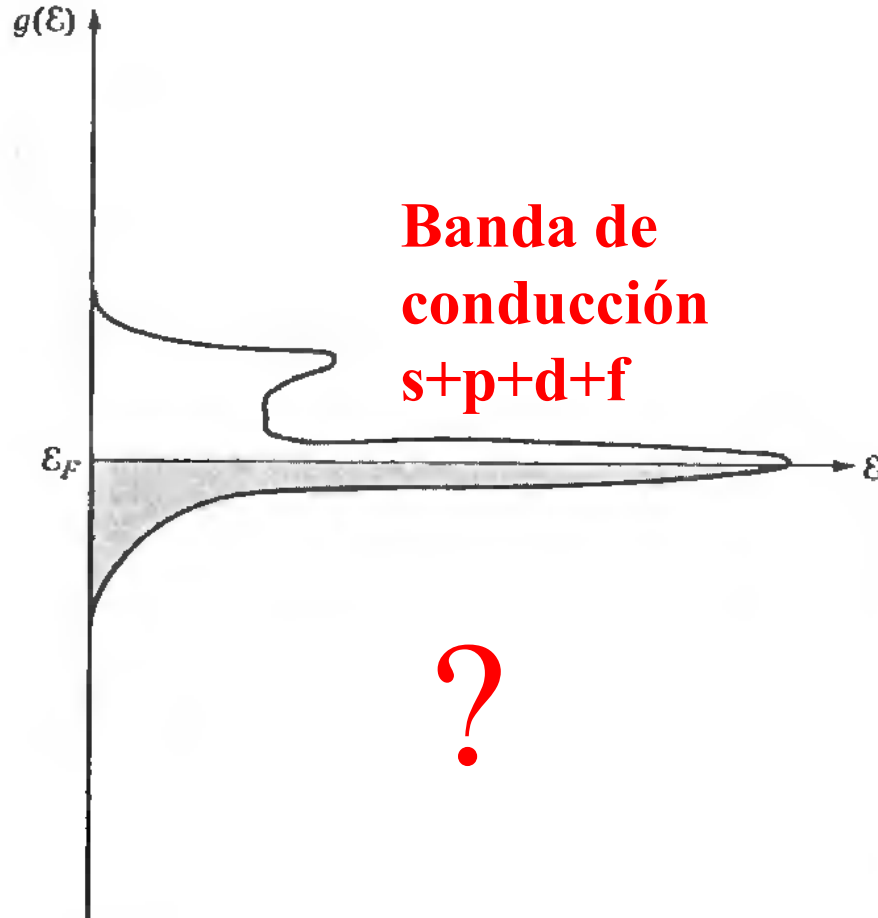


Superficie de Fermi del W



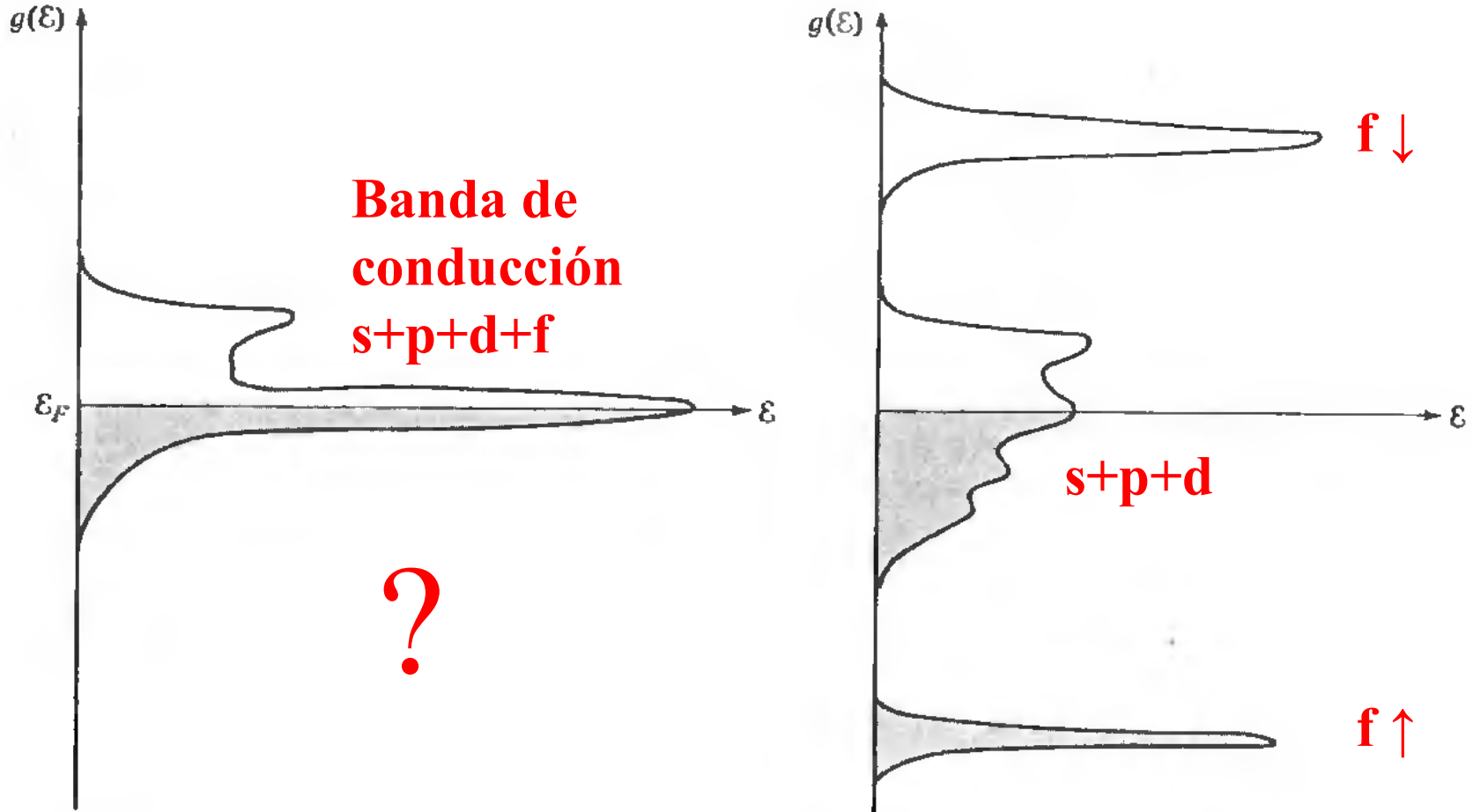
## Tierras raras

Los electrones “d” de un metal de transición se hibridizan con los “s” y “p” formando la banda de conducción.



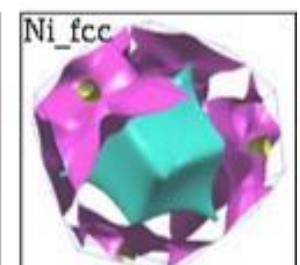
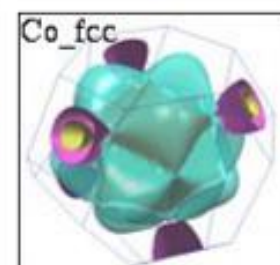
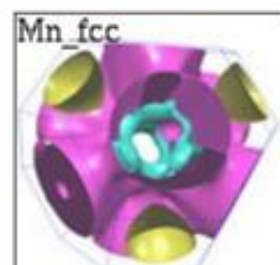
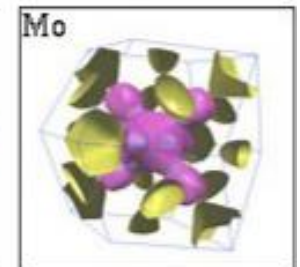
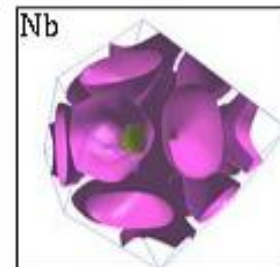
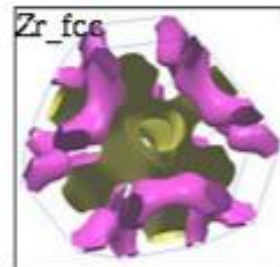
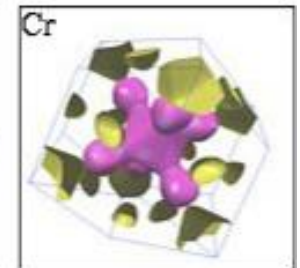
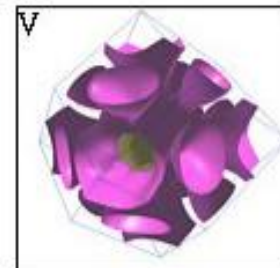
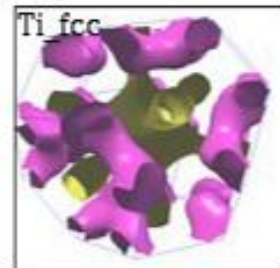
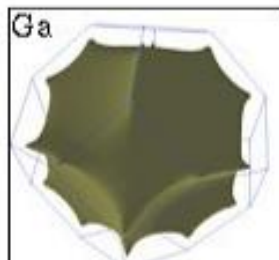
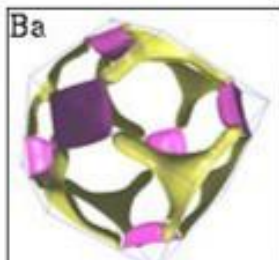
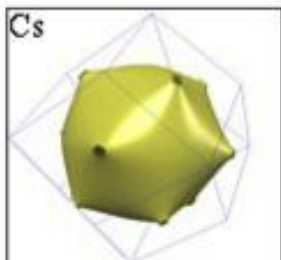
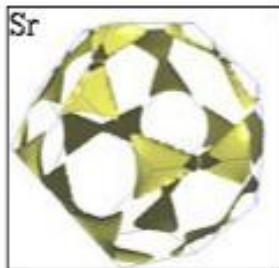
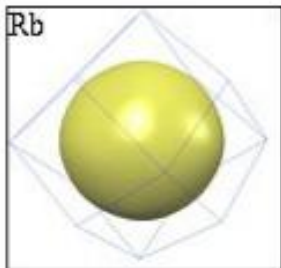
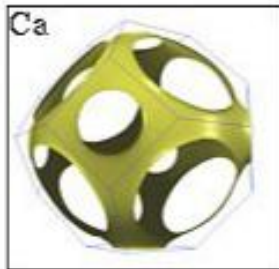
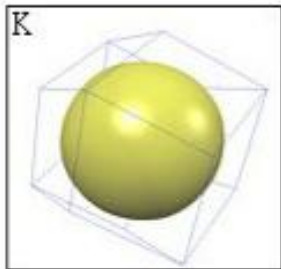
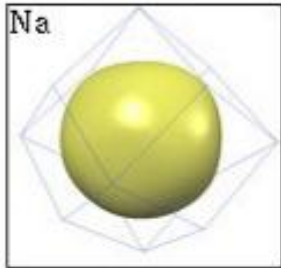
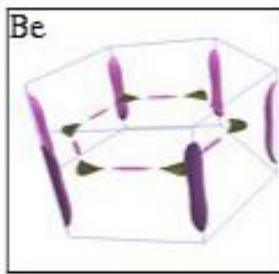
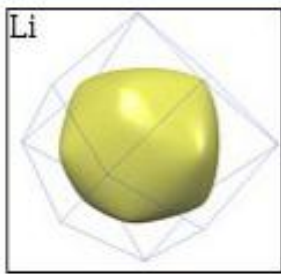
## Tierras raras

Los electrones “d” de un metal de transición se hibridizan con los “s” y “p” formando la banda de conducción.



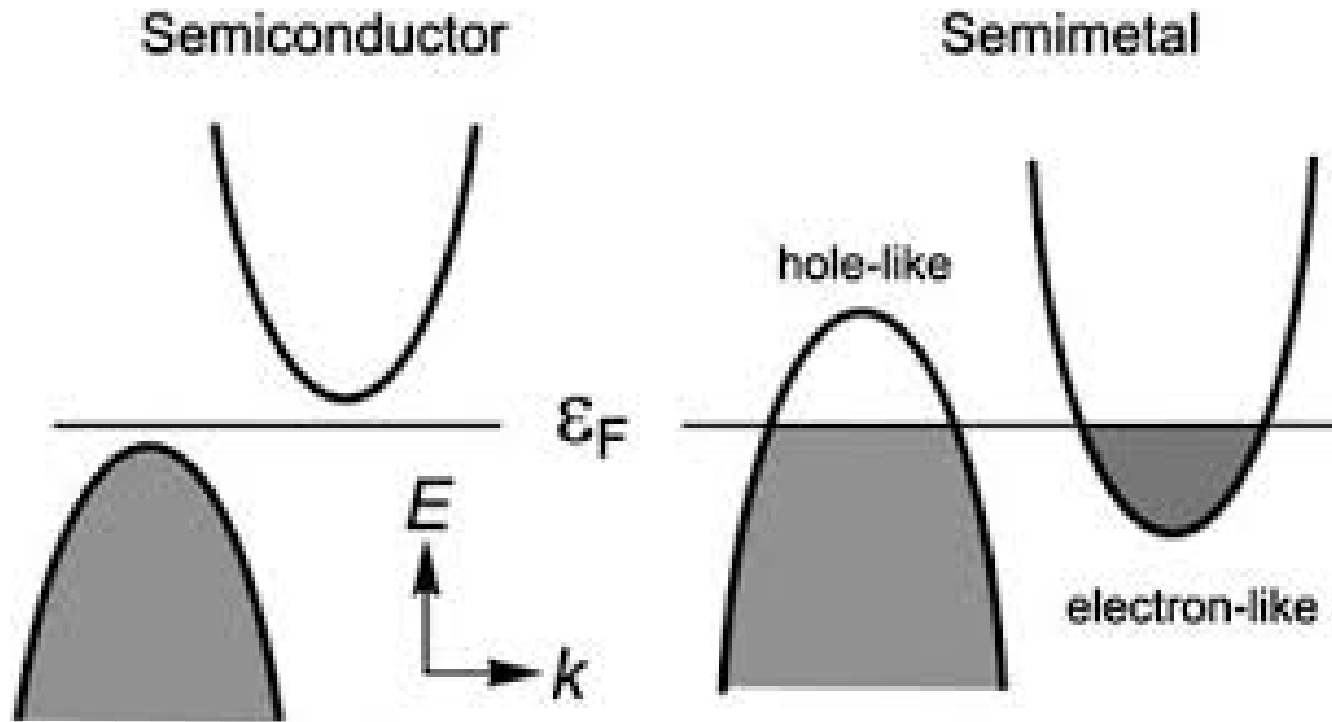
La aproximación de electrones independientes no es válida. Hay que considerar la repulsión coulombiana de los electrones f.

<http://www.phys.ufl.edu/fermisurface/>





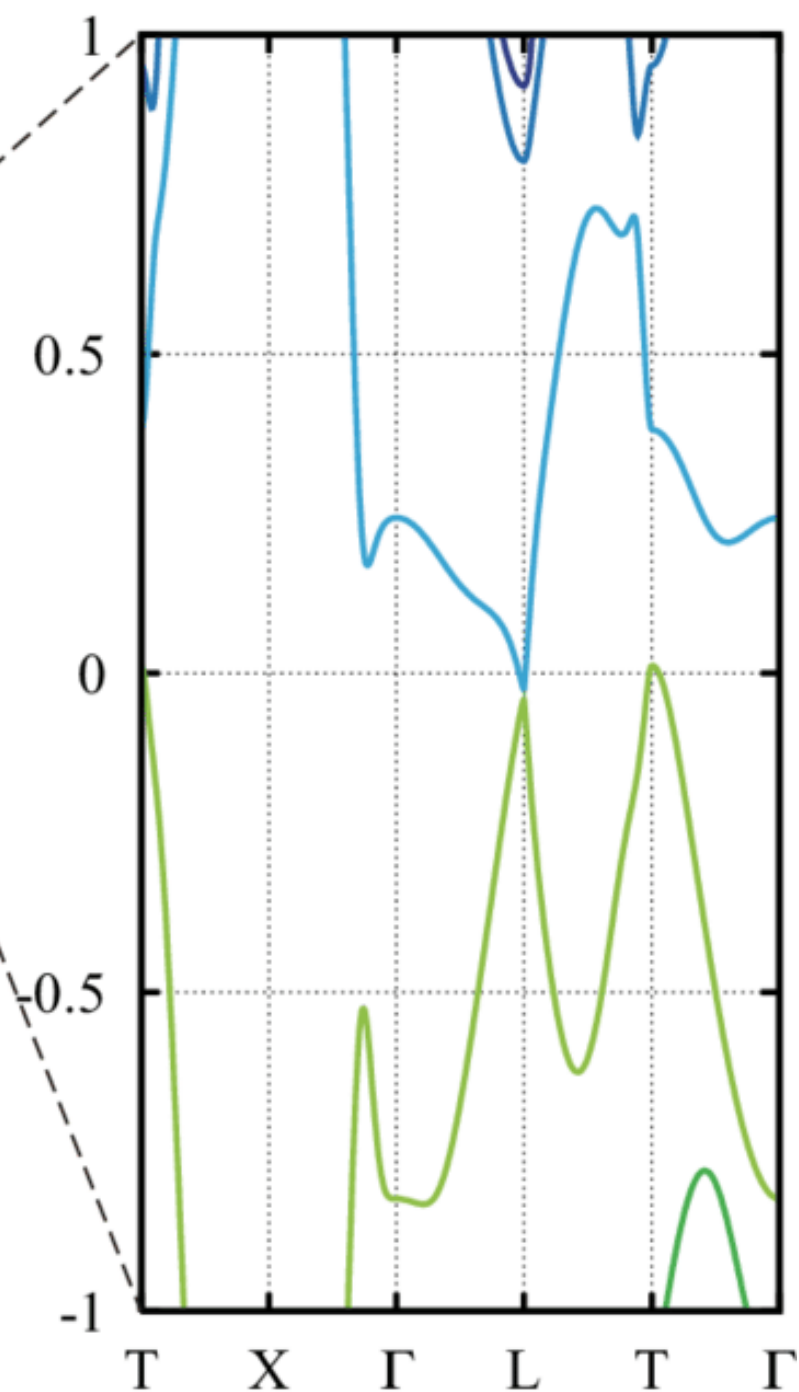
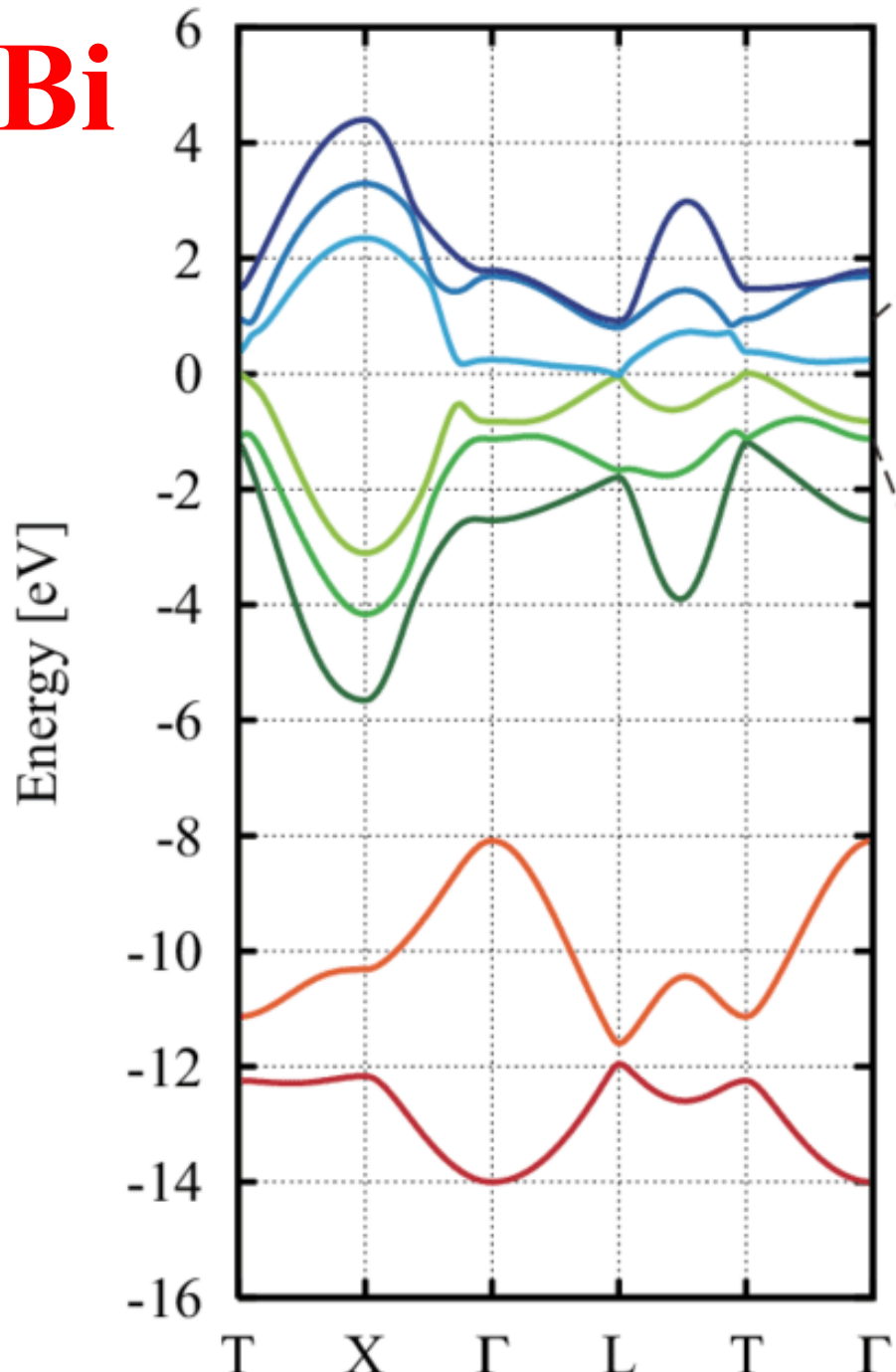
# Semimetales



Ej.: Bi, Grafito

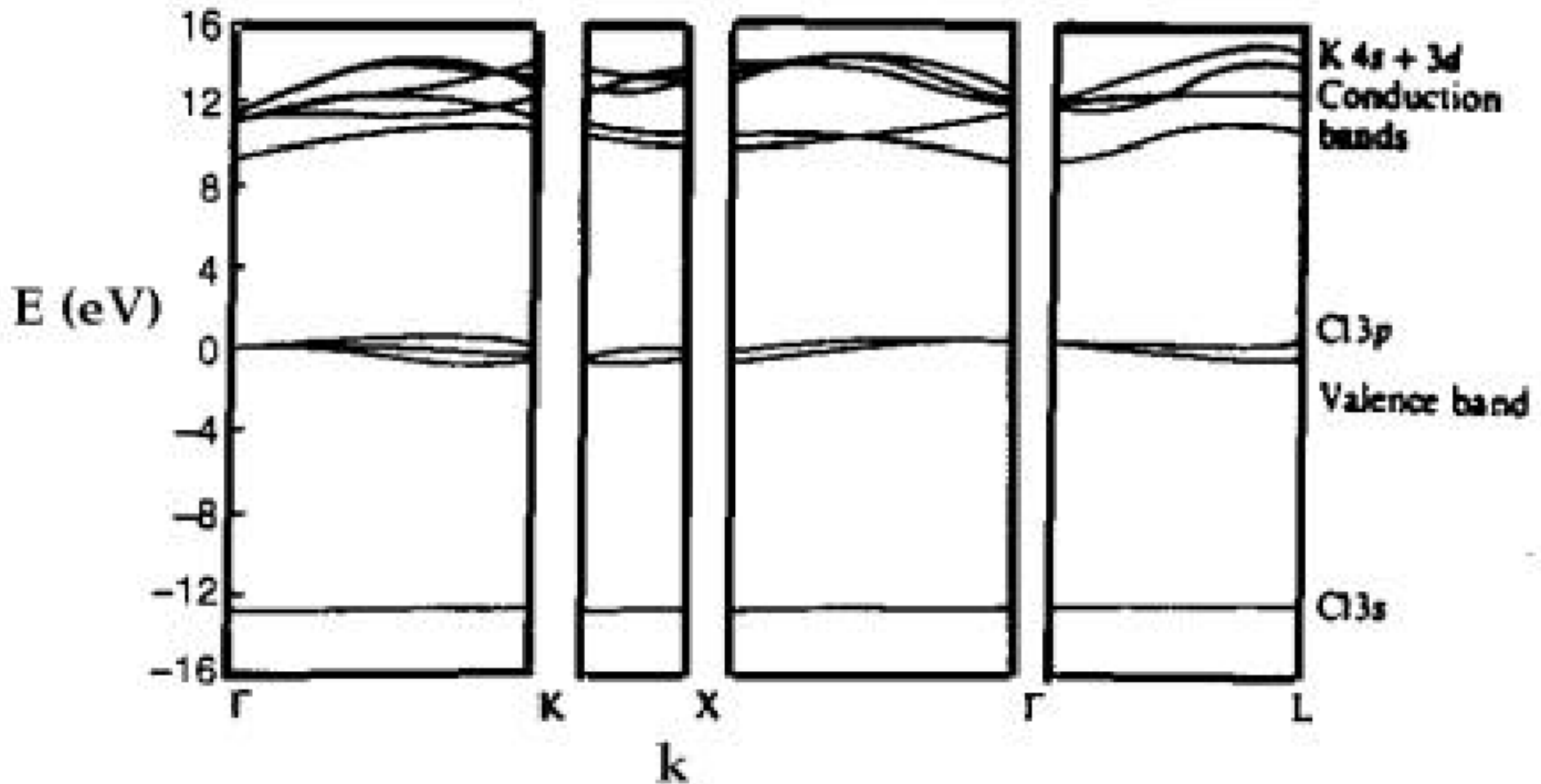
Number of carrier  $\ll 10^{22}/\text{cm}^3$

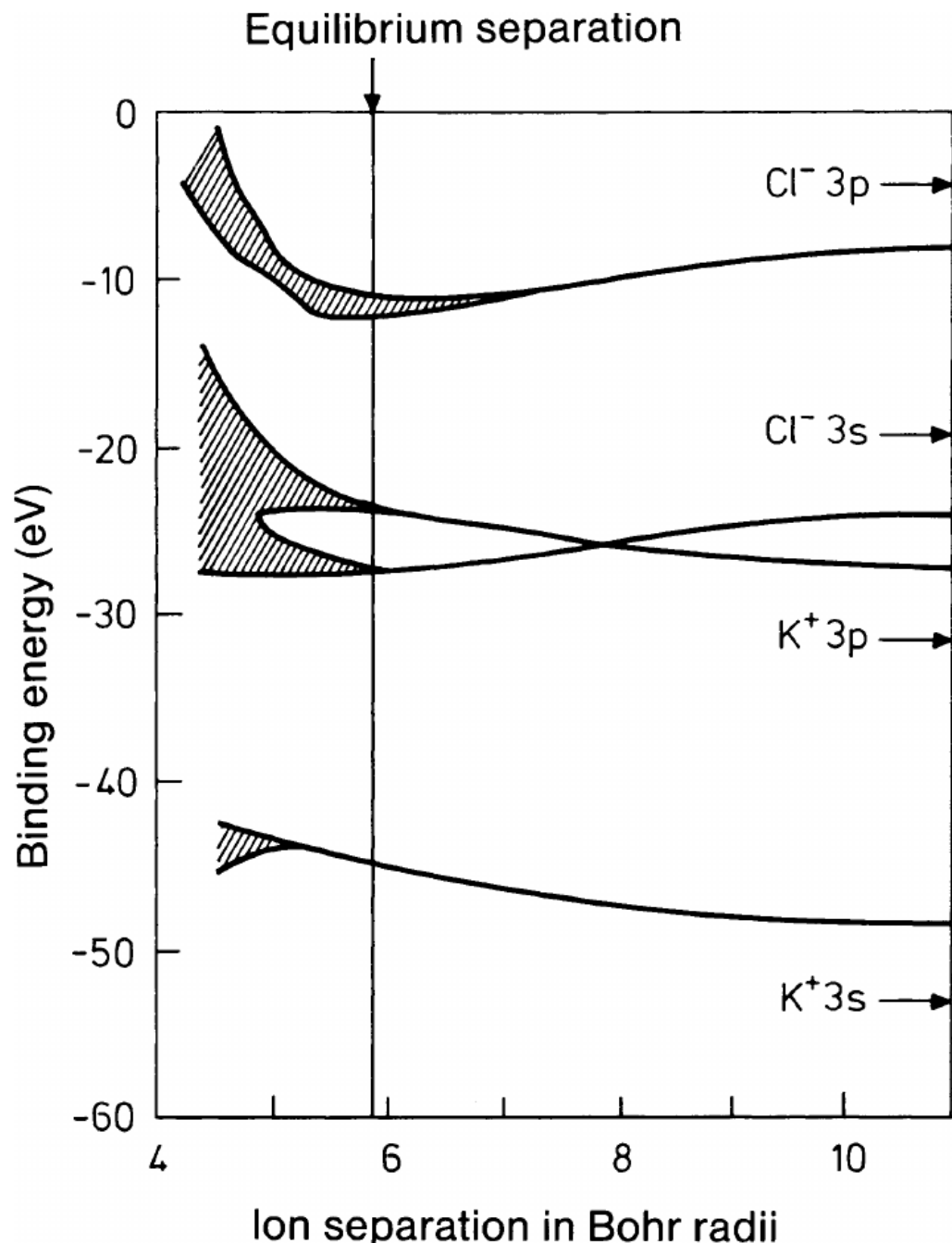
**Bi**



# Algunos compuestos binarios

KCl

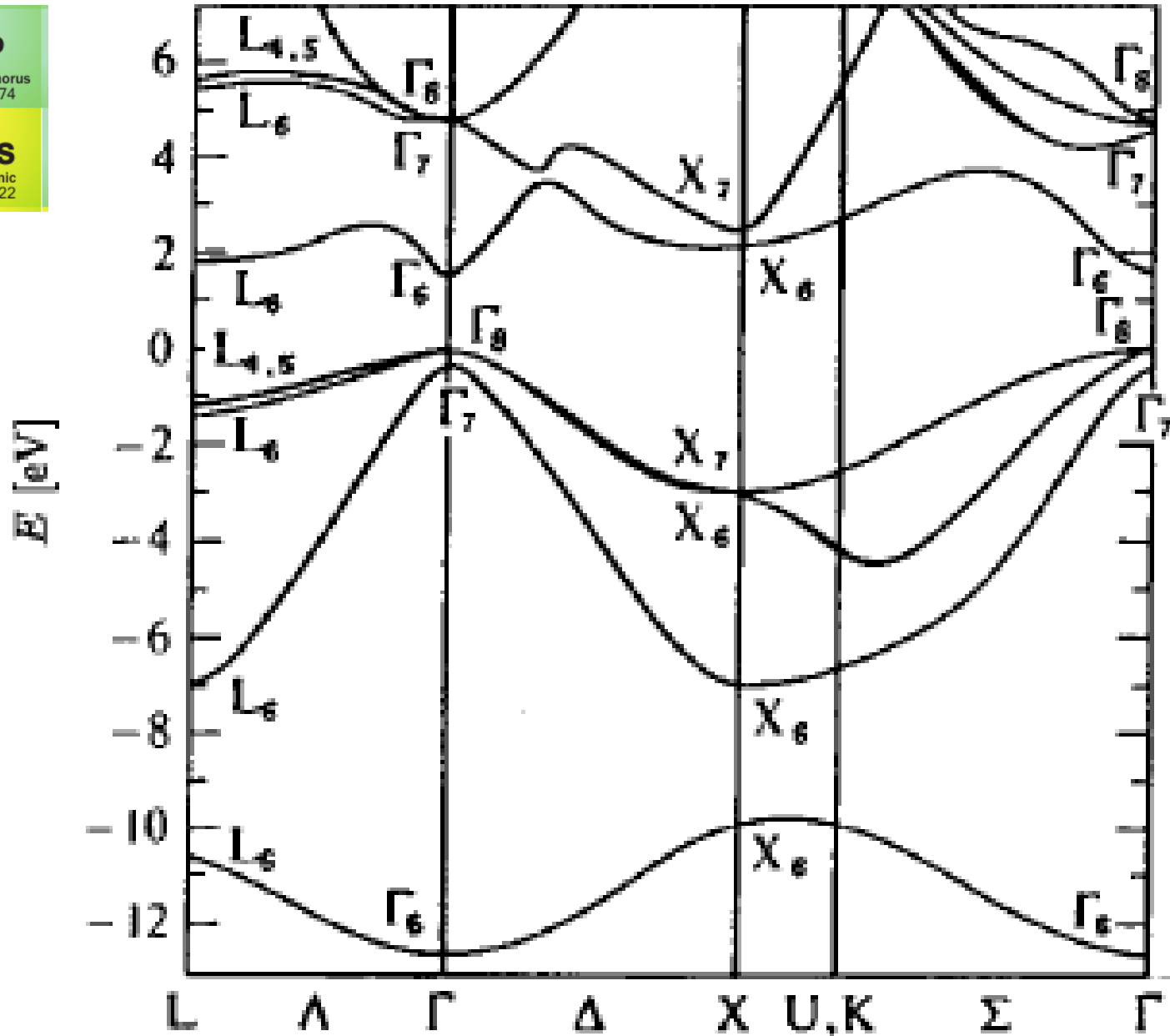




Compound	$\epsilon_g$ (eV)	Compound	$\epsilon_g$ (eV)	Compound	$\epsilon_g$ (eV)
LiF	13.7	LiCl	9.4	LiBr	7.6
NaF	11.5	NaCl	8.7	NaBr	7.5
KF	10.8	KCl	8.4	KBr	7.4
RbF	10.3	RbCl	8.2	RbBr	7.4
CsF	9.9	CsCl	8.3	CsBr	7.3

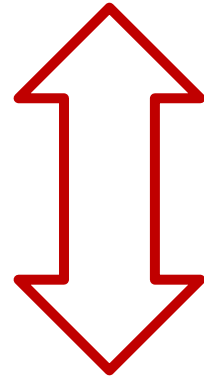
III-V compound	$\epsilon_g$ (eV)	II-VI compound	$\epsilon_g$ (eV)	I-VII compound	$\epsilon_g$ (eV)
AlSb	1.63	ZnO	3.20	AgF	2.8
GaP	2.27	ZnS	3.56	AgCl	3.25
GaAs	1.43	ZnSe	2.67	AgBr	2.68
GaSb	0.71	CdS	2.50	AgI	3.02
InP	1.26	CdSe	1.75	CuCl	3.39
InAs	0.36	CdTe	1.43	CuBr	3.07
InSb	0.18	HgS	2.27	CuI	3.11

13 <b>Al</b> Aluminum 26.982	14 <b>Si</b> Silicon 28.086	15 <b>P</b> Phosphorus 30.974
31 <b>Ga</b> Gallium 69.732	32 <b>Ge</b> Germanium 72.61	33 <b>As</b> Arsenic 74.922



GaAs

**Métodos ab-initio  
o de primeros principios**



**Métodos autoconsistentes**

**Teoría de la  
funcional densidad  
(DFT)**

**Hartree- Fock**

# Ya vimos la aproximación de Hartree

$$H\Psi = \sum_{i=1}^N \left( -\frac{\hbar^2}{2m} \nabla_i^2 \Psi - Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r}_i - \mathbf{R}|} \Psi \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \Psi = E\Psi.$$



**aprox.**

$$V_{\mathbf{N}}(\mathbf{r}) = -Ze^2 \sum_{\mathbf{R}} \frac{1}{|\mathbf{r} - \mathbf{R}|}. \quad V_{\mathbf{H}}(\mathbf{r}) = -e \int d\mathbf{r}' \rho(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|}.$$

llamando  $V_{\text{eff}}(\mathbf{r}) = V_{\mathbf{H}}(\mathbf{r}) + V_{\mathbf{N}}(\mathbf{r})$

$$\boxed{-\frac{\hbar^2}{8\pi^2 m} \nabla^2 \Psi_j(\mathbf{r}) + V_{\text{eff}}(\mathbf{r}) \Psi_j(\mathbf{r}) = \epsilon_j \Psi_j(\mathbf{r})}$$

donde  $\rho(\mathbf{r}) = \sum_{i \text{ occupied}} \Psi_j(\mathbf{r}) \Psi_j^*(\mathbf{r})$



# Density Functional Theory (Kohn y Sham 1965)

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{eff}(r) \right\} \Psi_i(r) = E_i \Psi_i(r)$$

$$V_{eff}(r) = V_{ion}(r) + V_H(r) + V_{XC}(r)$$

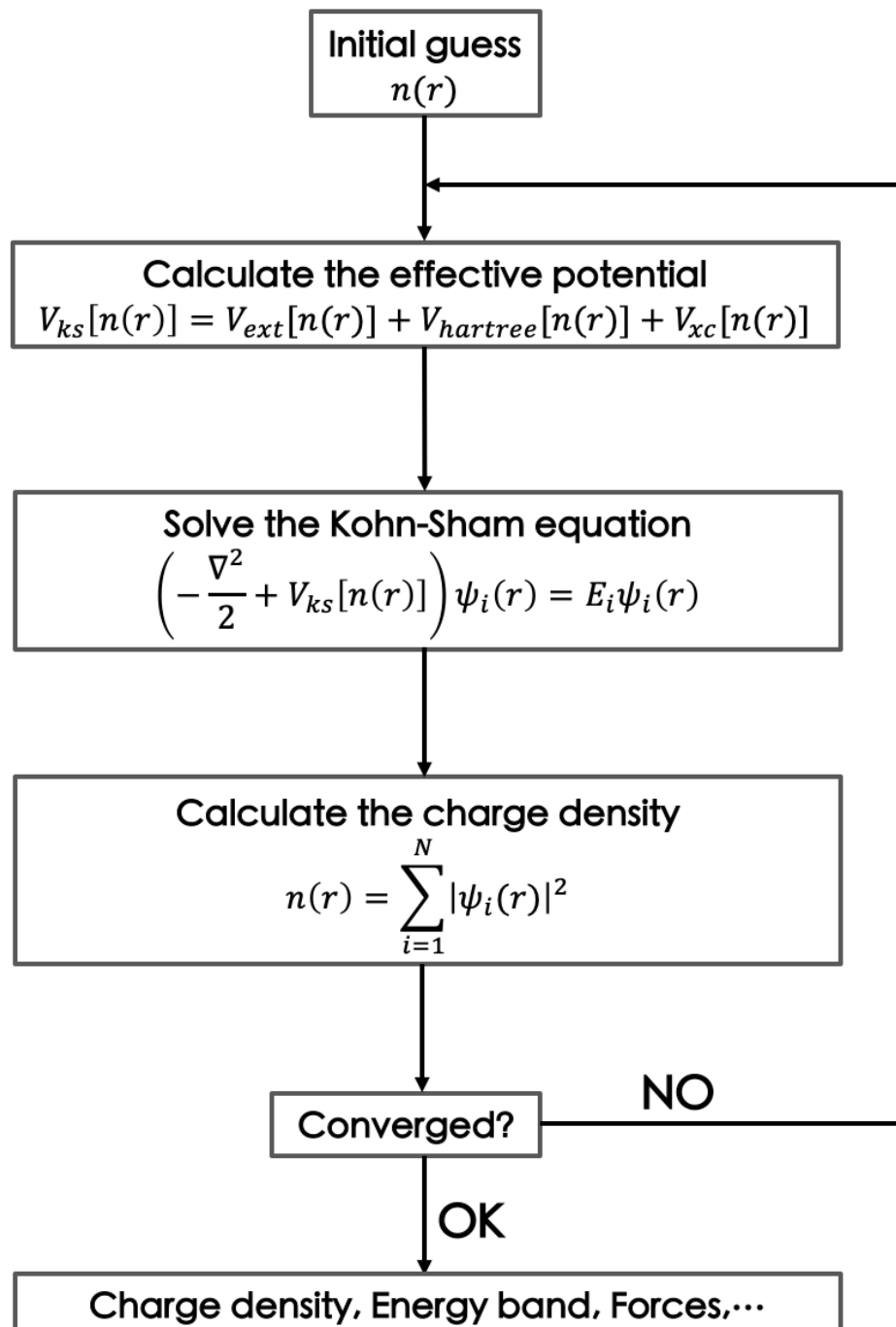
$V_{XC}(r)$  Potencial de intercambio y correlación

→ **LDA**  $E_{XC}^{LDA}[n] = \int \epsilon_{XC}(n)n(\vec{r})d^3r.$

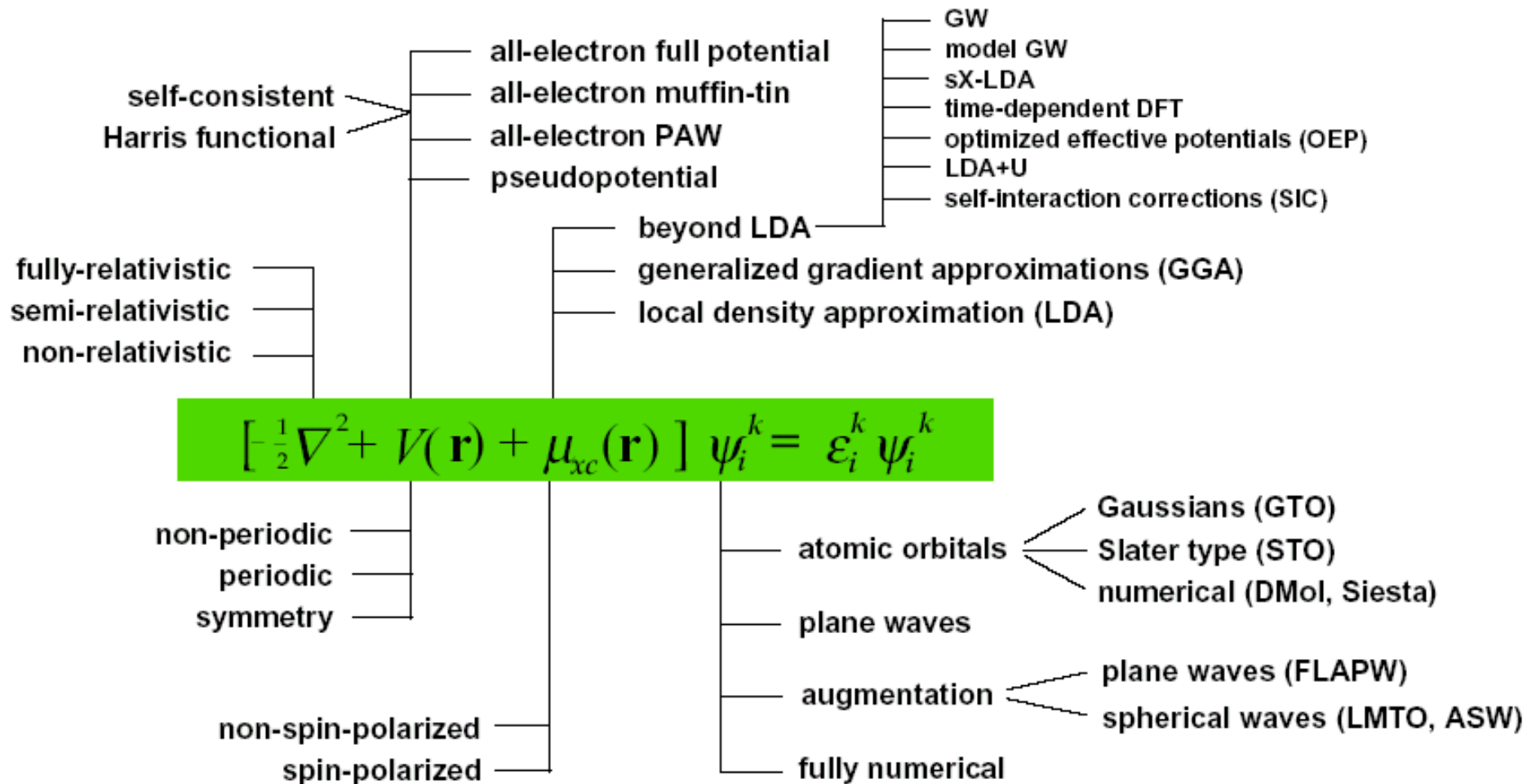
→ **GGA**  $E_{XC}^{GGA}[n_{\uparrow}, n_{\downarrow}] = \int \epsilon_{XC}(n_{\uparrow}, n_{\downarrow}, \vec{\nabla}n_{\uparrow}, \vec{\nabla}n_{\downarrow})n(\vec{r})d^3r.$

**Energía del estado fundamental :**

$$E_G[\rho(r)] = T[\rho(r)] + \int \rho(r)V_N(r) dr + \frac{1}{2} \int \rho(r)V_H(r) dr + E_{XC}[\rho(r)]$$



# DFT Implementations

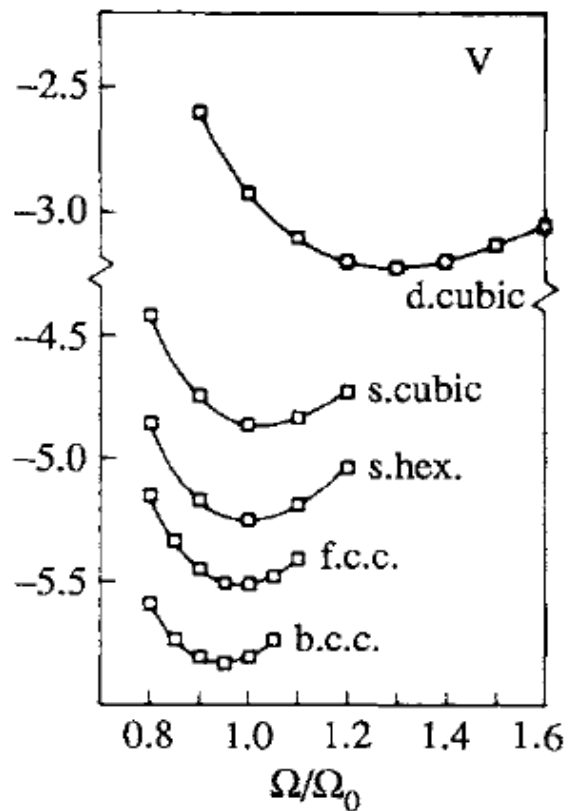
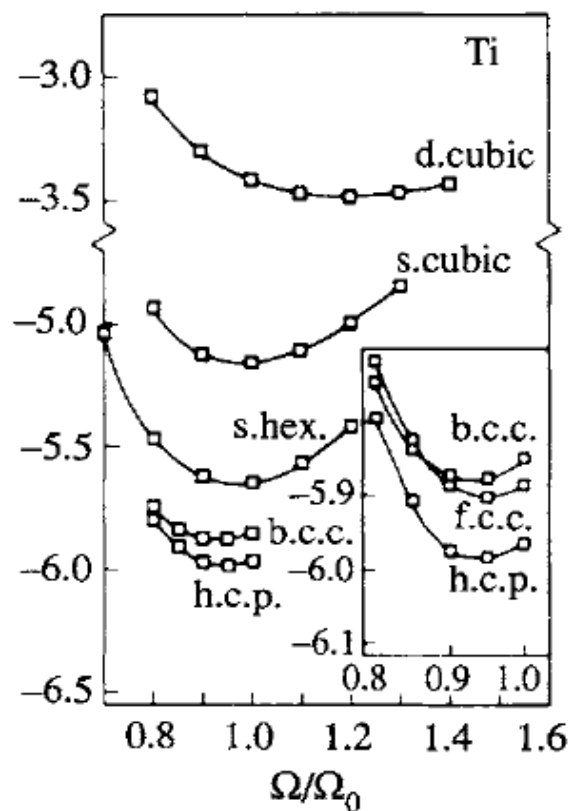
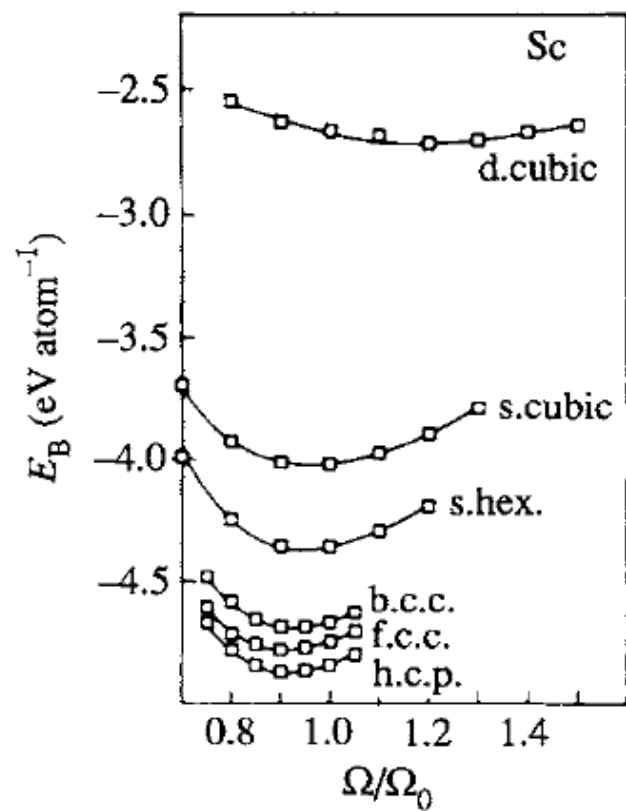


# Moléculas:

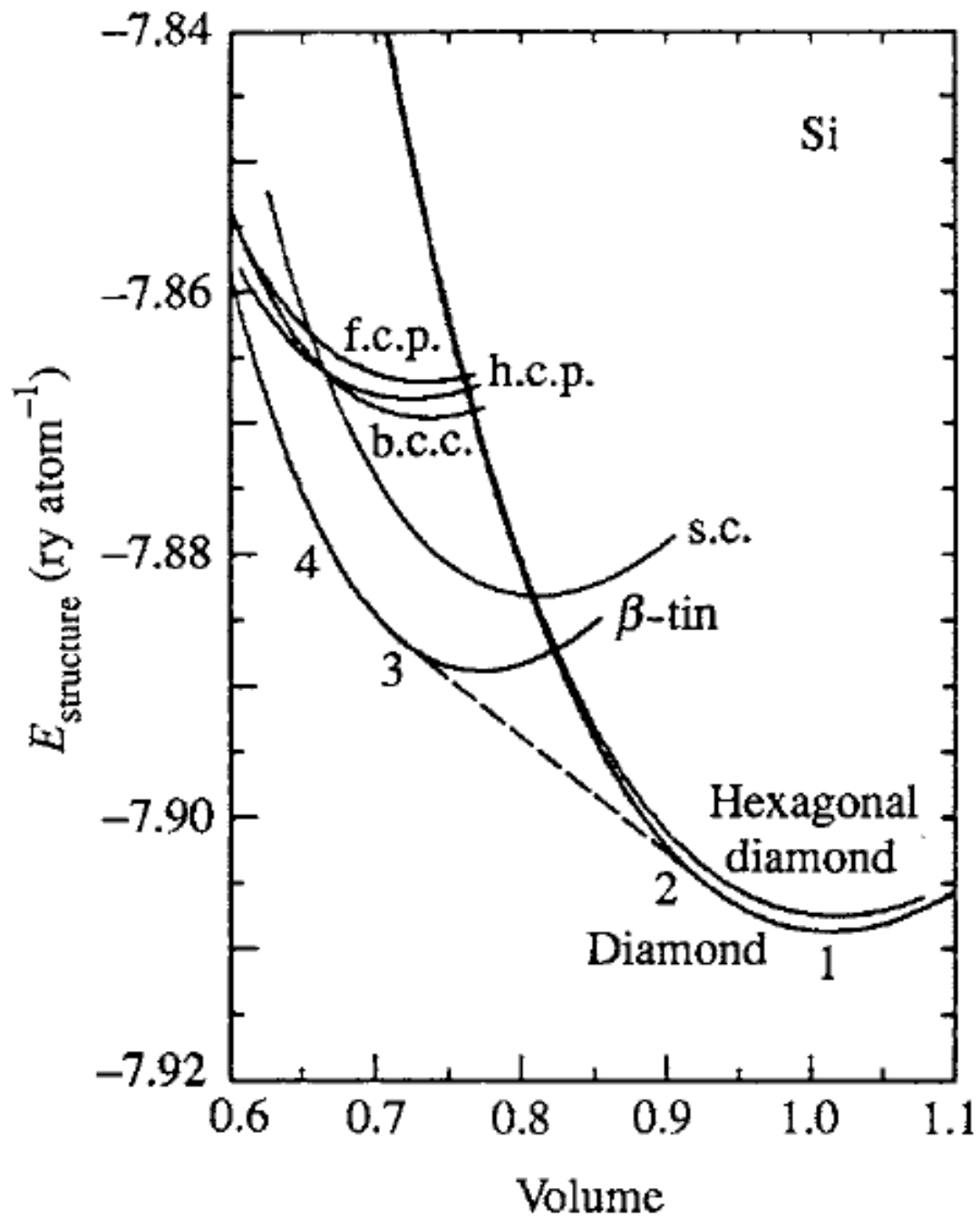
TABLE I. Equilibrium bond length  $R_0$  (Å) and atomization energy  $\Delta E$  (kcal/mol) of 19 covalent molecules.

Molecule	$R_0$				$\Delta E$			
	LDA	PBE	WC	Expt.	LDA	PBE	WC	Expt.
H <sub>2</sub>	0.764	0.749	0.754	0.741	113.5	104.8	104.2	109.5
LiH	1.601	1.602	1.605	1.595	67.7	60.1	59.4	57.8
CH <sub>4</sub>	1.096	1.095	1.094	1.087	462.7	420.3	426.3	419.3
NH <sub>3</sub>	1.021	1.020	1.020	1.012	338.1	302.8	307.1	297.4
OH	0.984	0.981	0.981	0.970	124.5	110.4	112.5	106.4
H <sub>2</sub> O	0.969	0.968	0.967	0.957	267.3	235.4	240.9	232.2
HF	0.931	0.930	0.929	0.917	162.5	142.6	146.6	140.8
Li <sub>2</sub>	2.649	2.670	2.682	2.673	31.0	27.3	26.8	24.4
LiF	1.548	1.573	1.564	1.564	163.7	146.3	149.1	138.9
C <sub>2</sub> H <sub>2</sub> (CC)	1.201	1.207	1.205	1.202	458.8	413.9	422.0	405.4
C <sub>2</sub> H <sub>2</sub> (CH)	1.074	1.070	1.071	1.063				
C <sub>2</sub> H <sub>4</sub> (CC)	1.323	1.333	1.329	1.339	632.6	571.7	582.1	562.6
C <sub>2</sub> H <sub>4</sub> (CH)	1.093	1.090	1.090	1.087				
HCN (HC)	1.079	1.075	1.076	1.066	359.6	325.2	330.6	311.9
HCN (CN)	1.150	1.158	1.155	1.153				
CO	1.127	1.136	1.132	1.128	298.1	268.5	274.8	259.3
N <sub>2</sub>	1.095	1.103	1.100	1.098	266.1	242.5	245.1	228.5
NO	1.146	1.157	1.153	1.151	197.8	171.6	176.4	152.9
O <sub>2</sub>	1.204	1.219	1.213	1.208	174.1	143.5	150.9	120.5
F <sub>2</sub>	1.388	1.417	1.405	1.412	77.4	52.7	59.0	38.5
P <sub>2</sub>	1.894	1.908	1.902	1.893	141.9	120.3	125.6	117.3
Cl <sub>2</sub>	1.994	2.018	2.005	1.988	82.5	66.0	71.4	58.0





Solid	$a_0$				$B_0$			
	LDA	PBE	WC	Expt. <sup>a</sup>	LDA	PBE	WC	Expt. <sup>a</sup>
Li (A2)	3.363	3.435	<b>3.449</b>	3.477	15.2	14.0	<b>13.4</b>	13.0
C (A4)	3.536	<b>3.575</b>	<b>3.558</b>	3.567	469	<b>434</b>	<b>451</b>	443
C (A9)	2.447	2.471	<b>2.460</b>	2.464				
Na (A2)	4.047	<b>4.196</b>	<b>4.199</b>	4.225	9.41	7.85	<b>7.32</b>	7.5
Al (A1)	3.983	<b>4.041</b>	4.023	4.047	84.3	<b>79.2</b>	80.6	73
Si (A4)	5.407	5.475	<b>5.437</b>	5.430	<b>96.4</b>	88.7	94.0	99.2
K (A2)	5.045	5.282	<b>5.256</b>	5.225	4.50	<b>3.61</b>	3.49	3.7
Ca (A1)	5.333	<b>5.530</b>	5.458	5.58	18.7	<b>17.3</b>	<b>17.4</b>	15
V (A2)	2.932	<b>3.001</b>	2.965	3.03	213	<b>183</b>	198	162
Fe (A2)	2.753	<b>2.830</b>	2.791	2.868	256	<b>194</b>	227	167
Ni (A1)	3.423	<b>3.518</b>	3.468	3.524	259	<b>200</b>	231	184
Cu (A1)	3.522	<b>3.632</b>	3.573	3.615	191	<b>141</b>	168	133
Ge (A4)	<b>5.632</b>	5.769	5.686	5.652	<b>72.7</b>	59.5	67.8	75.8
Rb (A2)	5.374	5.670	<b>5.609</b>	5.59	3.59	<b>2.77</b>	2.71	3.06
Sr (A1)	5.786	<b>6.027</b>	5.914	6.08	14.4	11.4	<b>12.2</b>	12
Nb (A2)	3.250	<b>3.312</b>	3.280	3.30	193	<b>171</b>	183	170
Mo (A2)	3.116	<b>3.164</b>	<b>3.139</b>	3.15	294	260	<b>279</b>	272
Rh (A1)	3.759	3.834	<b>3.795</b>	3.798	320	<b>259</b>	292	269
Pd (A1)	3.848	3.948	<b>3.892</b>	3.881	231	170	<b>207</b>	195
Ag (A1)	4.007	4.152	<b>4.065</b>	4.069	140.4	91.0	<b>118.9</b>	109



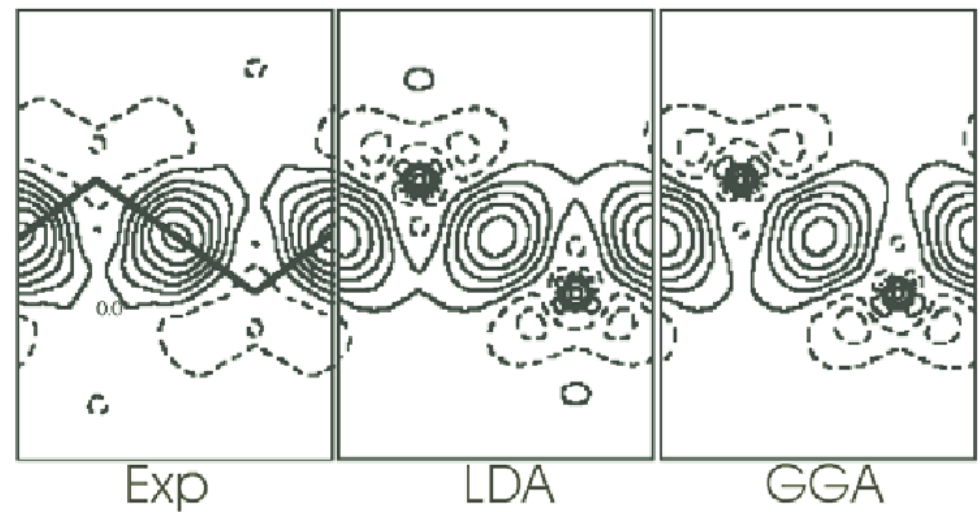
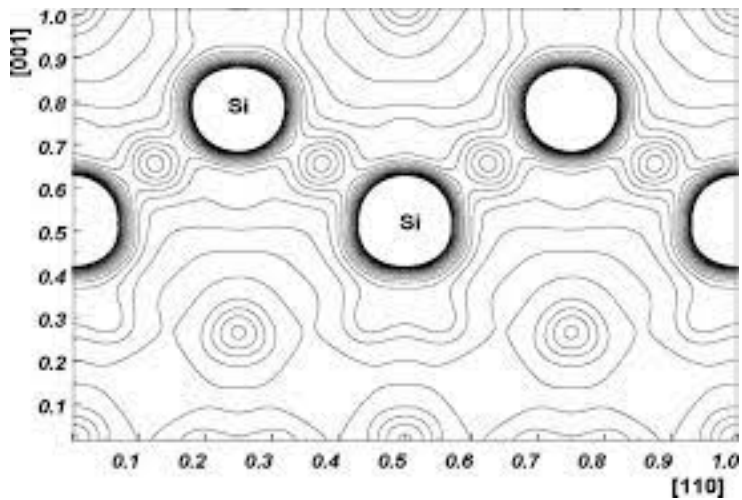
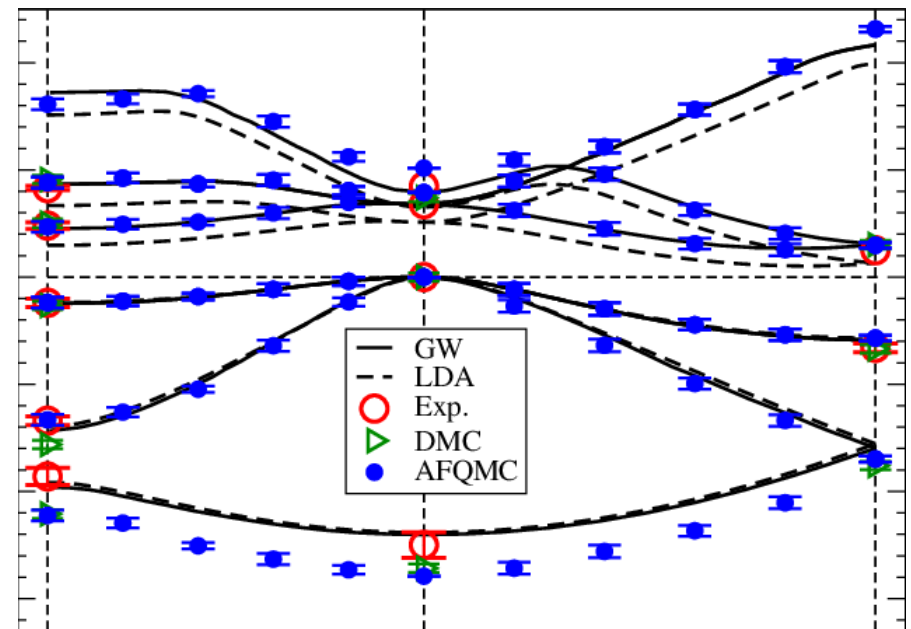
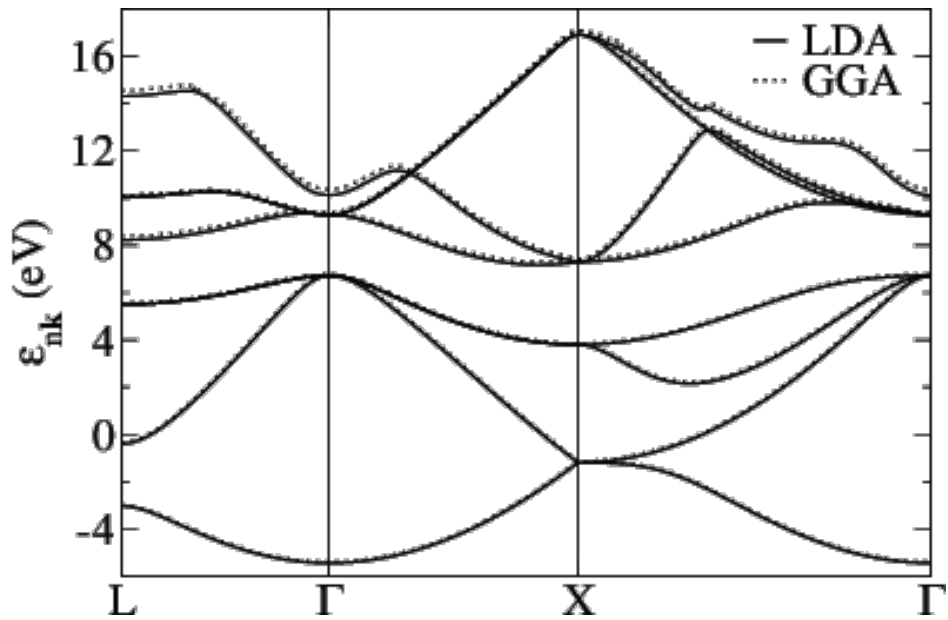
Al aplicar presión:

diamante  $\longrightarrow$   $\beta$ -tin

**Comprobación experimental !!!**

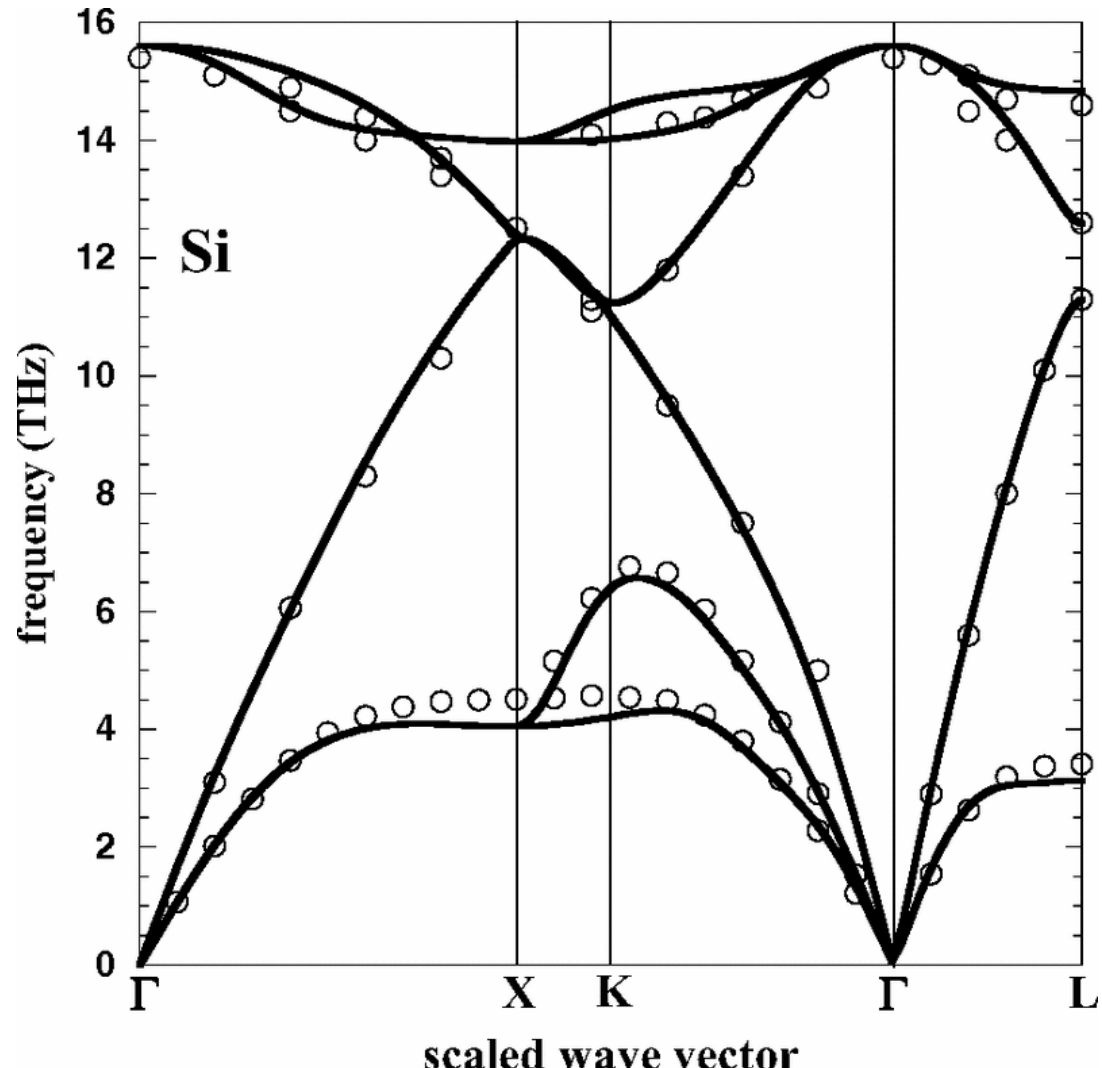


# Propiedades electrónicas en la estructura de equilibrio



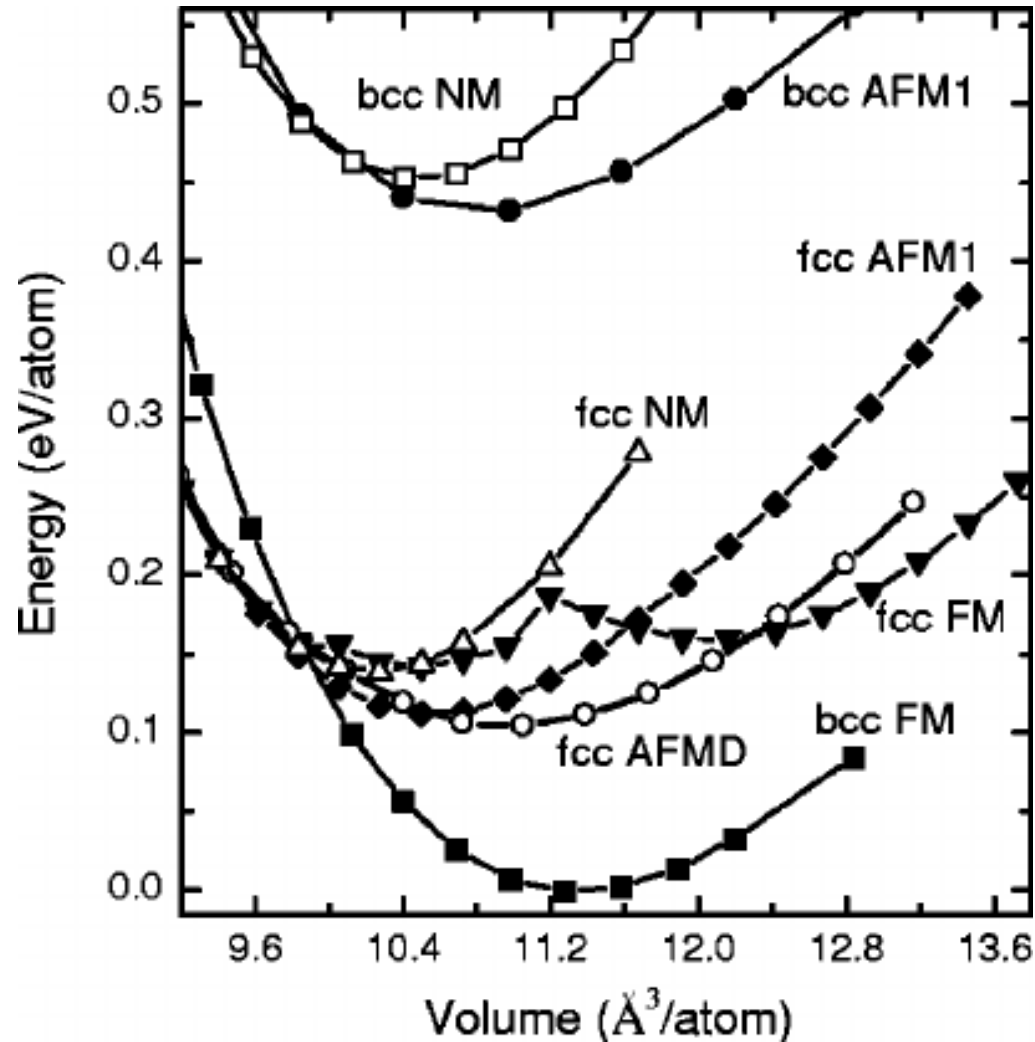
Actualmente es posible determinar muchas propiedades de materiales desde primeros principios. Por ejemplo:

- **Fonones**



# - Sistemas magnéticos

## Fe



**Además: constantes elásticas, propiedades eléctricas, ópticas, superficiales, etc.**