



# Physique des solides

Une introduction

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# Retour sur le modèle de Sommerfeld

$$\vec{j} = \rho \langle \vec{v}_{\text{stat}} \rangle = \frac{nq^2}{m} \tau \vec{E} = \sigma \vec{E}$$

Pauli

phonons

Bandes



# Electrons : Semi-conducteurs

1. Méthodes des liaisons fortes
  1. De l'atome à la molécule
  2. Retour sur la structure diamant
  3. La chaîne polymère
  
2. Bandes, structures et remplissage
  1. Influence du potentiel : masse effective
  2. Isolants, conducteurs
  
3. Semi-conducteurs
  1. Isolants et Semi-conducteurs intrinsèques
  2. Semi-conducteurs extrinsèques
  3. Jonctions



# 1 Méthode des liaisons fortes

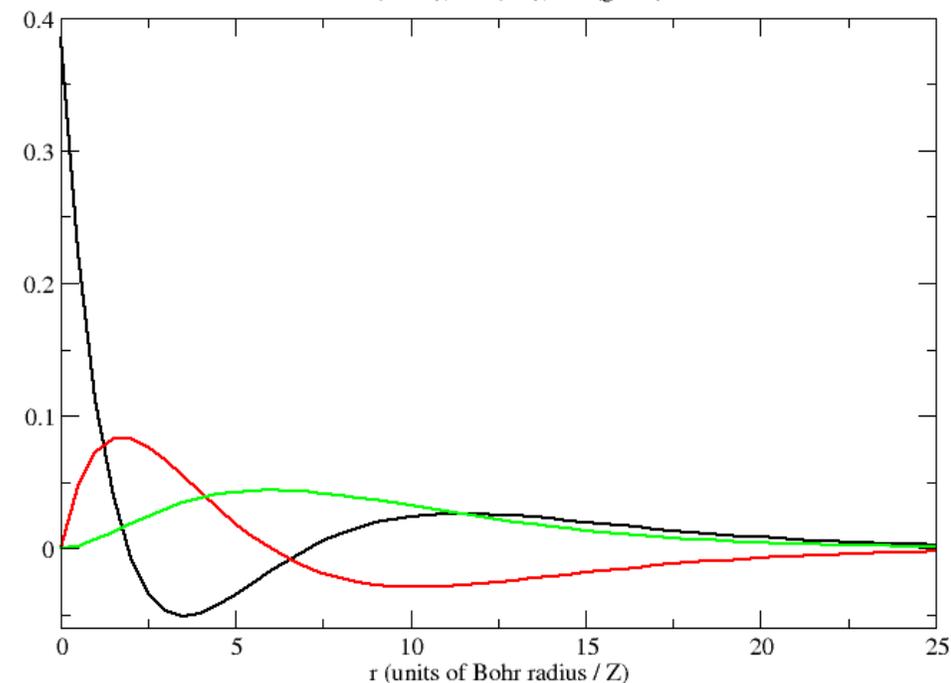
## Atomes et molécules

Electron Configurations in the Periodic Table

1 H 1s																	2 He 1s
3 Li 2s	4 Be											5 B 2p	6 C	7 N	8 O	9 F	10 Ne
11 Na 3s	12 Mg											13 Al 3p	14 Si	15 P	16 S	17 Cl	18 Ar
19 K 4s	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn 3d	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga 4p	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb 5s	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc 4d	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In 5p	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs 6s	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re 5d	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl 6p	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr 7s	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh 6d	108 Hs	109 Mt	110	111	112	113	114				
		58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd 4f	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu		
		90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm 5f	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		

atomic radial wave functions (n=3)

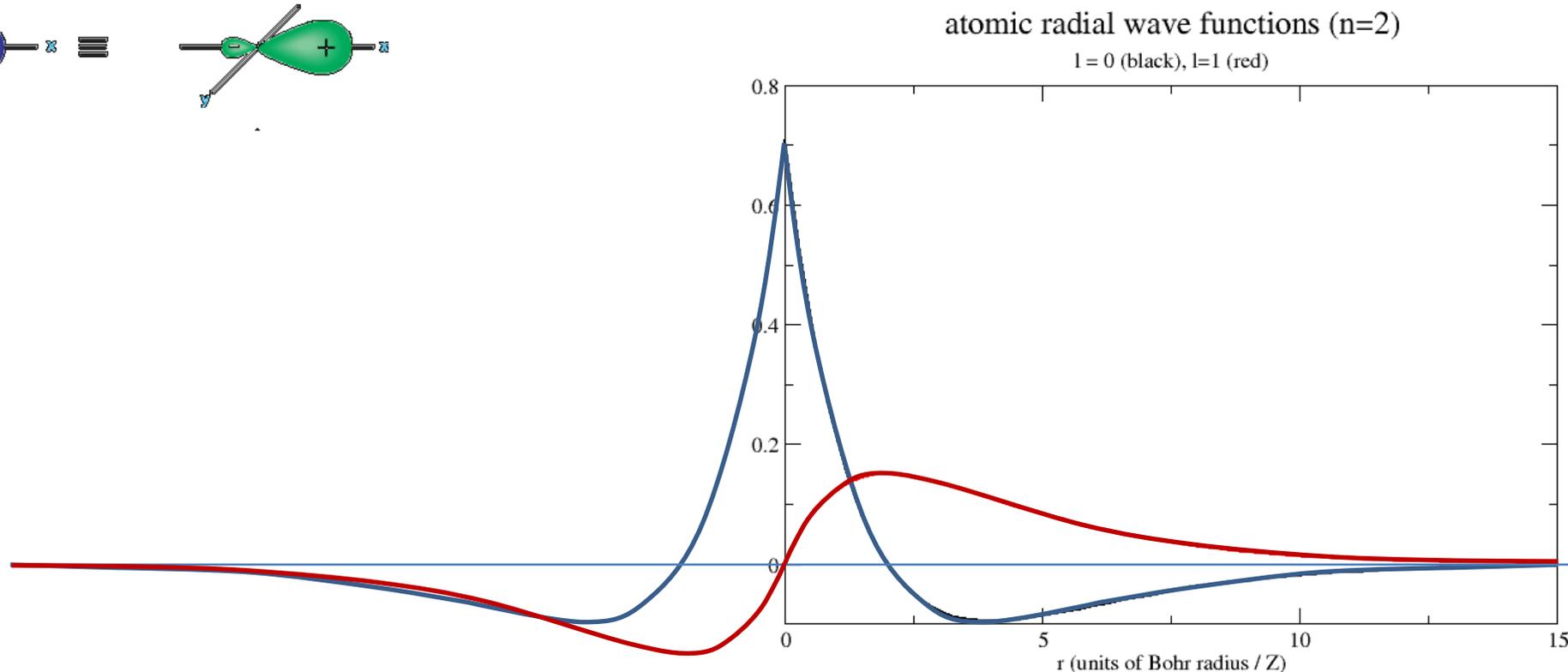
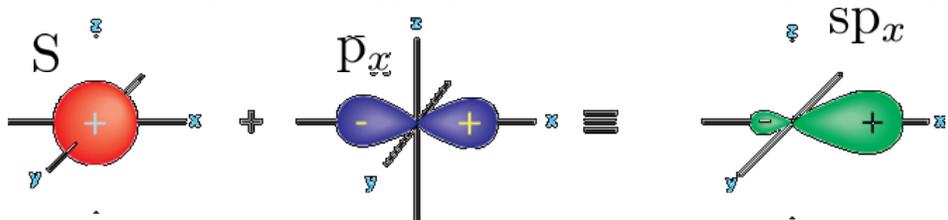
l=0 (black), l=1 (red), l=2 (green)





# 1 Méthode des liaisons fortes

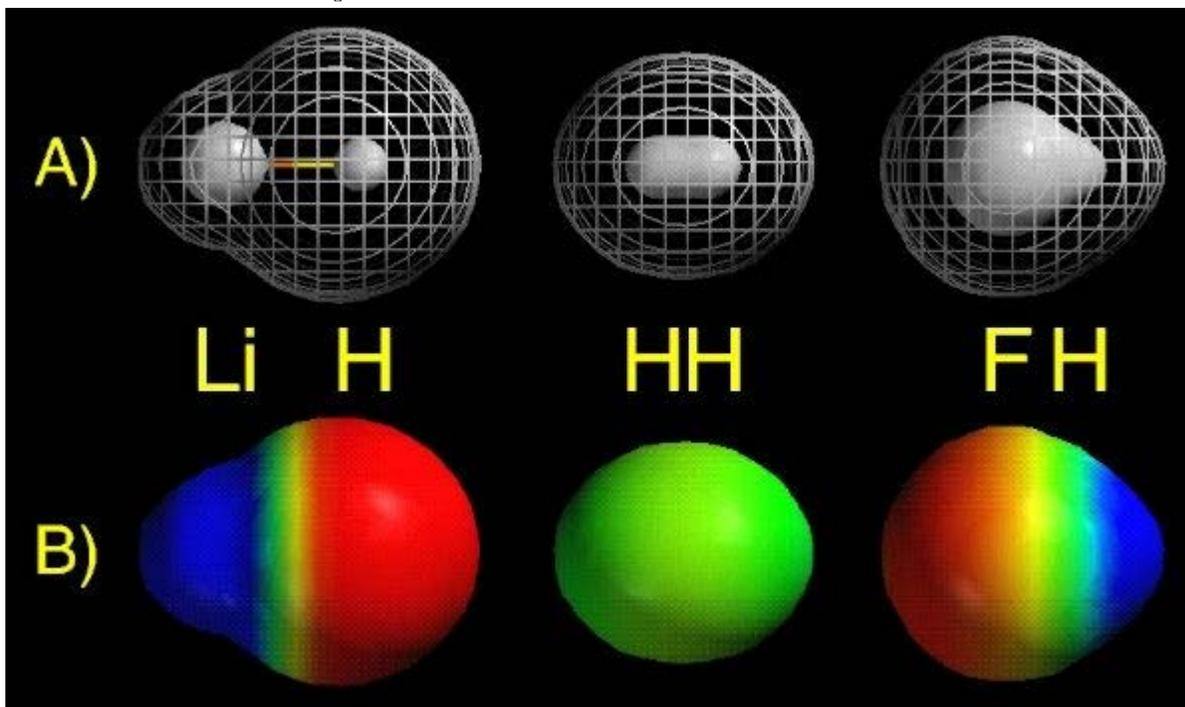
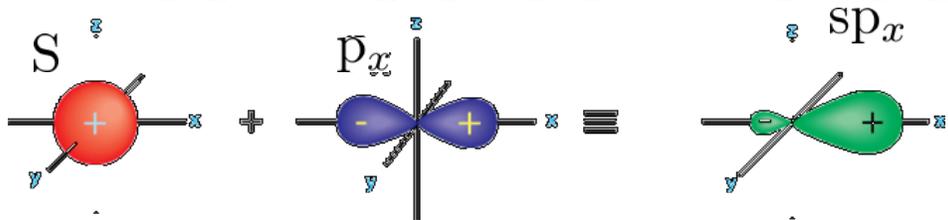
## Atomes et molécules





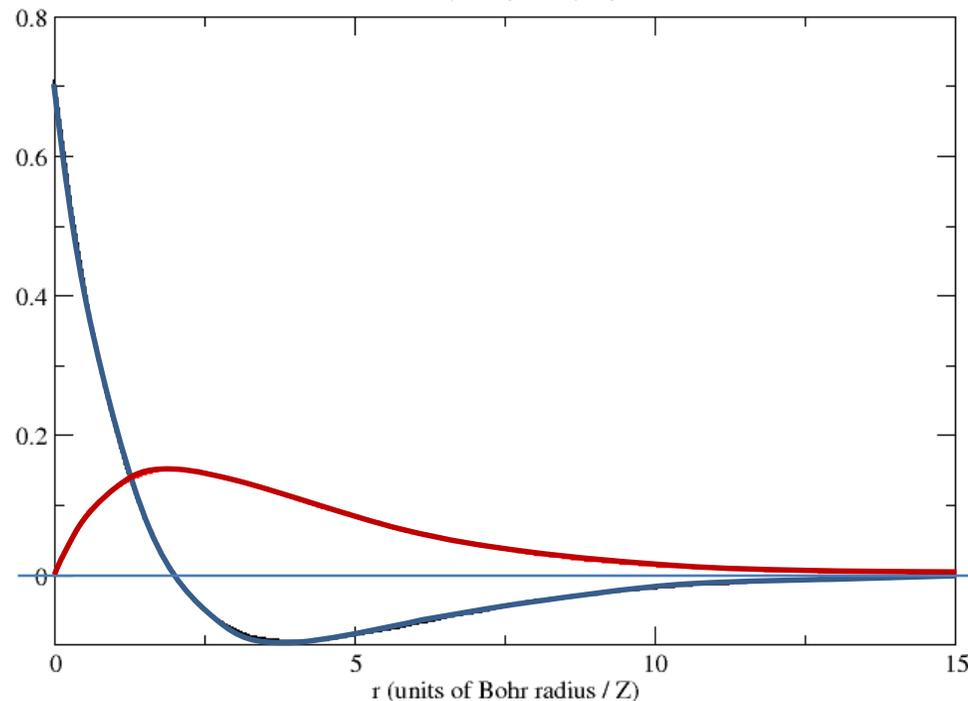
# 1 Méthode des liaisons fortes

## Atomes et molécules



atomic radial wave functions (n=2)

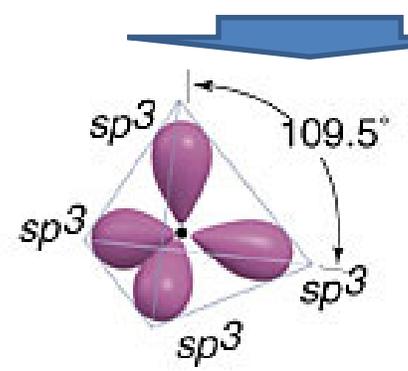
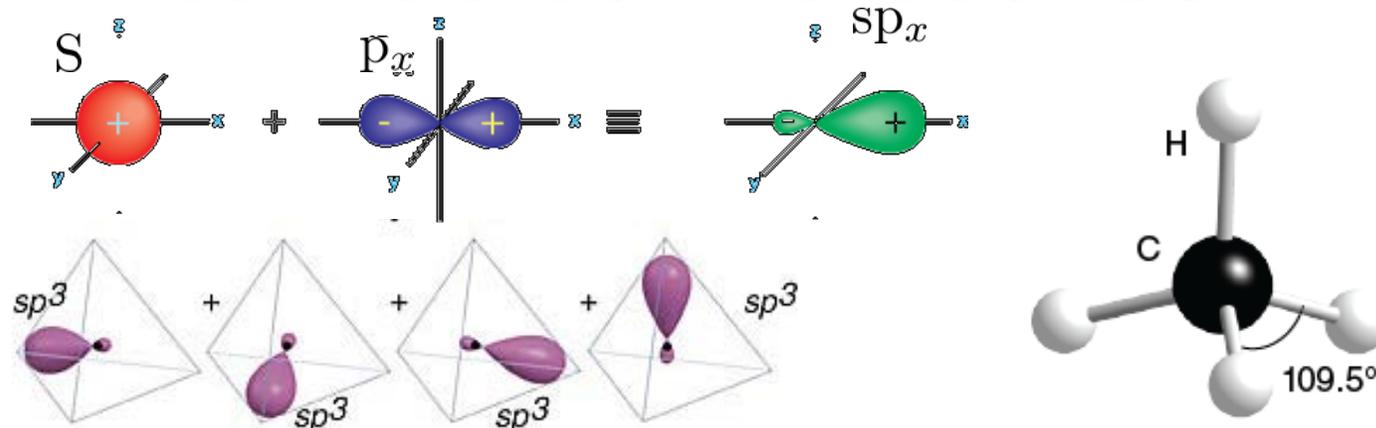
l = 0 (black), l = 1 (red)





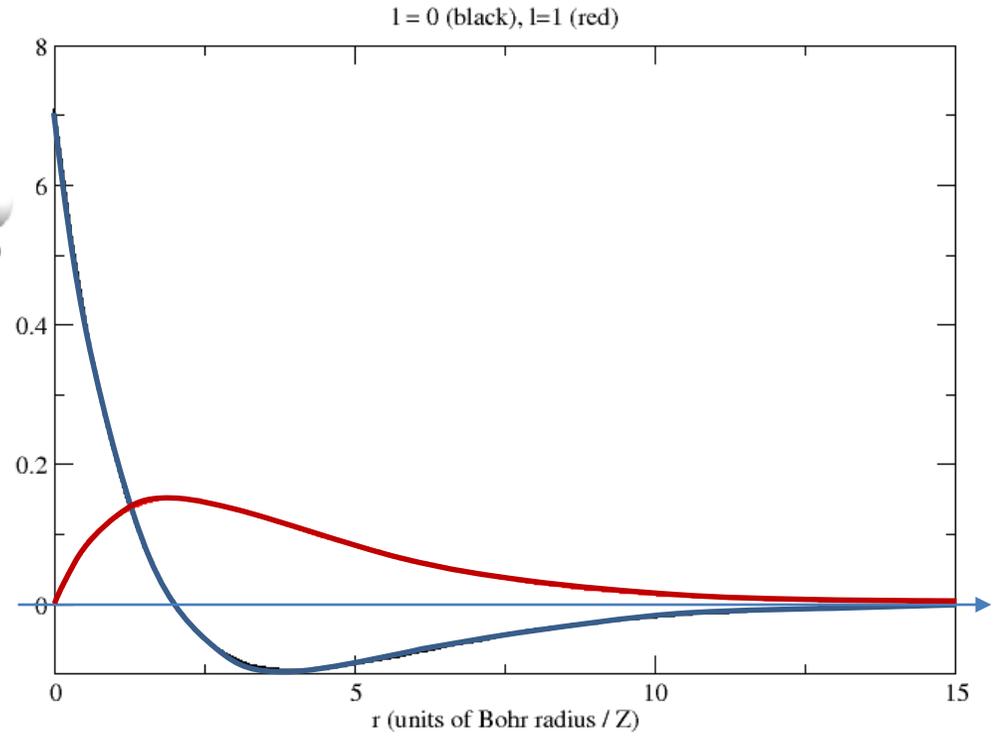
# 1 Méthode des liaisons fortes

## Atomes et molécules



$$\begin{aligned}
 |\psi_1\rangle &= \frac{1}{2} [|\phi_s\rangle + |\phi_x\rangle + |\phi_y\rangle + |\phi_z\rangle] \\
 |\psi_2\rangle &= \frac{1}{2} [|\phi_s\rangle + |\phi_x\rangle - |\phi_y\rangle - |\phi_z\rangle] \\
 |\psi_3\rangle &= \frac{1}{2} [|\phi_s\rangle - |\phi_x\rangle + |\phi_y\rangle - |\phi_z\rangle] \\
 |\psi_4\rangle &= \frac{1}{2} [|\phi_s\rangle - |\phi_x\rangle - |\phi_y\rangle - |\phi_z\rangle]
 \end{aligned}$$

atomic radial wave functions (n=2)

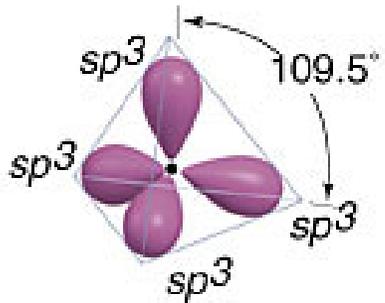




# 1 Méthode des liaisons fortes

## Structure diamant

# Sn

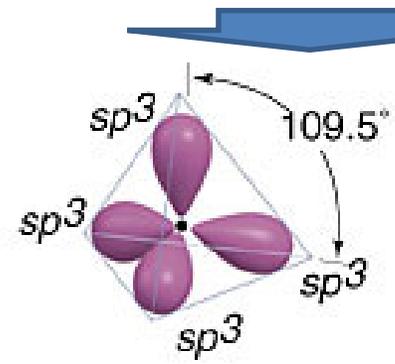
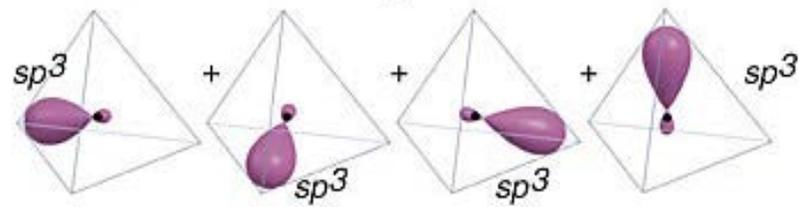
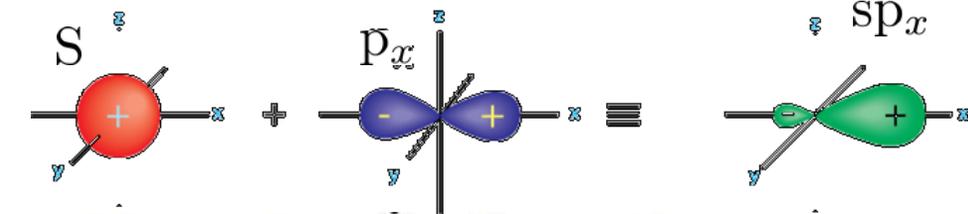


										8A	
										4.003	
										2 He	
										0.31	
										helium	
										noble gas	
										$1s^2$	
										19.00	
										20.18	
										0.42	
										10 Ne	
										0.38	
										neon	
										noble gas	
										$[He]2s^2 2p^6$	
3A	4A	5A	6A	7A							
10.81	8.3	12.01	11.3	14.01	14.5	6.00	13.6	19.00	17.4	20.18	
5 B	6 C	7 N	8 O	9 F	10 Ne						
0.87	0.67	0.56	0.48	0.42	0.38						
boron	carbon	nitrogen	oxygen	fluorine	neon						
metalloid	non metal	non metal	non metal	halogen	noble gas						
$[He]2s^2 2p^1$	$[He]2s^2 2p^2$	$[He]2s^2 2p^3$	$[He]2s^2 2p^4$	$[He]2s^2 2p^5$	$[He]2s^2 2p^6$						
26.98	5.99	28.08	5.15	30.97	10.5	32.06	10.4	35.45	13.	39.95	
13 Al	14 Si	15 P	16 S	17 Cl	18 Ar						
1.18	1.11	0.98	0.87	0.79	0.71						
aluminum	silicon	phosphorus	sulfur	chlorine	argon						
poor metal	metalloid	non metal	non metal	halogen	noble gas						
$[Ne]3s^2 3p^1$	$[Ne]3s^2 3p^2$	$[Ne]3s^2 3p^3$	$[Ne]3s^2 3p^4$	$[Ne]3s^2 3p^5$	$[Ne]3s^2 3p^6$						
58.69	7.64	63.55	7.73	65.38	9.39	69.72	6.	72.63	7.9	74.92	
28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr			
1.49	1.45	1.42	1.36	1.25	1.14	1.03	0.94	0.87			
nickel	copper	zinc	gallium	germanium	arsenic	selenium	bromine	krypton			
transition metal	transition metal	transition metal	poor metal	metalloid	metalloid	metalloid	halogen	noble gas			
$[Ar]4s^2 3d^8$	$[Ar]4s^1 3d^{10}$	$[Ar]4s^2 3d^{10}$	$[Ar]4s^2 3d^{10} 4p^1$	$[Ar]4s^2 3d^{10} 4p^2$	$[Ar]4s^2 3d^{10} 4p^3$	$[Ar]4s^2 3d^{10} 4p^4$	$[Ar]4s^2 3d^{10} 4p^5$	$[Ar]4s^2 3d^{10} 4p^6$			
106.4	8.34	107.9	7.58	112.4	8.99	114.8	5.79	118.7	7.34	21.8	
46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe			
1.69	1.65	1.61	1.56	1.45	1.33	1.23	1.15	1.08			
palladium	silver	cadmium	indium	tin	antimony	tellurium	iodine	xenon			
transition metal	transition metal	transition metal	poor metal	poor metal	metalloid	metalloid	halogen	noble gas			
$[Kr]4d^{10}$	$[Kr]5s^1 4d^{10}$	$[Kr]5s^2 4d^{10}$	$[Kr]5s^2 4d^{10} 5p^1$	$[Kr]5s^2 4d^{10} 5p^2$	$[Kr]5s^2 4d^{10} 5p^3$	$[Kr]5s^2 4d^{10} 5p^4$	$[Kr]5s^2 4d^{10} 5p^5$	$[Kr]5s^2 4d^{10} 5p^6$			
195.1	9.02	197.0	9.23	200.6	10.4	204.4	6.11	207.2	7.42	209.0	
78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn			
1.77	1.74	1.71	1.56	1.54	1.43	1.35	1.27	1.20			
platinum	gold	mercury	thallium	lead	bismuth	polonium	astatine	radon			
transition metal	transition metal	transition metal	poor metal	poor metal	poor metal	poor metal	halogen	noble gas			
$[Xe]6s^1 4f^{14} 5d^9$	$[Xe]6s^1 4f^{14} 5d^{10}$	$[Xe]6s^2 4f^{14} 5d^{10}$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^1$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^2$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^3$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^4$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^5$	$[Xe]6s^2 4f^{14} 5d^{10} 6p^6$			
281.	281.	285.	286.	289.	289.	293.	293.	294.			
110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og			
transition metal	transition metal	transition metal	poor metal	poor metal	poor metal	poor metal	halogen	noble gas			
$[Rn]7s^1 5f^{14} 6d^9$	$[Rn]7s^1 5f^{14} 6d^{10}$	$[Rn]7s^2 5f^{14} 6d^{10}$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^1$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^2$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^3$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^4$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^5$	$[Rn]7s^2 5f^{14} 6d^{10} 7p^6$			
157.3	6.15	158.9	5.86	162.5	5.94	164.9	6.02	167.3	6.11	168.9	
64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu				
2.33	2.25	2.28	2.26	2.26	2.22	2.22	2.17				
gadolinium	terbium	dysprosium	holmium	erbium	thulium	ytterbium	lutetium				
lanthanide	lanthanide	lanthanide	lanthanide	lanthanide	lanthanide	lanthanide	lanthanide				
$[Xe]6s^2 4f^7 5d^1$	$[Xe]6s^2 4f^9$	$[Xe]6s^2 4f^{10}$	$[Xe]6s^2 4f^{11}$	$[Xe]6s^2 4f^{12}$	$[Xe]6s^2 4f^{13}$	$[Xe]6s^2 4f^{14}$	$[Xe]6s^2 4f^{14} 5d^1$				
247.	6.02	247.	6.23	251.	6.3	252.	6.42	257.	6.5	258.	
96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr				
actinide	actinide	actinide	actinide	actinide	actinide	actinide	actinide				
$[Rn]7s^2 5f^7 6d^1$	$[Rn]7s^2 5f^9$	$[Rn]7s^2 5f^{10}$	$[Rn]7s^2 5f^{11}$	$[Rn]7s^2 5f^{12}$	$[Rn]7s^2 5f^{13}$	$[Rn]7s^2 5f^{14}$	$[Rn]7s^2 5f^{14} 7p^1$				



# 1 Méthode des liaisons fortes

## Atomes et molécules

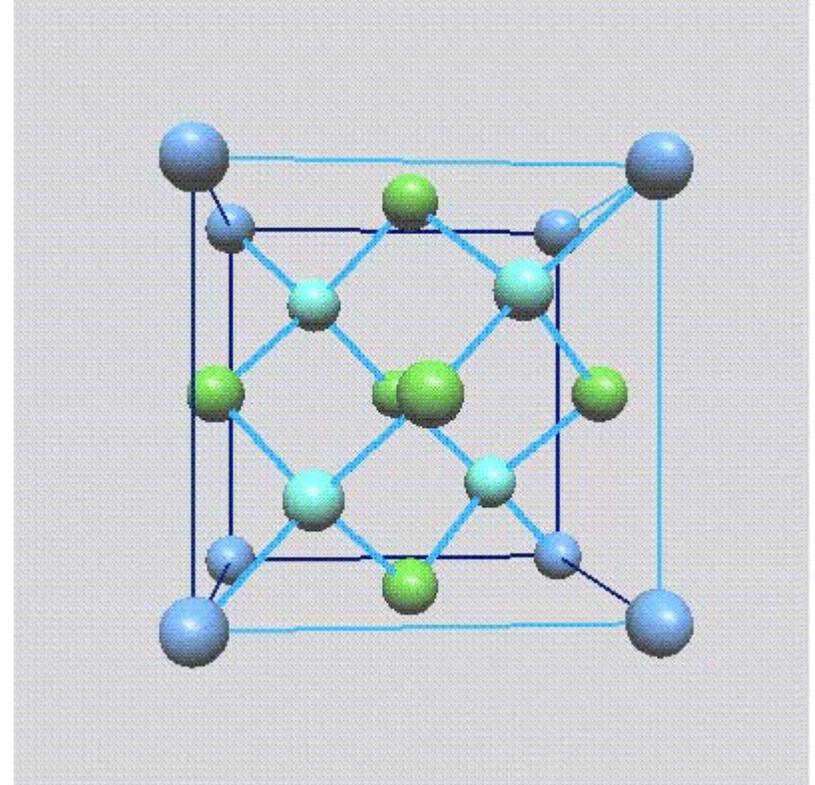


$$|\psi_1\rangle = \frac{1}{2} [|\phi_s\rangle + |\phi_x\rangle + |\phi_y\rangle + |\phi_z\rangle]$$

$$|\psi_2\rangle = \frac{1}{2} [|\phi_s\rangle + |\phi_x\rangle - |\phi_y\rangle - |\phi_z\rangle]$$

$$|\psi_3\rangle = \frac{1}{2} [|\phi_s\rangle - |\phi_x\rangle + |\phi_y\rangle - |\phi_z\rangle]$$

$$|\psi_4\rangle = \frac{1}{2} [|\phi_s\rangle - |\phi_x\rangle - |\phi_y\rangle - |\phi_z\rangle]$$

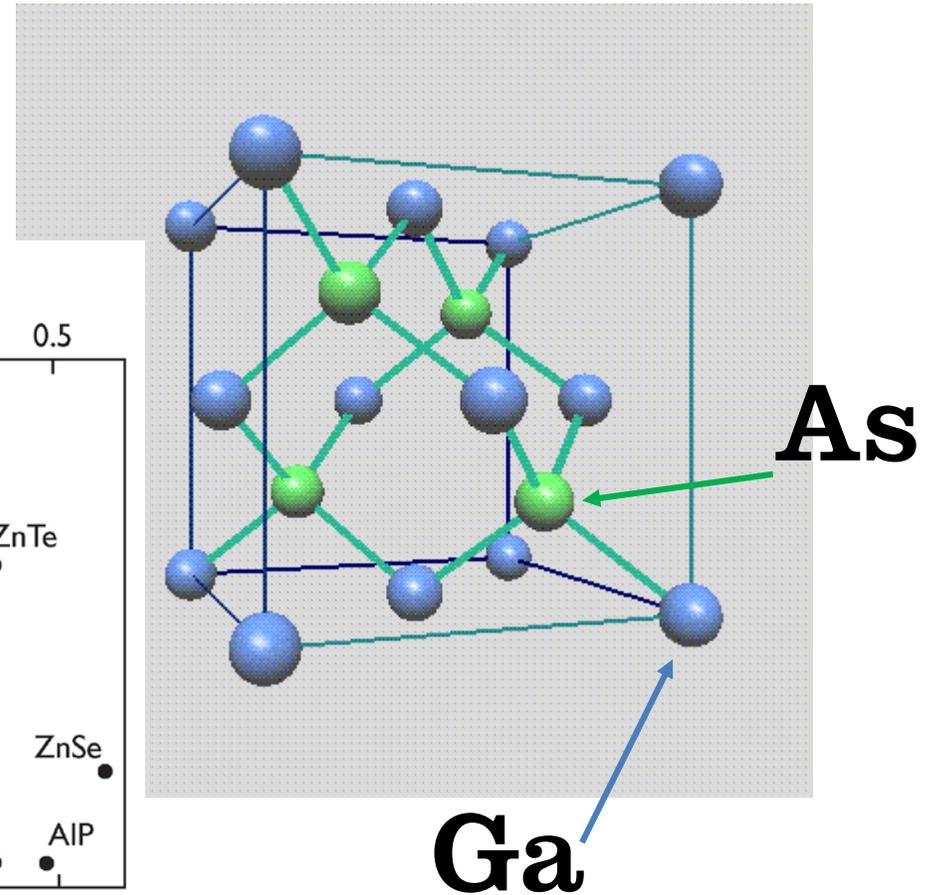
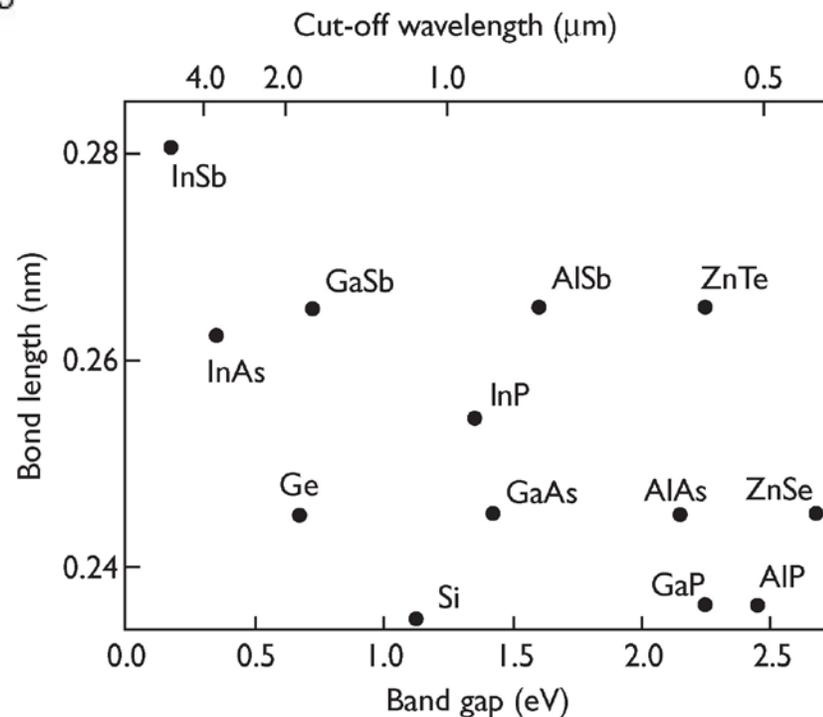
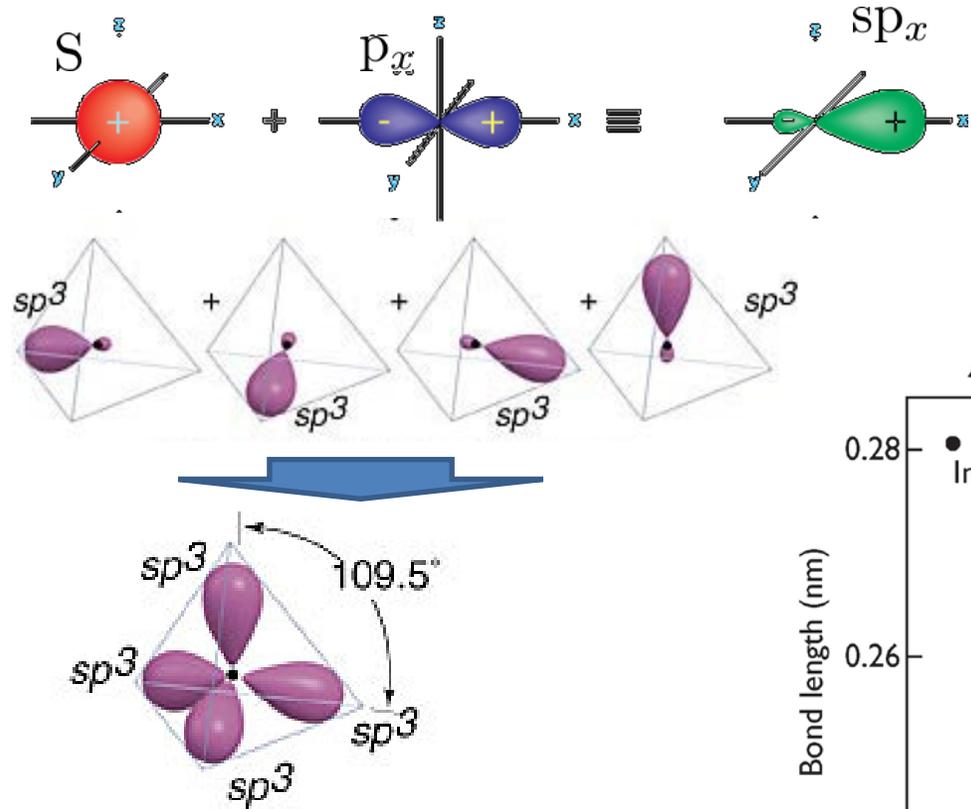






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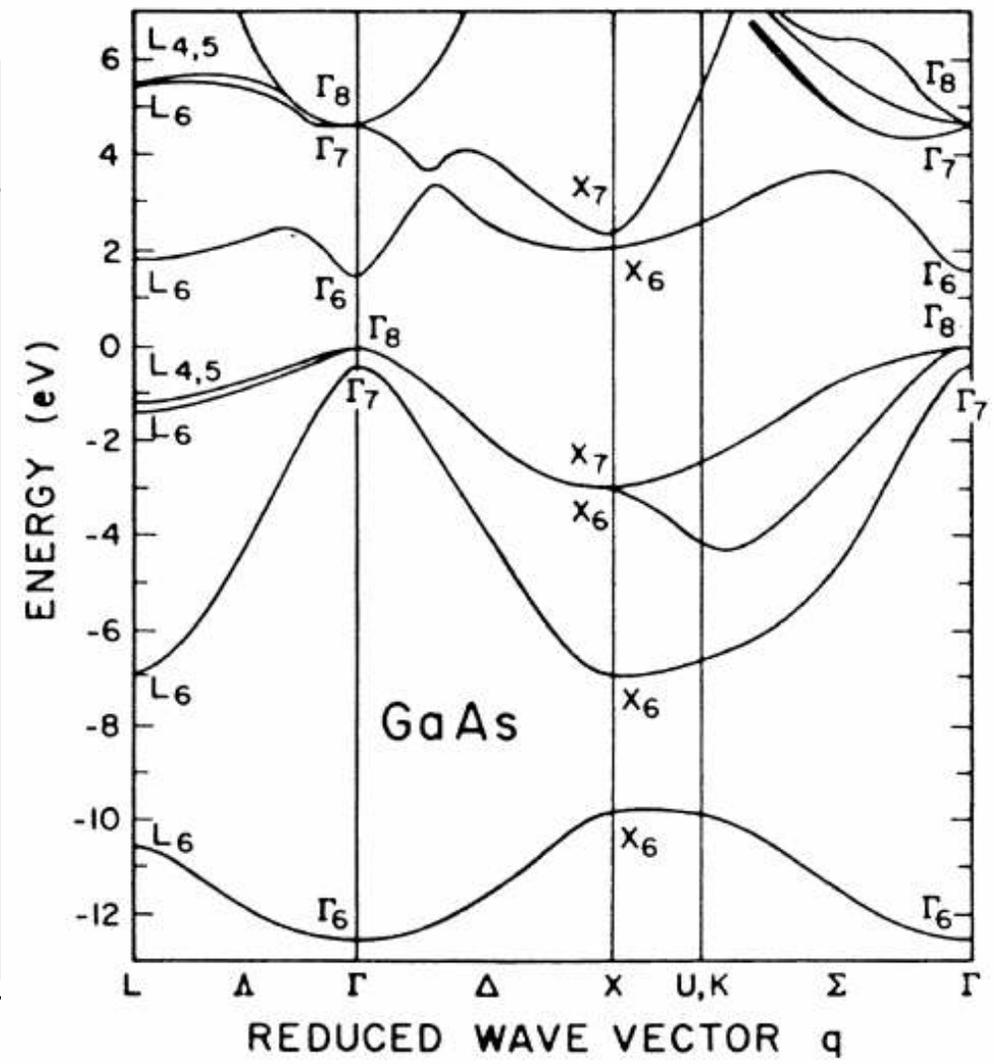
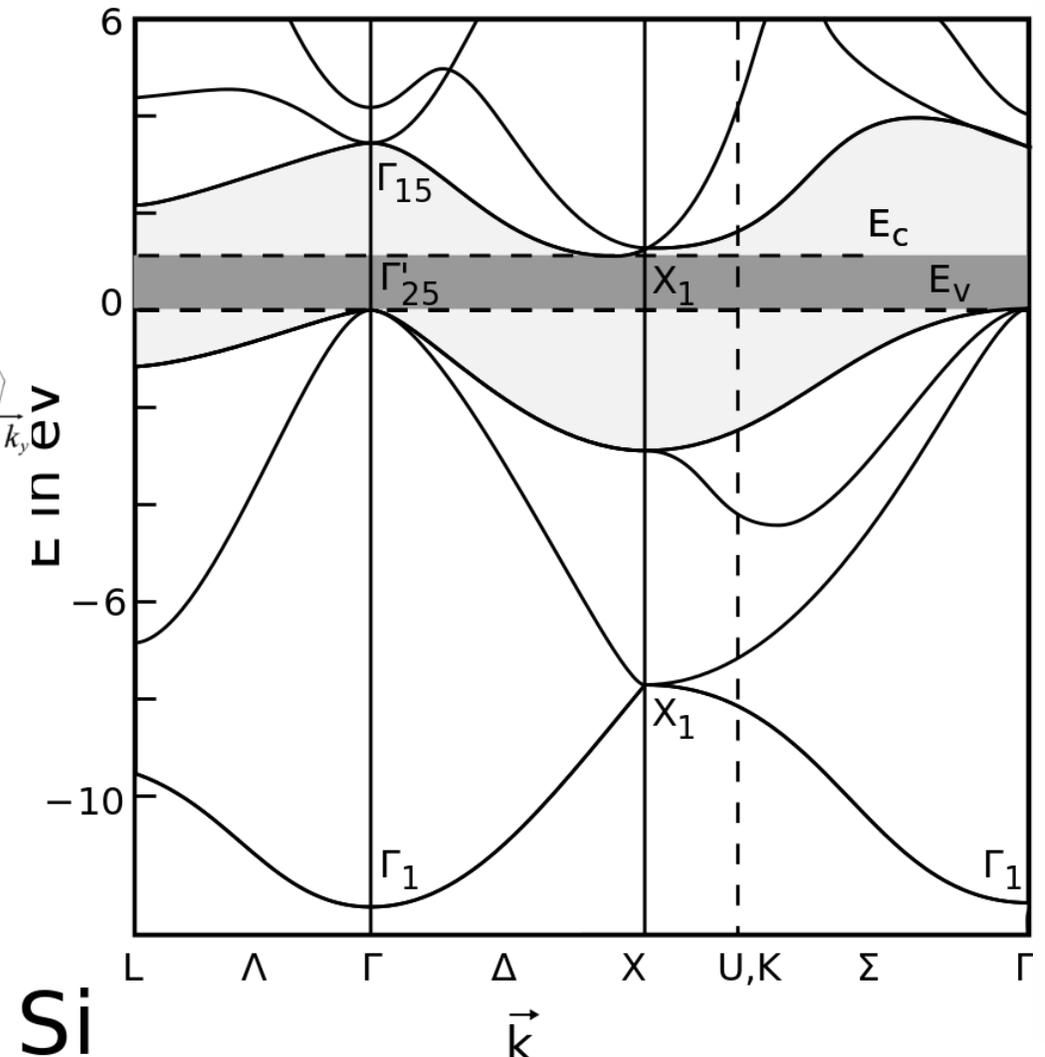
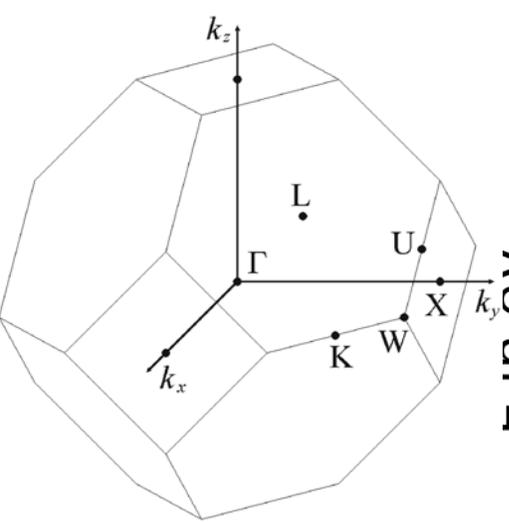
## Atomes et molécules





# 1- Méthode des liaisons fortes

## Zone réduite





# 1- Méthode des liaisons fortes

## Chaîne polymère : cristal 1D

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

$$\psi_{j,k}(x) = \sum_n \phi_j(x - na)e^{ikna} \qquad \text{avec} \quad \hat{H}_0\phi_j(x) = \varepsilon_j\phi_j(x)$$



# 1- Méthode des liaisons fortes

## Chaîne polymère : cristal 1D

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

$$\psi_{s,\mathbf{k}}(x) = \sum_n \phi_s(x - na)e^{ikna} \quad \text{avec} \quad \hat{H}_0\phi_j(x) = \varepsilon_j\phi_j(x)$$

$$\psi_{p,\mathbf{k}}(x) = \sum_n \phi_p(x - na)e^{ikna}$$



# 1- Méthode des liaisons fortes

## Chaîne polymère : cristal 1D

$$\hat{H}\psi_{j,k}(x) = \varepsilon_j(k)\psi_{j,k}(x)$$

**1<sup>er</sup> voisins et  
fonctions réelles**

$$\varepsilon_s(k) \approx \varepsilon_s + V_{ss} \cos ka$$

**avec**  $\hat{H}_0\phi_j(x) = \varepsilon_j\phi_j(x)$

$$\varepsilon_p(k) \approx \varepsilon_p + V_{pp} \cos ka$$



# 1- Méthode des liaisons fortes

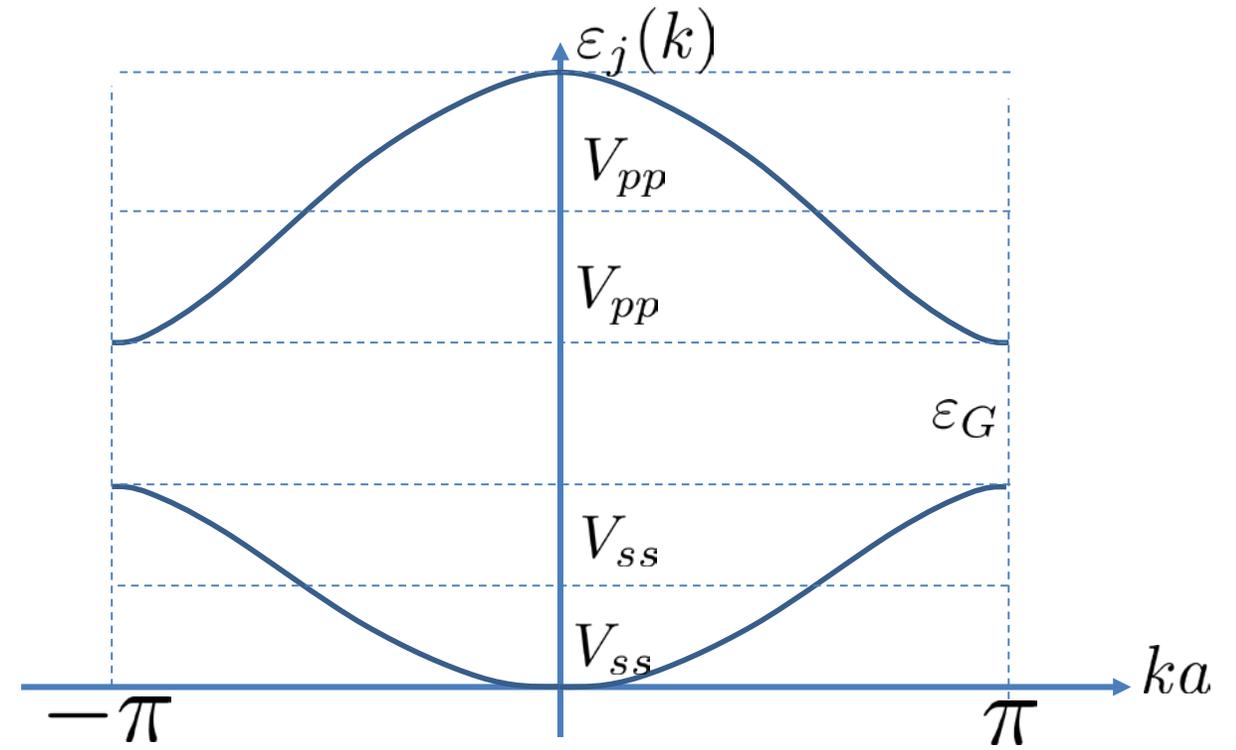
## Chaîne polymère : cristal 1D

$$\hat{H}\psi_{j,k}(x) = \varepsilon_j(k)\psi_{j,k}(x)$$

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# 1- Méthode des liaisons fortes

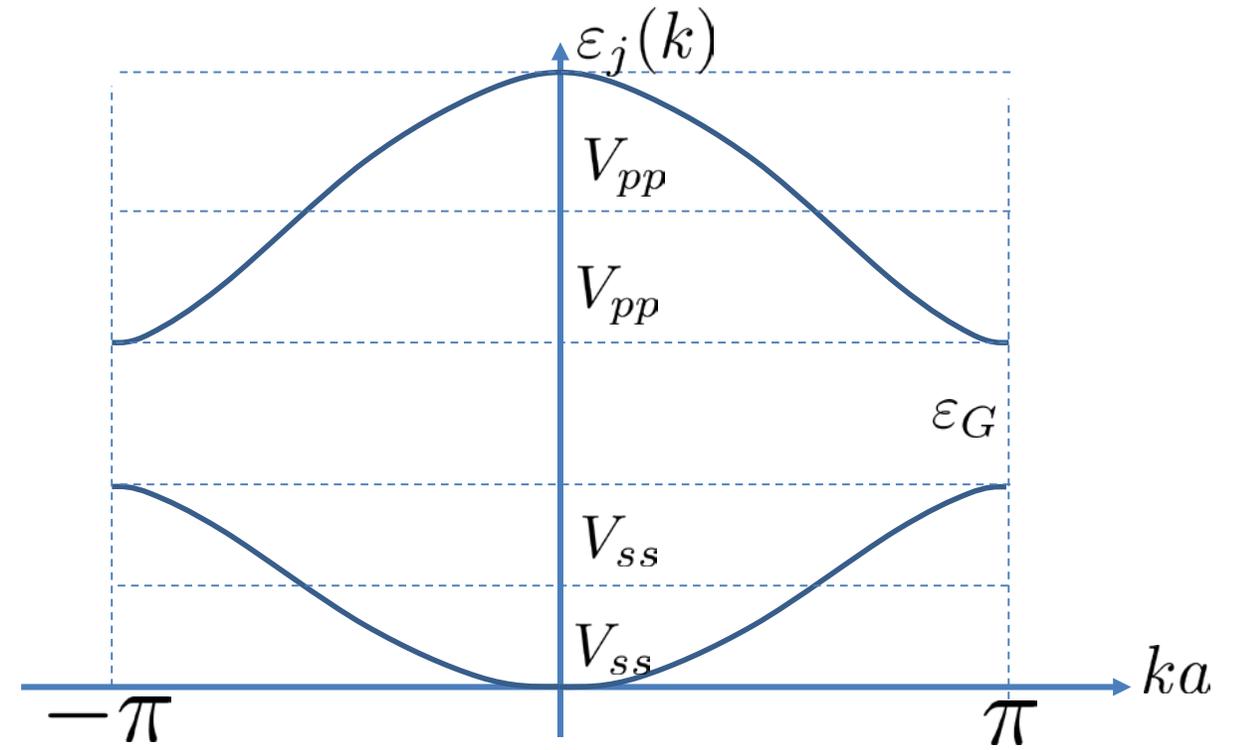
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**1<sup>er</sup> voisins et fonctions réelles**





# 2- Bandes, structure et remplissage

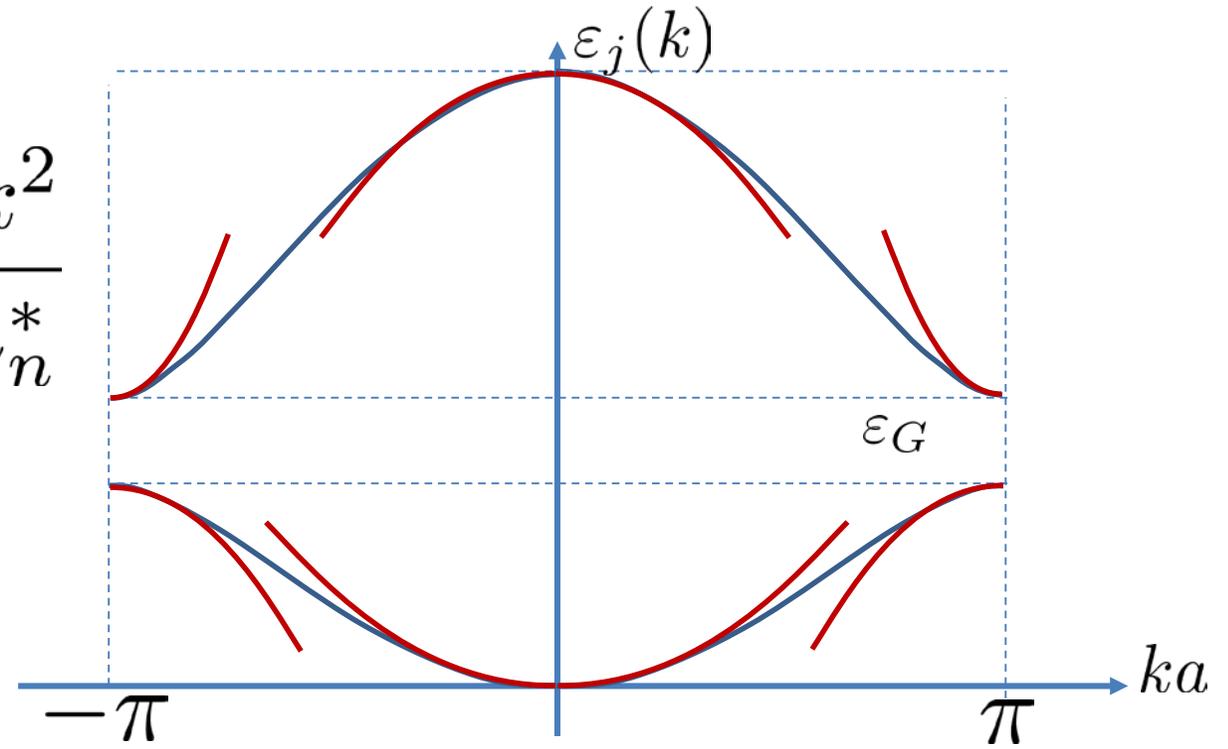
**Masse effective**

$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$$

**Paraboloïde local**

$$\varepsilon_n(k) \approx \frac{\hbar^2 k^2}{2m_n^*}$$

**Approximation des bandes paraboliques**



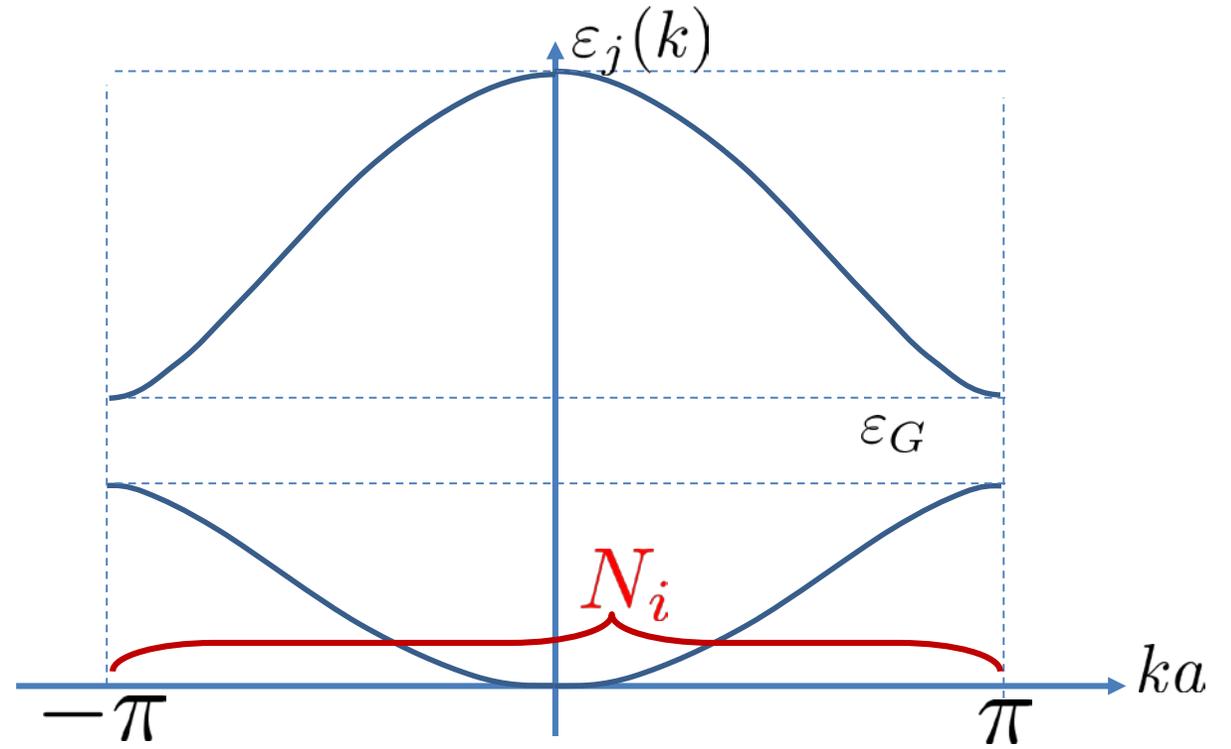


# 2- Bandes, structure et remplissage

## Electrons et trous

$$k_i = n_i \frac{2\pi}{L_i} \quad L_i = N_i a_i$$

Il y a  $N_1 \times N_2 \times N_3$  vecteurs accessibles dans la Z.B.





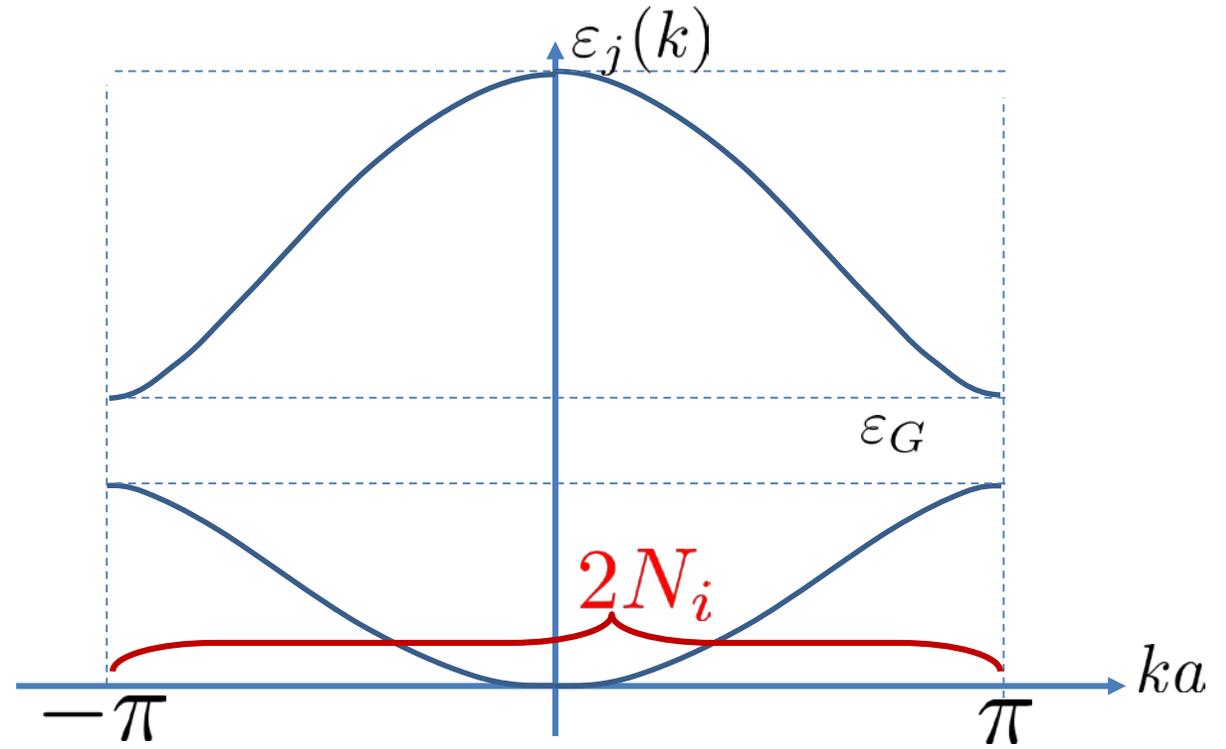
# 2- Bandes, structure et remplissage

## Electrons et trous

table

$$k_i = n_i \frac{2\pi}{L_i} \quad L_i = N_i a_i$$

Il y a  $2^3 \times N_1 \times N_2 \times N_3$  états accessibles dans la Z.B.





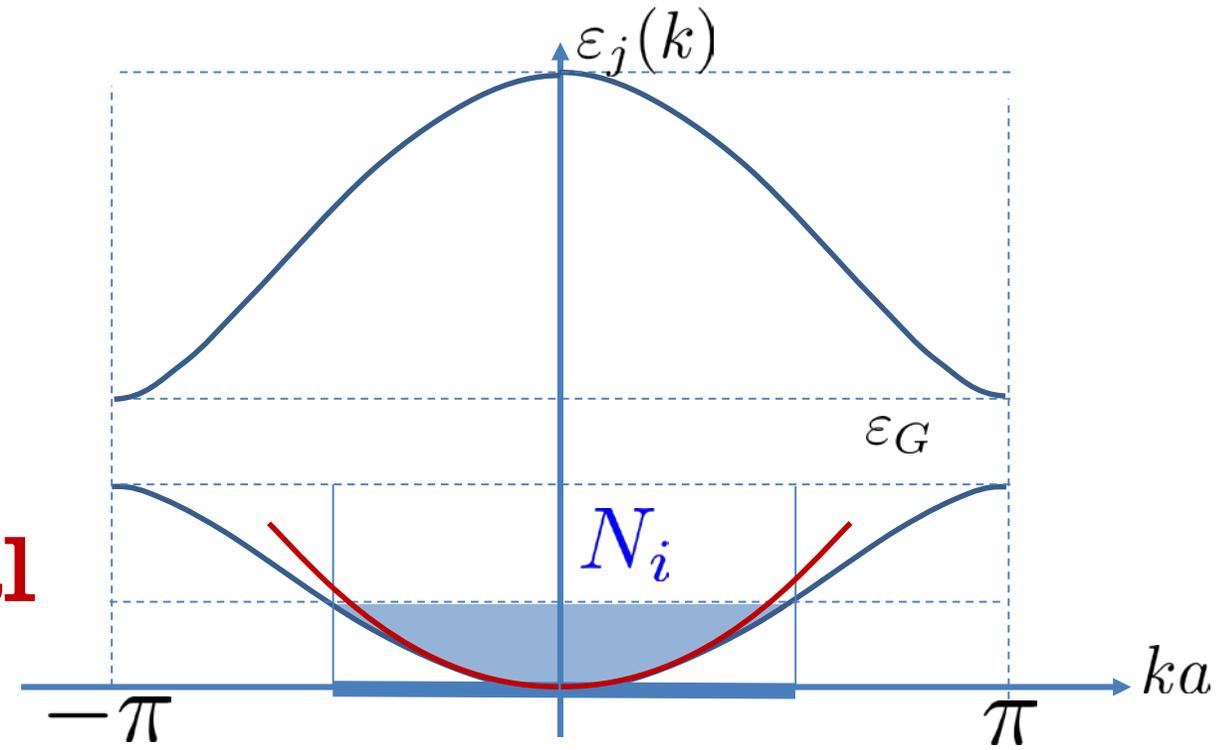
# 2- Bandes, structure et remplissage

## Electrons et trous

Nombre **impair** d'électrons par maille

Il y a  $2^3 \times N_1 \times N_2 \times N_3$  **états** accessibles dans la Z.B.

**Métal**



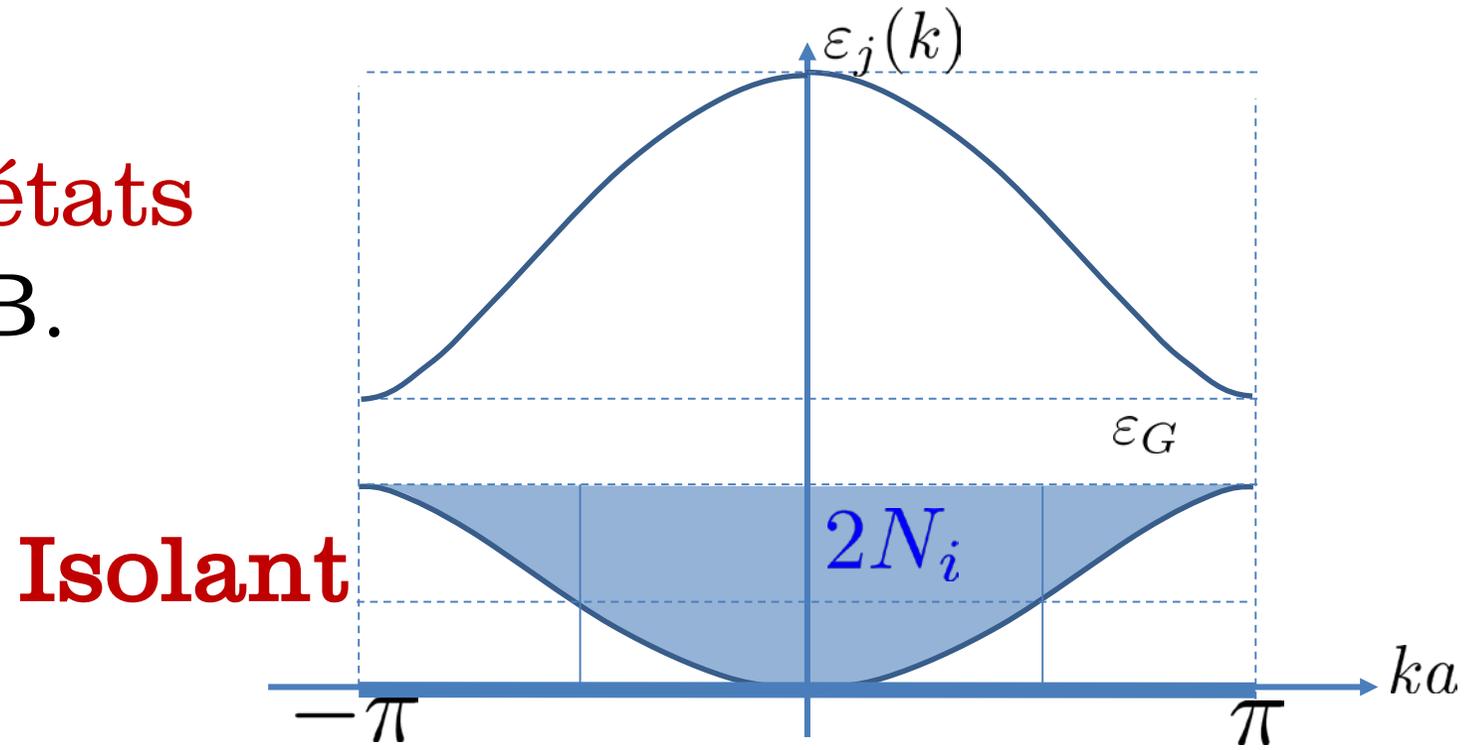


# 2- Bandes, structure et remplissage

## Electrons et trous

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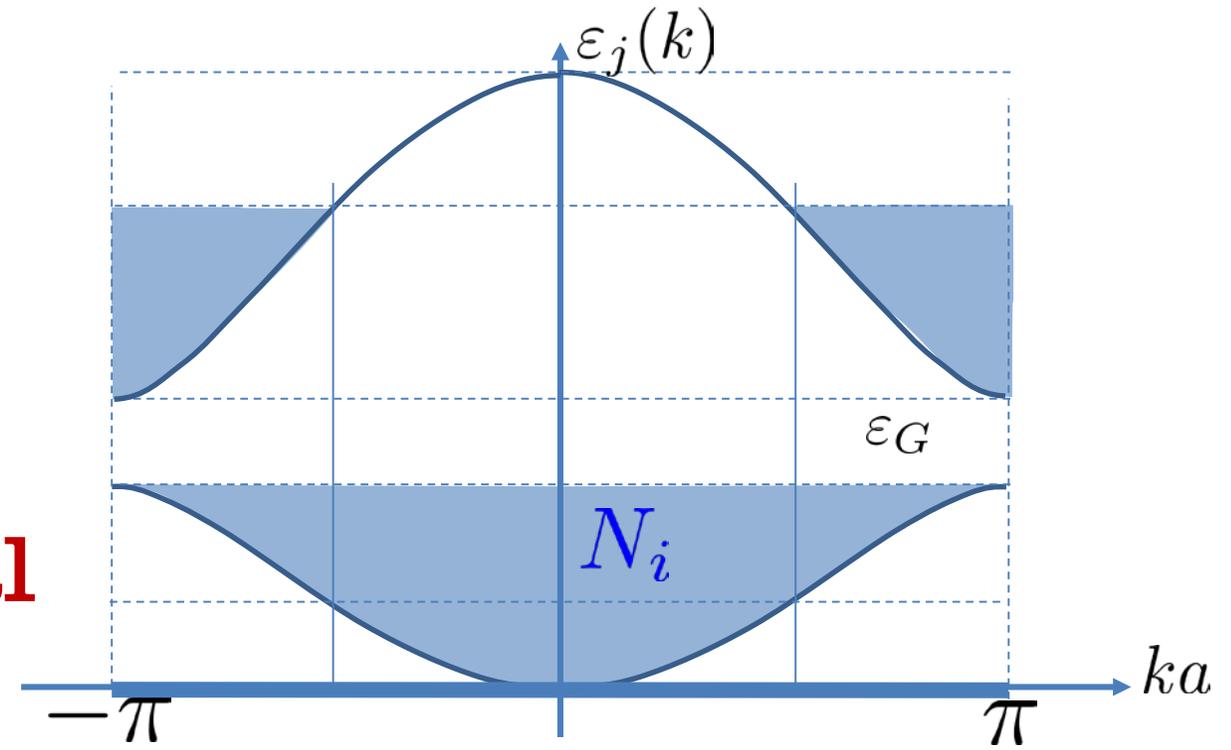
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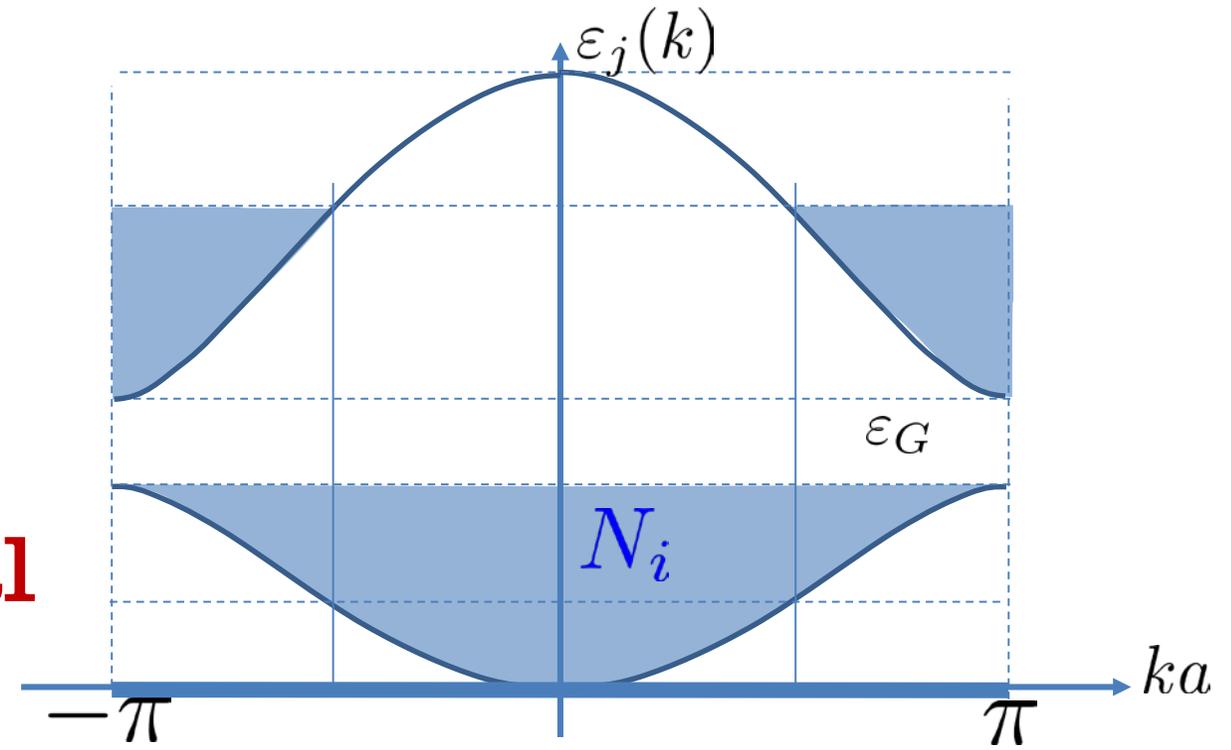
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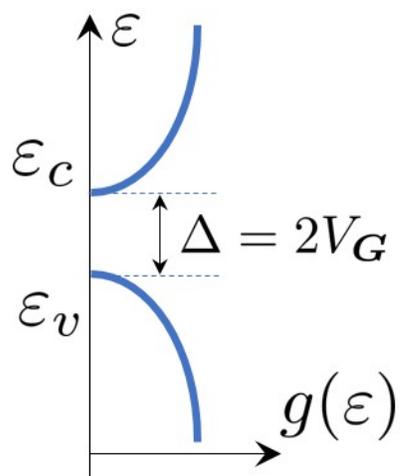
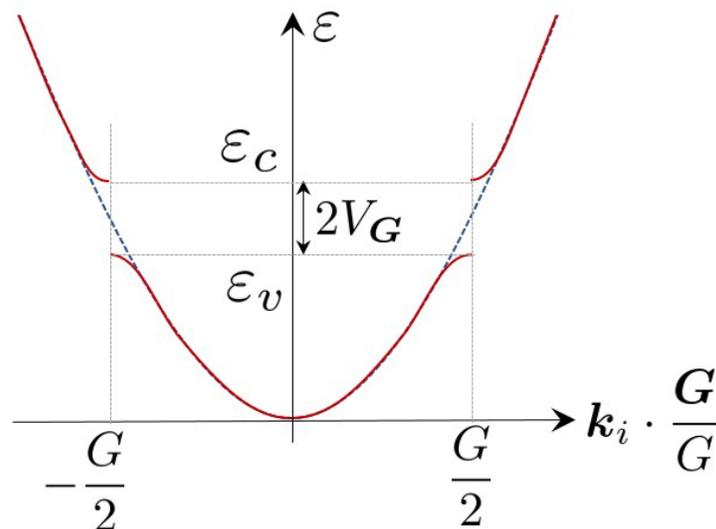
**Métal**



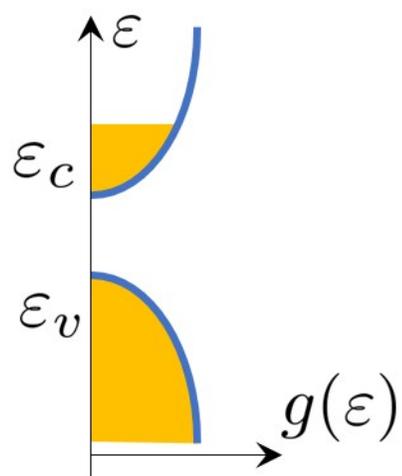


# 3. Semi-conducteurs et jonctions

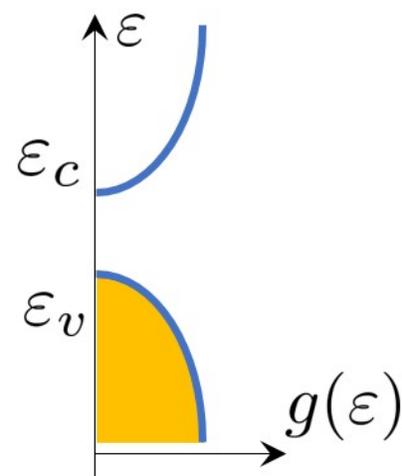
## Zone réduite



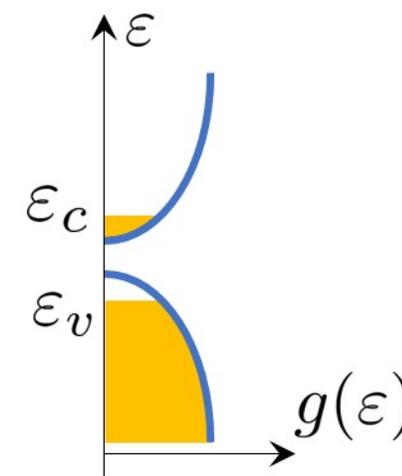
(a)



(b)



(c)



(d)



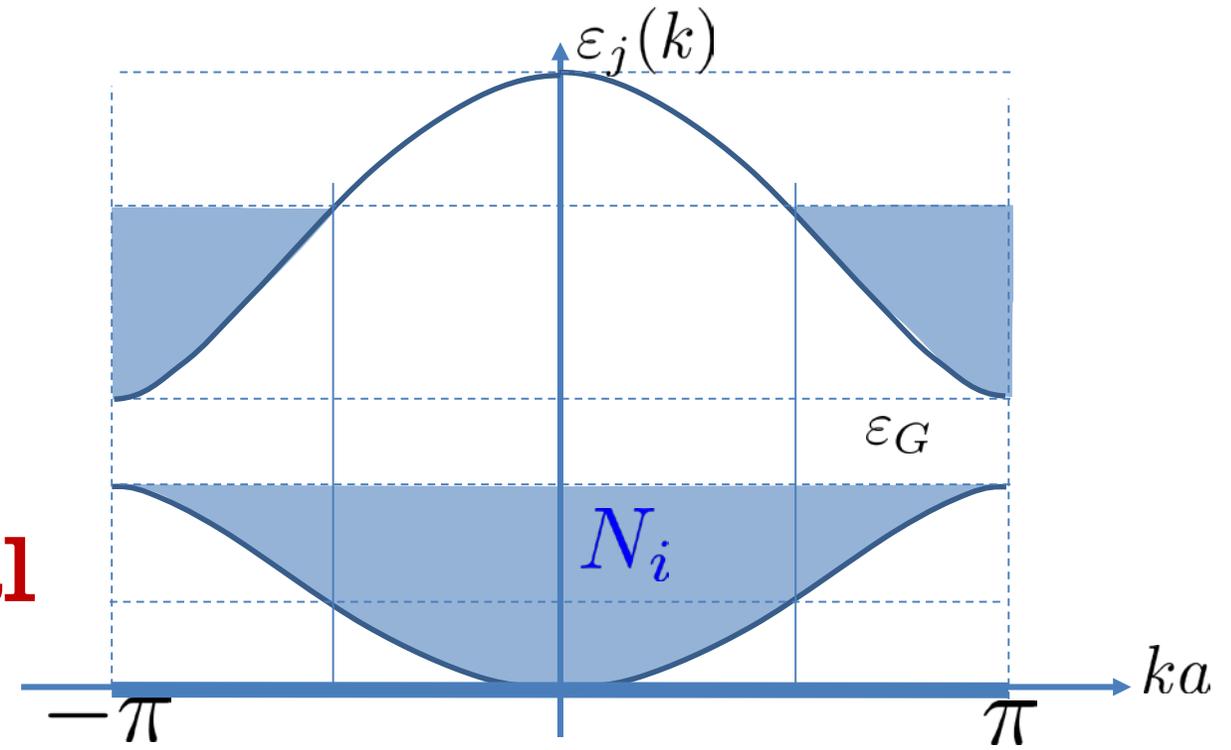
## 2- Bandes, structure et remplissage

**Electrons et trous**  $\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$

Nombre **impair** d'électrons par maille

Il y a  $2^3 \times N_1 \times N_2 \times N_3$  **états** accessibles dans la Z.B.

**Métal**





# 3. Semi-conducteurs et jonctions

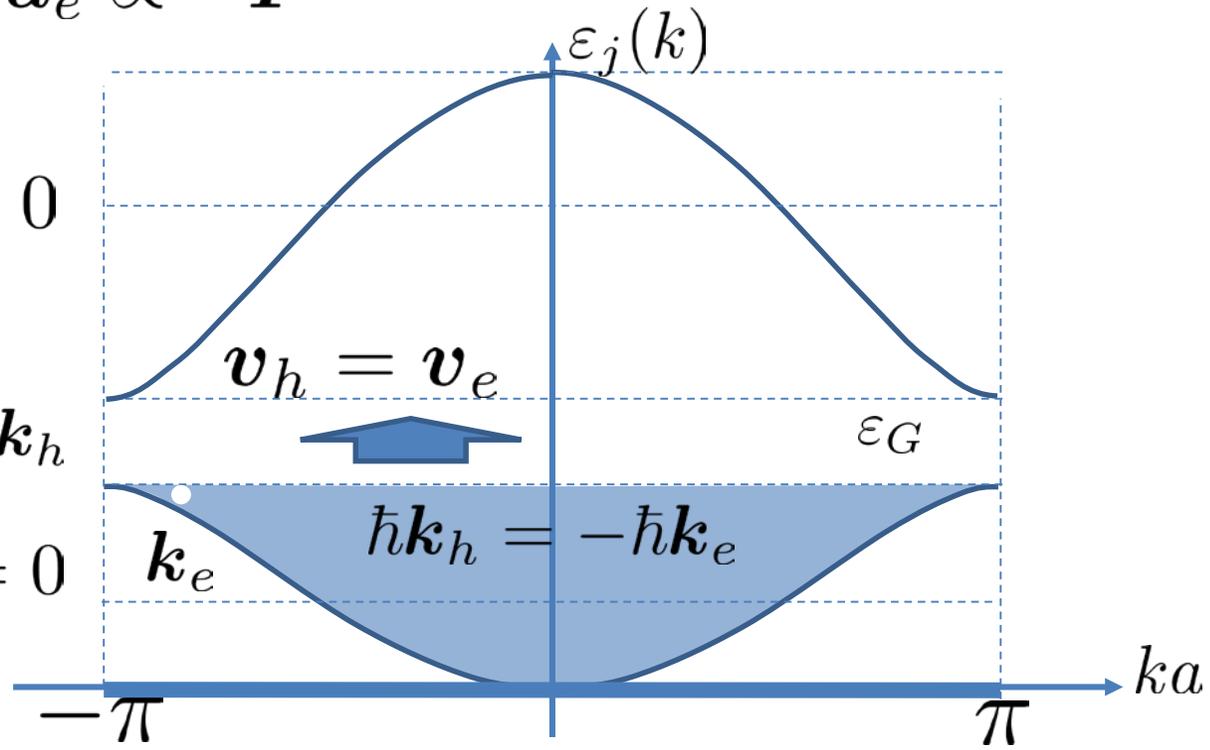
$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$$

$$a_e = \frac{1}{m^*} F \quad \Rightarrow \quad a_e \propto -F$$

$$m_h^* = -m_e^* > 0$$

$$\sum_{val} \hbar \mathbf{k} - \hbar \mathbf{k}_e = \hbar \mathbf{k}_h$$

$$\sum_{val} \hbar \mathbf{k} = 0$$





### 3. Semi-conducteurs et jonctions

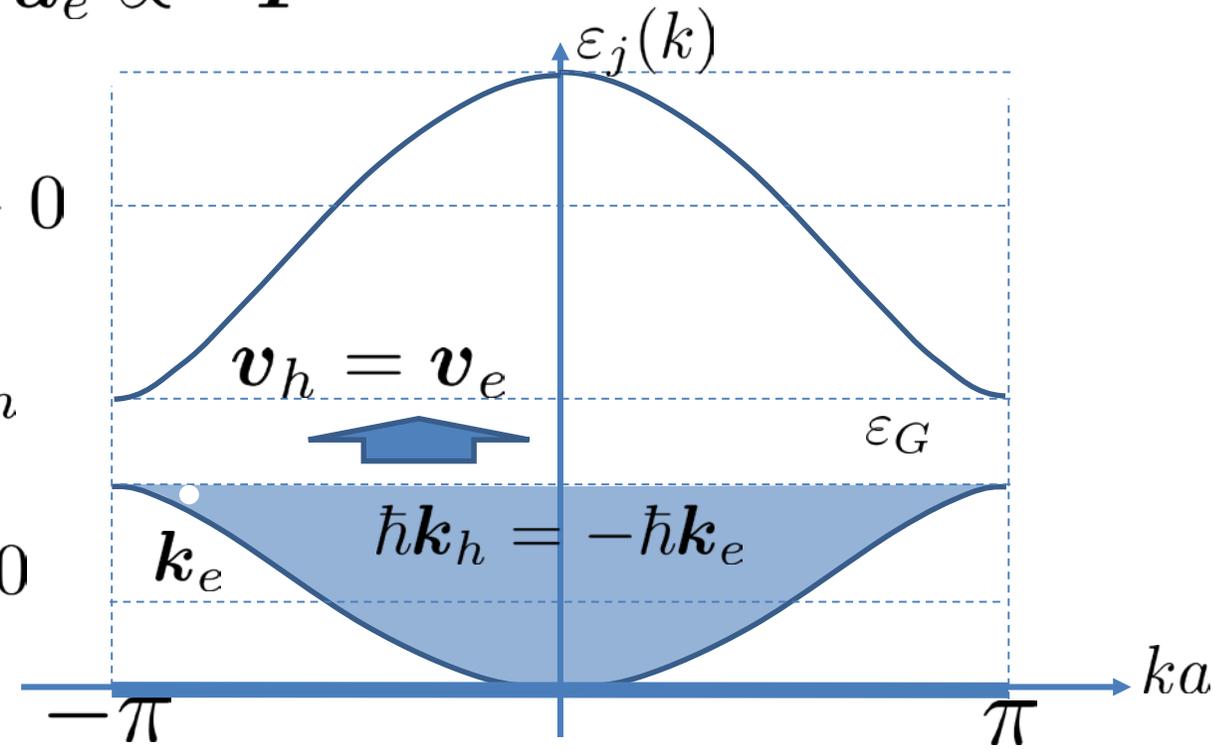
$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$$

$$\mathbf{a}_e = \frac{1}{m^*} \mathbf{F} \quad \Rightarrow \quad \mathbf{a}_e \propto -\mathbf{F}$$

$$q_h^* = -q_e^* > 0 \quad m_h^* = -m_e^* > 0$$

$$\mathbf{j}_h = \sum_{val} \mathbf{j} - \frac{q_e}{V} \mathbf{v}_e = \frac{q_h}{V} \mathbf{v}_h$$

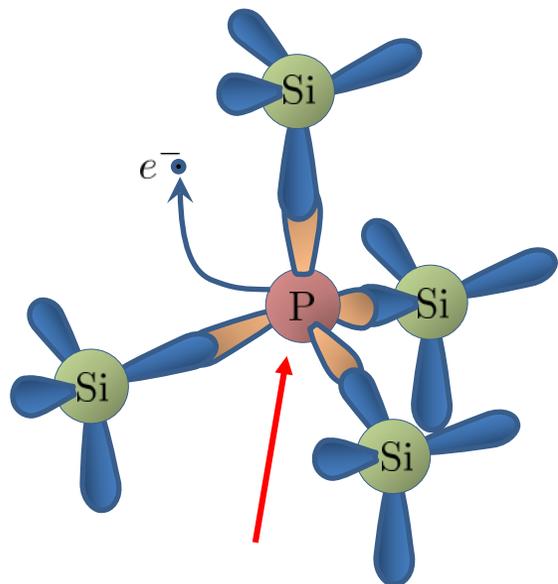
$$\sum_{val} \mathbf{j} = 0$$



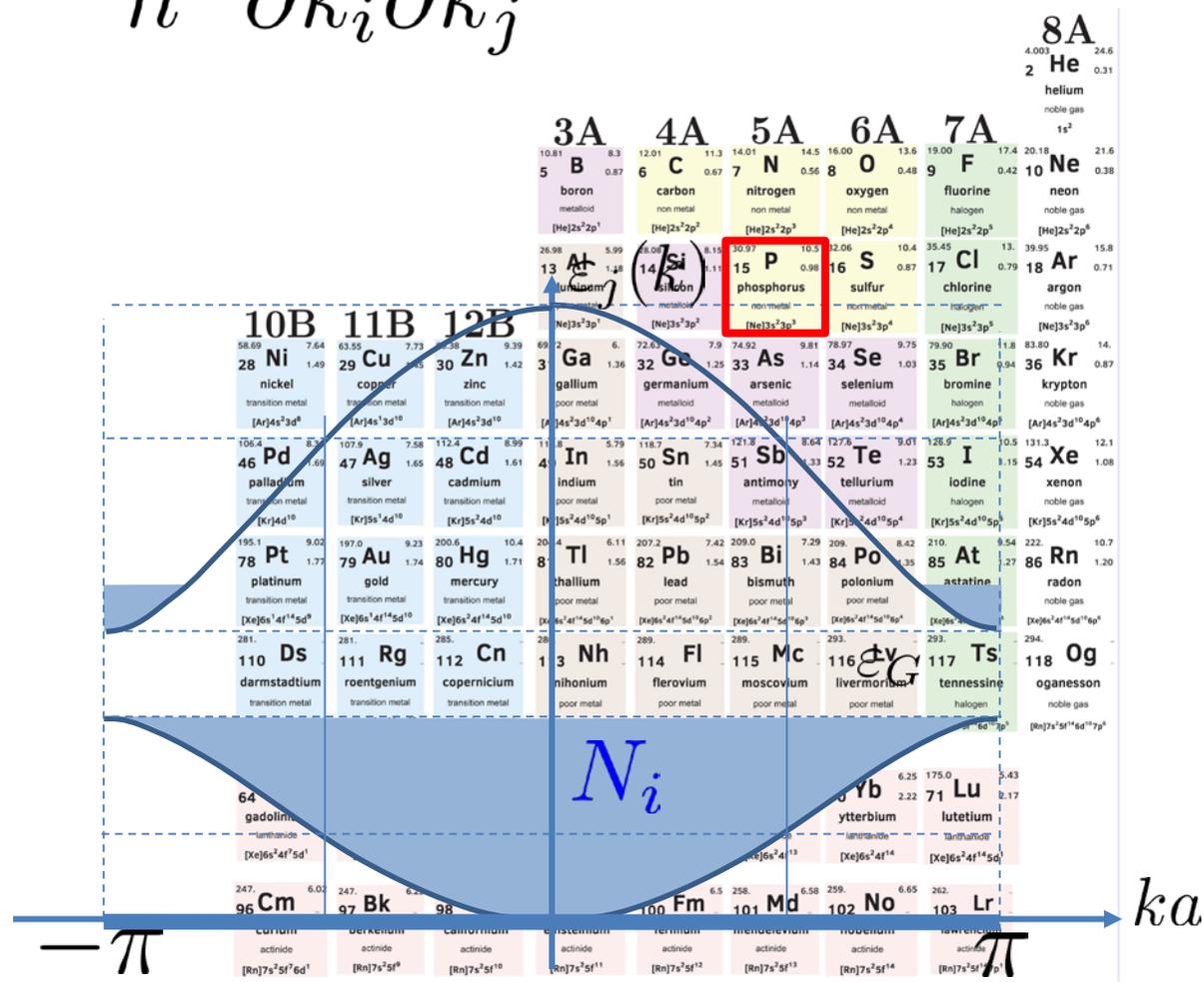
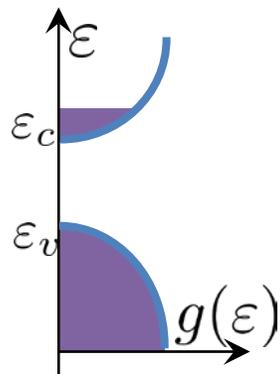
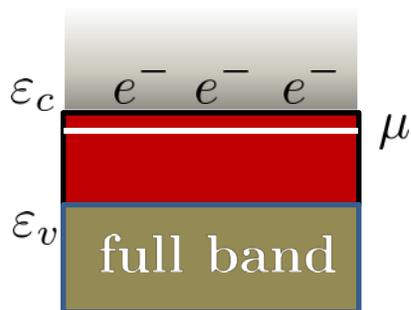


# 3. Semi-conducteurs et jonctions

$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$$



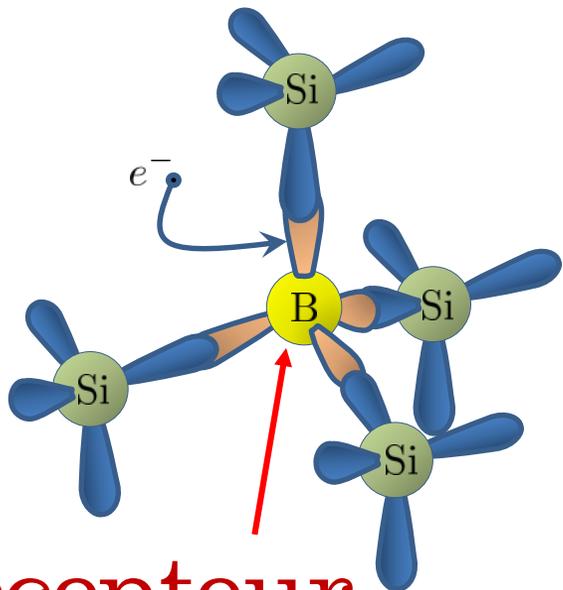
donneur



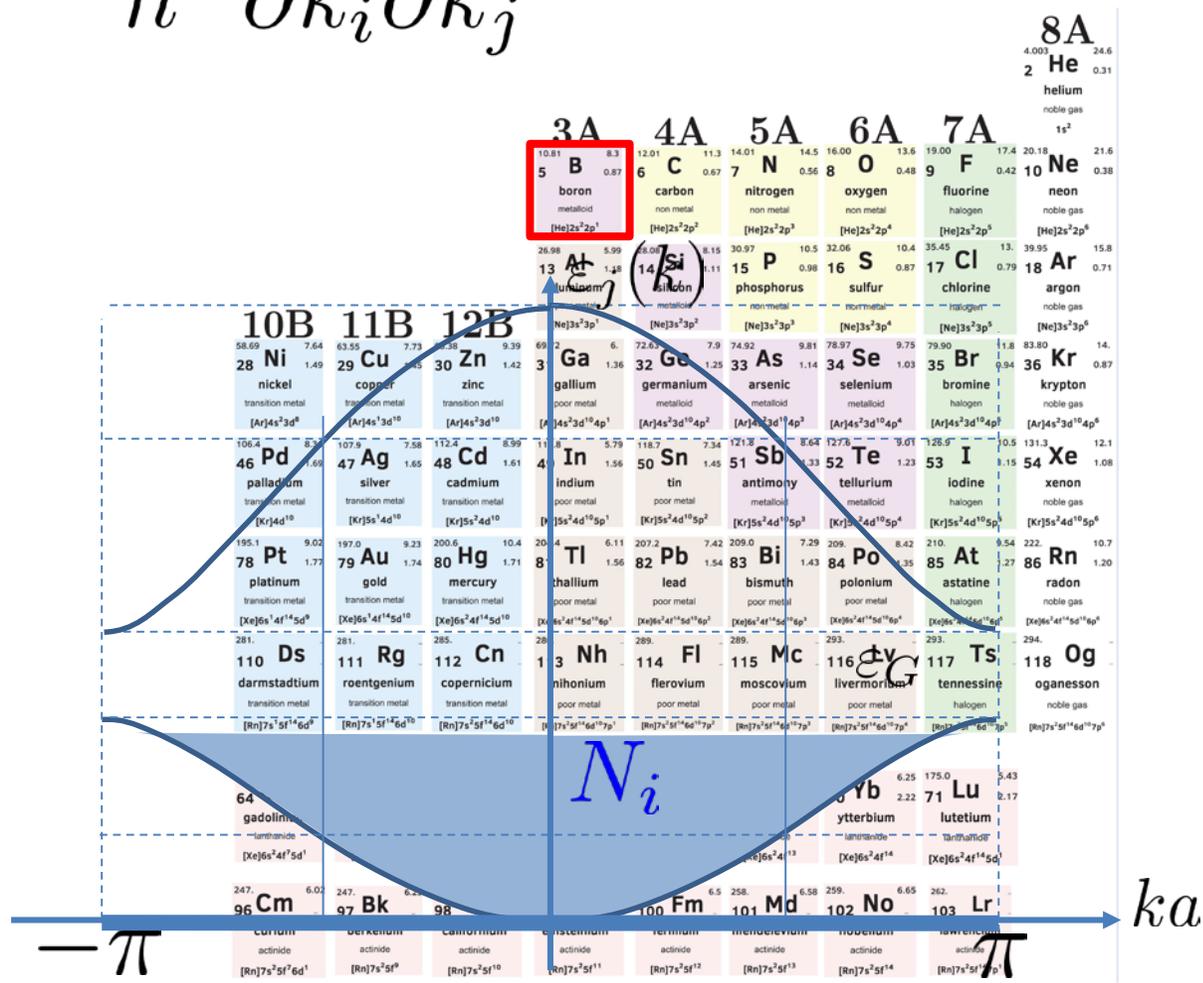
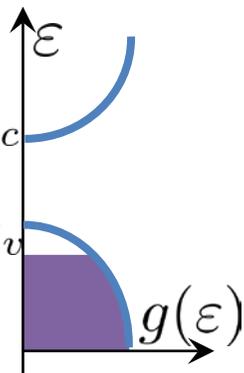
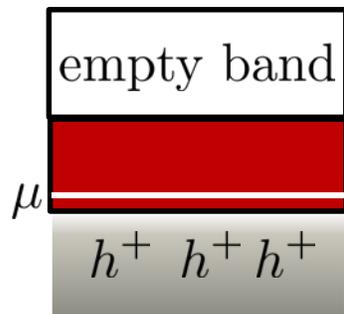


# 3. Semi-conducteurs et jonctions

$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}$$

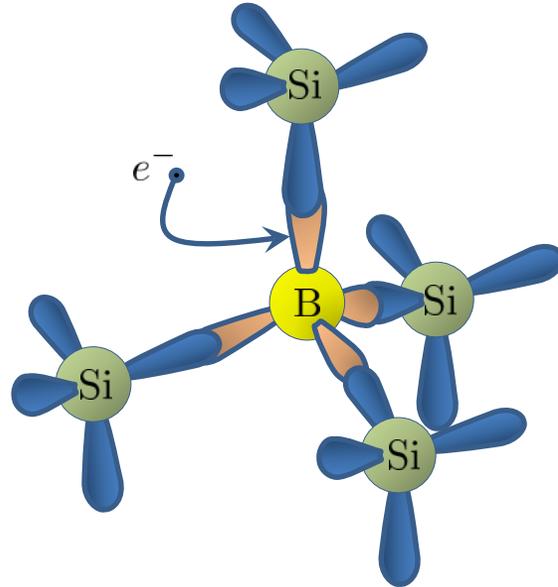
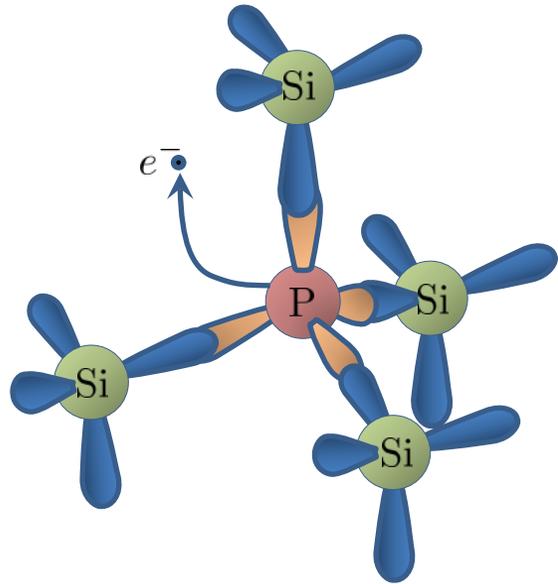


accepteur

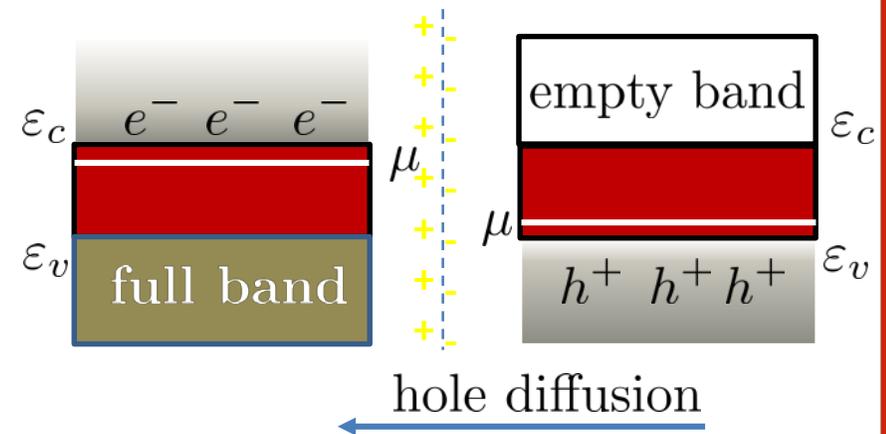
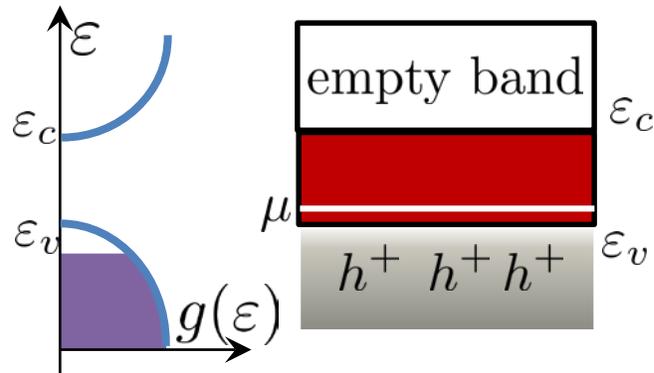
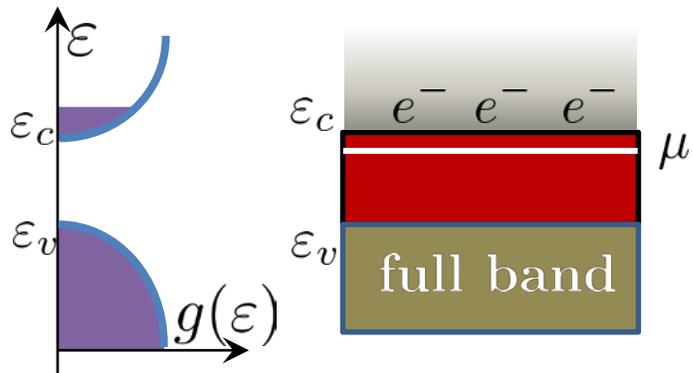




# 3. Semi-conducteurs et jonctions

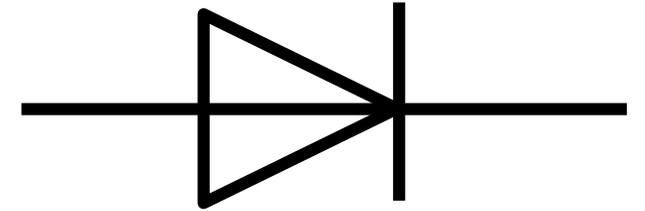
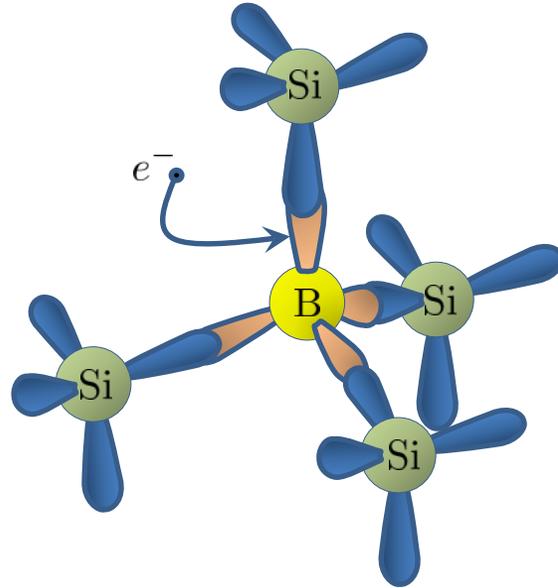
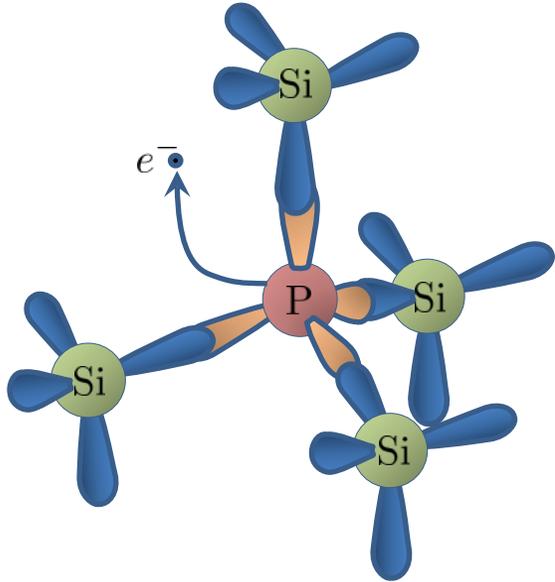


electron diffusion

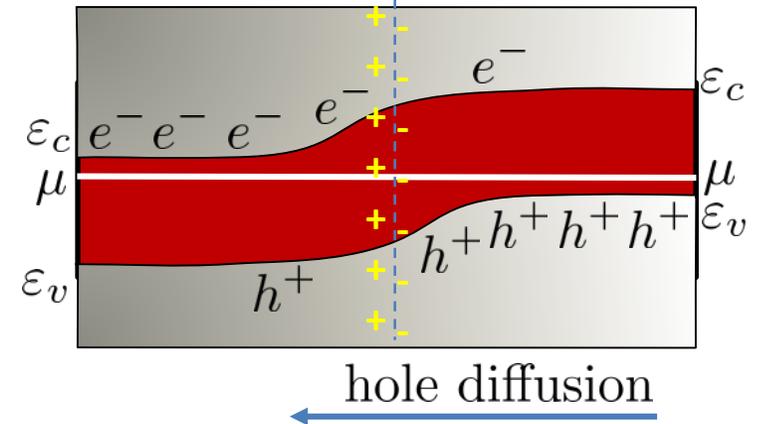




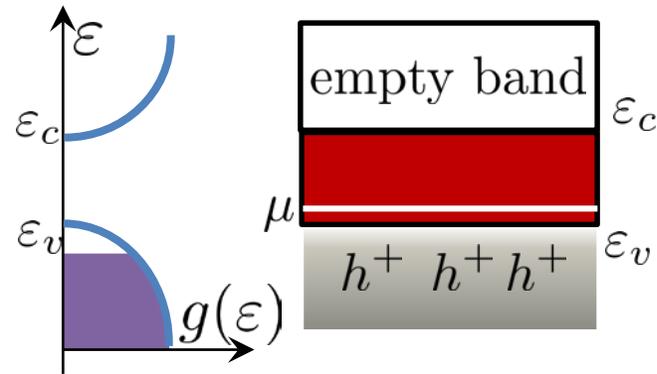
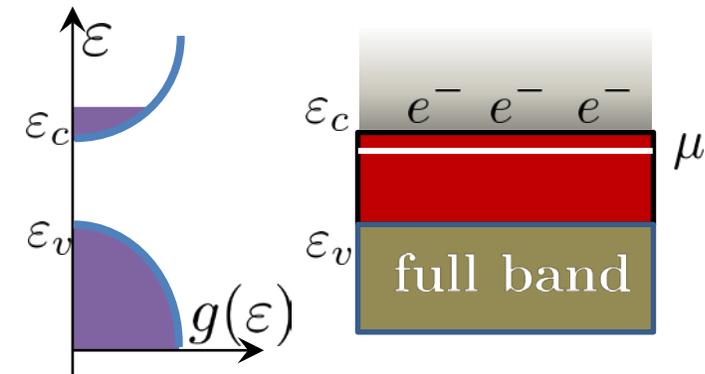
# 3. Semi-conducteurs et jonctions



electron diffusion



hole diffusion



(d)