

La science quantique

Une vision singulière

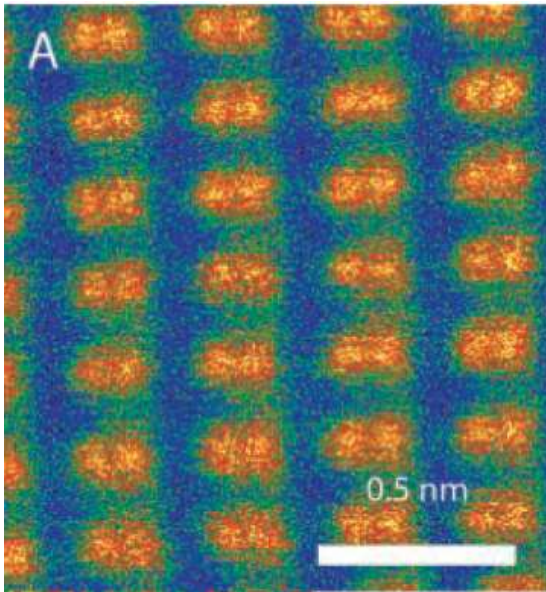
V) Bandes et hétérostructures

P.A. Besse

Formation de bandes

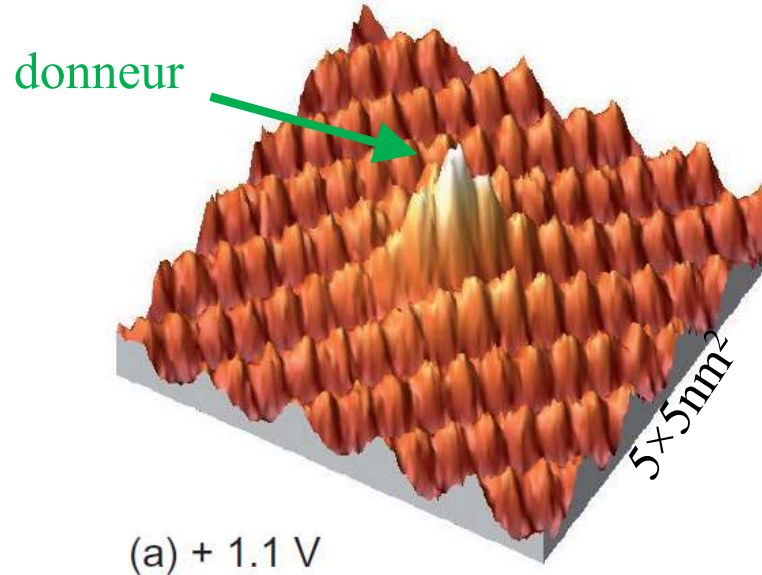
Réseau cristallin: images STM (Scanning Tunnel Microscope)

Silicium
[112]-orientation



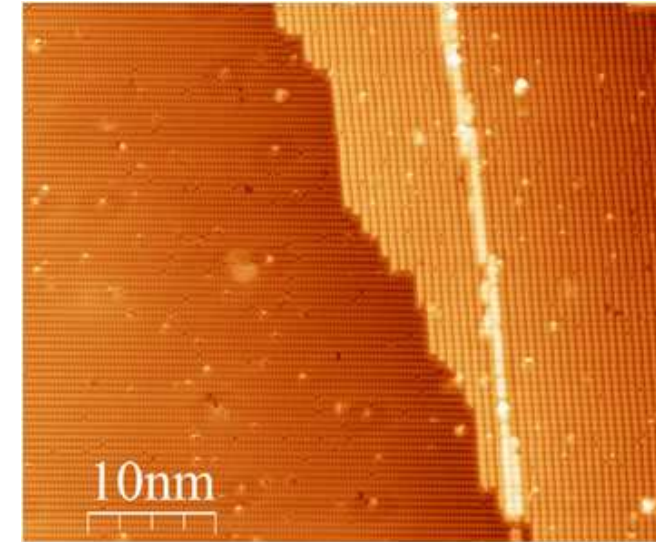
P.D.Nellist et al. « Direct Sub-Angstrom Imaging of a Crystal Lattice », Science, Vol. 305, 2004, p. 1741

N-doped Si
(111)-2×1 surface



C.Sürgers et al., «Electronic disorder of P- and B-doped Si at the metal-insulator transition investigated by scanning tunnelling microscopy and electronic transport», New Journal of Physics 15 (2013)

Silicium
(100)-surface

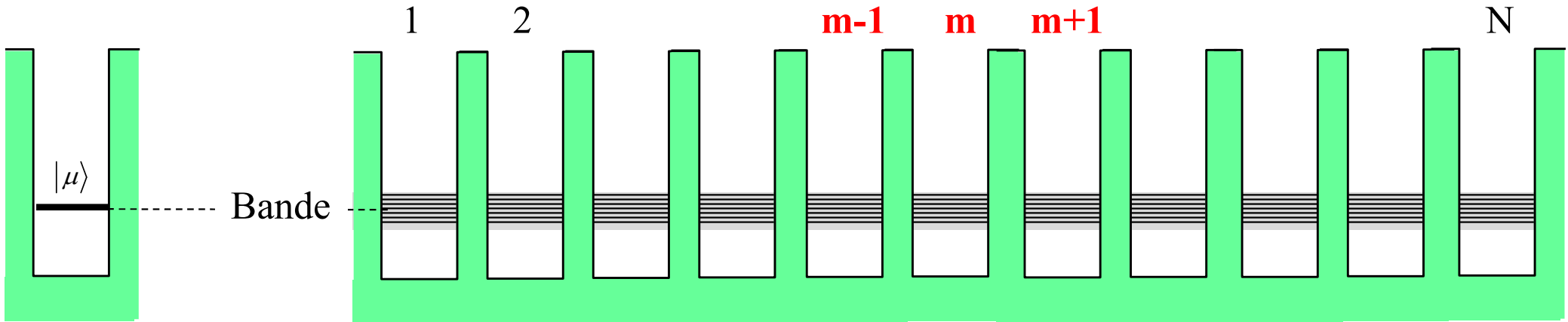


<http://www.nist.gov/pml/div683/grp02/abdm.cfm>



Le silicium et un réseau cristallin, on peut le décrire par des «modes globaux» et interpréter les particules comme des «paquets d'ondes» dans ce réseau.

Chaîne de puits couplés



$$H = \begin{pmatrix}
 \bar{E} & -T & 0 & 0 & 0 & 0 & 0 & -T \\
 -T & \bar{E} & -T & 0 & 0 & 0 & 0 & 0 \\
 0 & \dots & \dots & \dots & 0 & 0 & 0 & 0 \\
 0 & 0 & -T & \bar{E} & -T & 0 & 0 & 0 \\
 0 & 0 & 0 & -T & \bar{E} & -T & 0 & 0 \\
 0 & 0 & 0 & 0 & -T & \bar{E} & -T & 0 \\
 0 & 0 & 0 & 0 & 0 & \dots & \dots & -T \\
 -T & 0 & 0 & 0 & 0 & 0 & -T & \bar{E}
 \end{pmatrix}$$

$$|\psi\rangle \cong \begin{pmatrix}
 \alpha_1 \\
 \alpha_2 \\
 \vdots \\
 \alpha_{m-1} \\
 \alpha_m \\
 \alpha_{m+1} \\
 \vdots \\
 \alpha_N
 \end{pmatrix} \cdot \begin{pmatrix}
 |\mu(x-x_1)\rangle \\
 |\mu(x-x_2)\rangle \\
 \vdots \\
 |\mu(x-x_{m-1})\rangle \\
 |\mu(x-x_m)\rangle \\
 |\mu(x-x_{m+1})\rangle \\
 \vdots \\
 |\mu(x-L)\rangle
 \end{pmatrix}$$

Recherche des modes et valeurs propres:

$$H = \begin{pmatrix} \bar{E} & -T & 0 & 0 & 0 & 0 & 0 & -T \\ -T & \bar{E} & -T & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & \dots & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & -T & \bar{E} & -T & 0 & 0 & 0 \\ 0 & 0 & 0 & -T & \bar{E} & -T & 0 & 0 \\ 0 & 0 & 0 & 0 & -T & \bar{E} & -T & 0 \\ 0 & 0 & 0 & 0 & 0 & \dots & \dots & -T \\ -T & 0 & 0 & 0 & 0 & 0 & -T & \bar{E} \end{pmatrix}$$

Supposition:

$$|\varphi_\delta\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{i(1)\delta} \\ e^{i(2)\delta} \\ \vdots \\ e^{i(m-1)\delta} \\ e^{i(m)\delta} \\ e^{i(m+1)\delta} \\ \vdots \\ e^{i(N)\delta} \end{pmatrix}$$

$$H \cdot |\varphi_\delta\rangle = E |\varphi_\delta\rangle$$



$$-T \cdot e^{i(m-1)\delta} + \bar{E} \cdot e^{i(m)\delta} - T \cdot e^{i(m+1)\delta} = E \cdot e^{i(m)\delta}$$



$$E(\delta) = \bar{E} - 2T \cdot \cos(\delta)$$

	Vecteurs de Fourier	Orbitales
$ \varphi_\delta\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{i(1)\delta} \\ e^{i(2)\delta} \\ \vdots \\ e^{i(m-1)\delta} \\ e^{i(m)\delta} \\ e^{i(m+1)\delta} \\ \vdots \\ e^{i(N)\delta} \end{pmatrix}$	$\xrightarrow[\substack{\delta = K \cdot a \\ x_m = m \cdot a}]{}$	$ \varphi_\delta\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} e^{iK \cdot x_1} \\ e^{iK \cdot x_2} \\ \vdots \\ e^{iK \cdot x_{m-1}} \\ e^{iK \cdot x_m} \\ e^{iK \cdot x_{m+1}} \\ \vdots \\ e^{iK \cdot L} \end{pmatrix}$
		$\begin{aligned} &\cdot \mu(x-x_1)\rangle \\ &\cdot \mu(x-x_2)\rangle \\ &\cdot \mu(x-x_{m-1})\rangle \\ &\cdot \mu(x-x_m)\rangle \\ &\cdot \mu(x-x_{m+1})\rangle \\ &\cdot \mu(x-L)\rangle \end{aligned}$

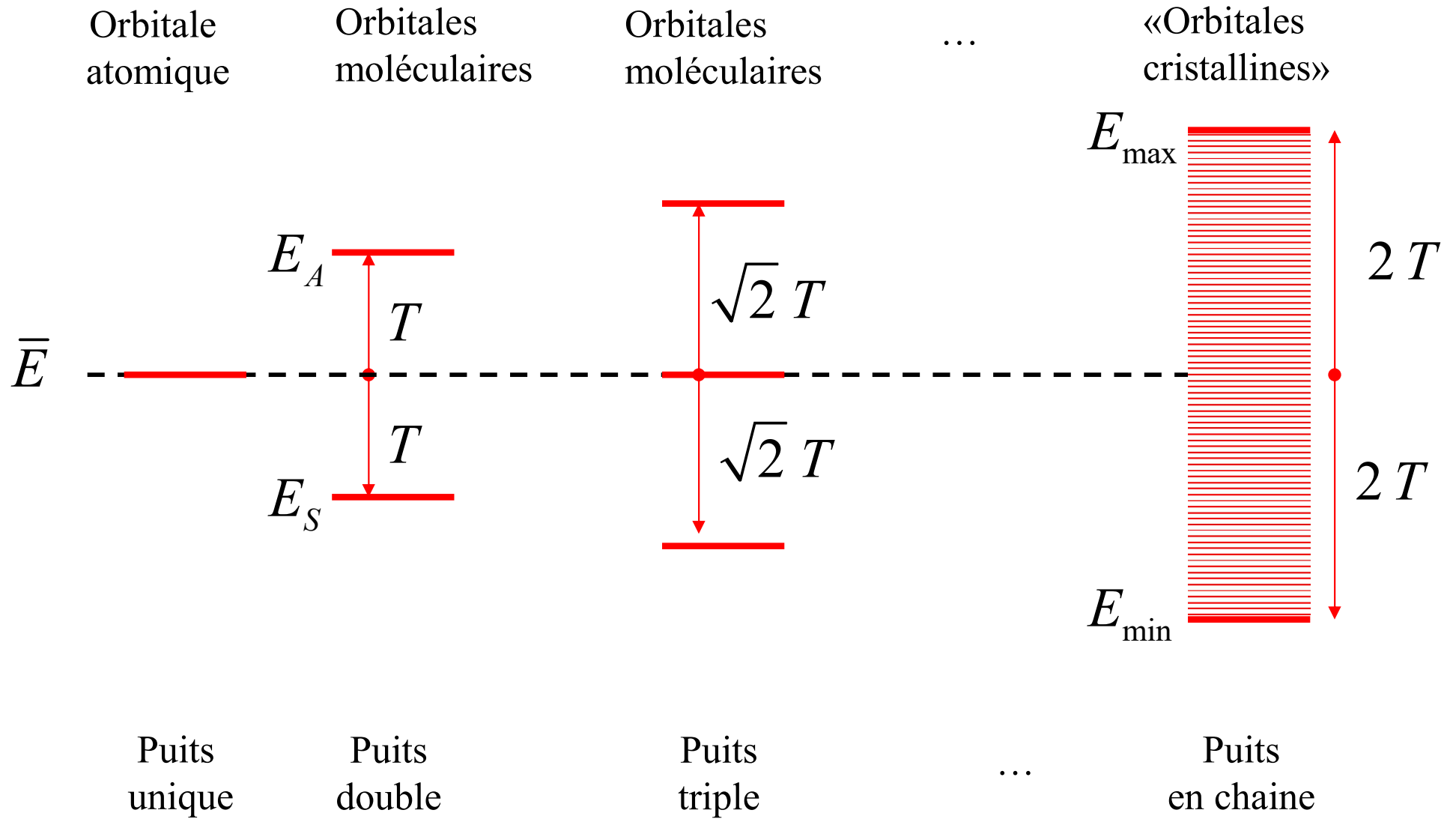
Les vecteurs **K**
sont équidistants

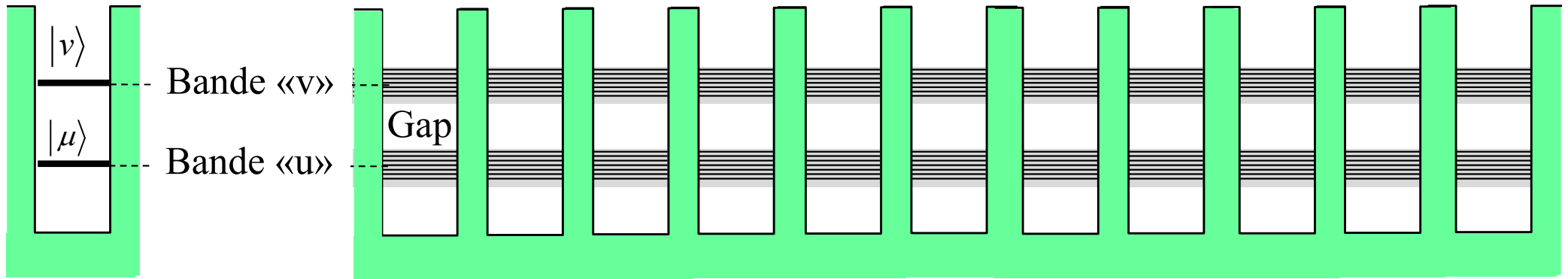
Périodicité:

$$K_n \cdot L = n \cdot 2\pi \Rightarrow K_n = n \cdot \frac{2\pi}{L}$$

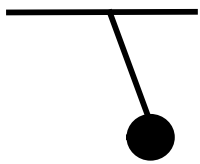
$$n = -\frac{N}{2}, \dots, \frac{N-1}{2}$$

Chaine de puits couplés

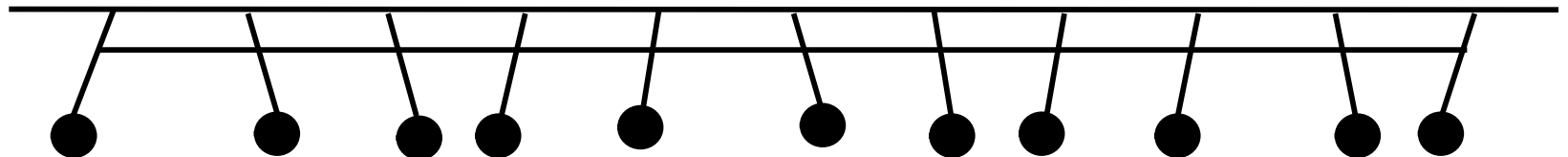




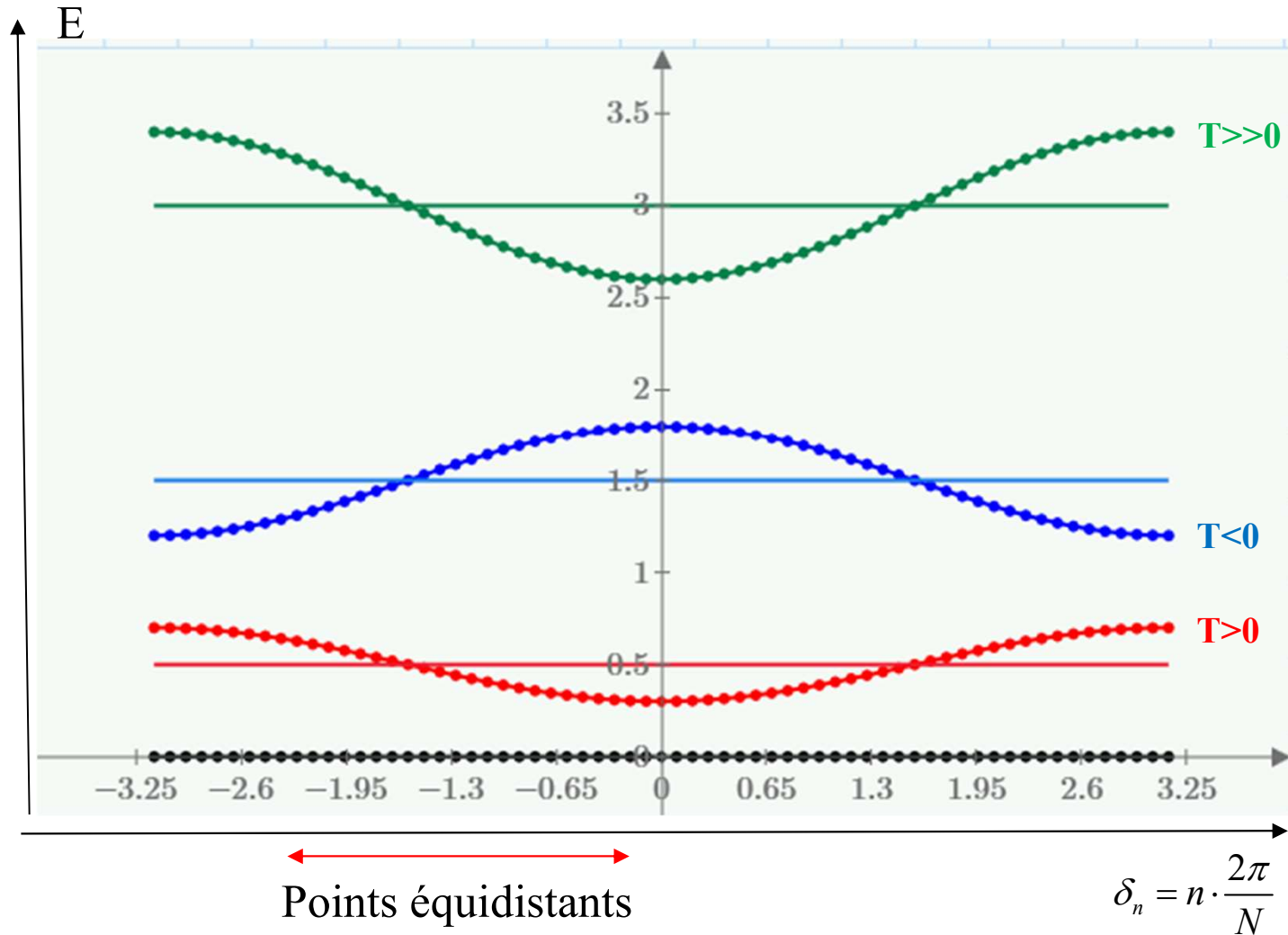
Atome



Cristal



Relation de dispersion et bandes



$$E(\delta) = \bar{E} - 2T \cdot \cos(\delta)$$

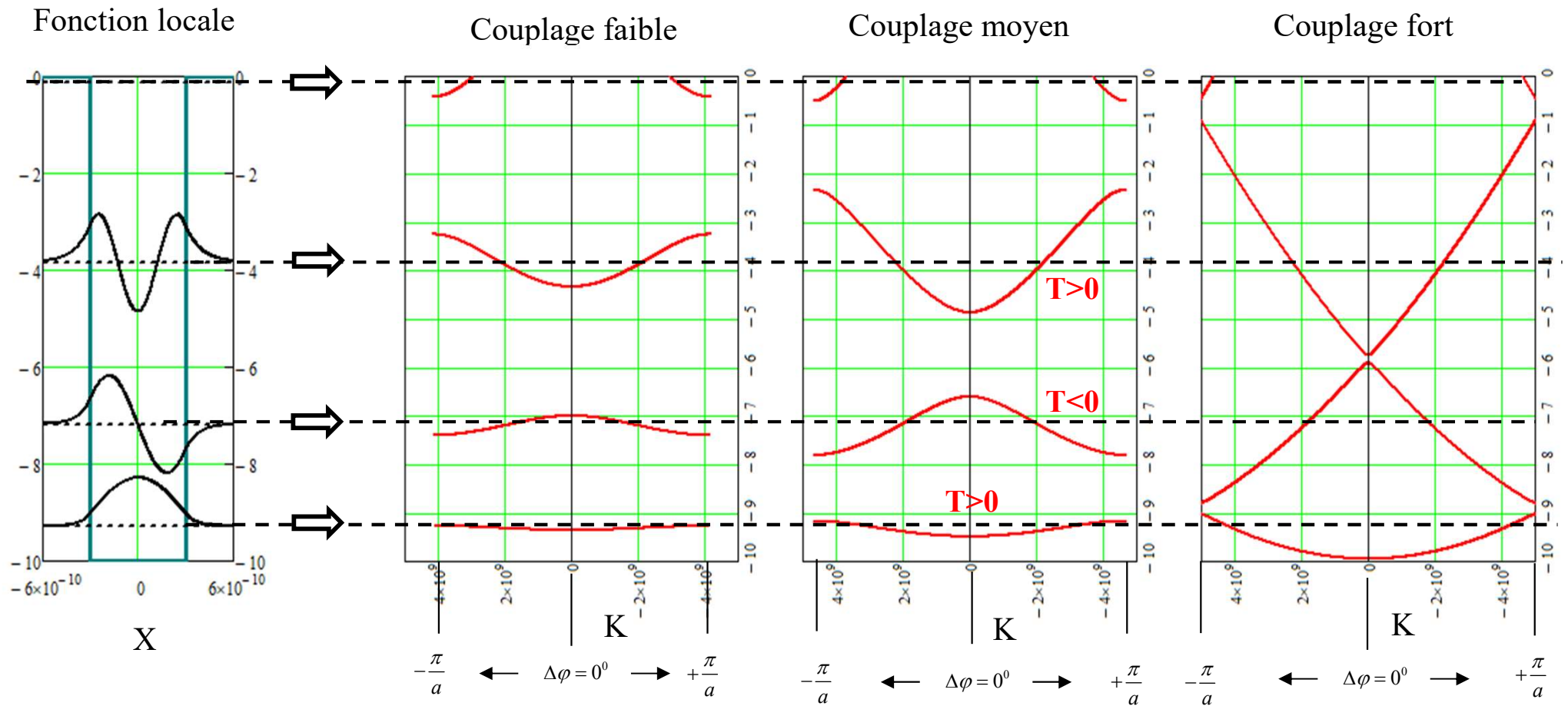
$$K_n = \frac{\delta_n}{a} = n \cdot \frac{2\pi}{L}$$

$$n = -\frac{N}{2}, \dots, \frac{N-1}{2}$$

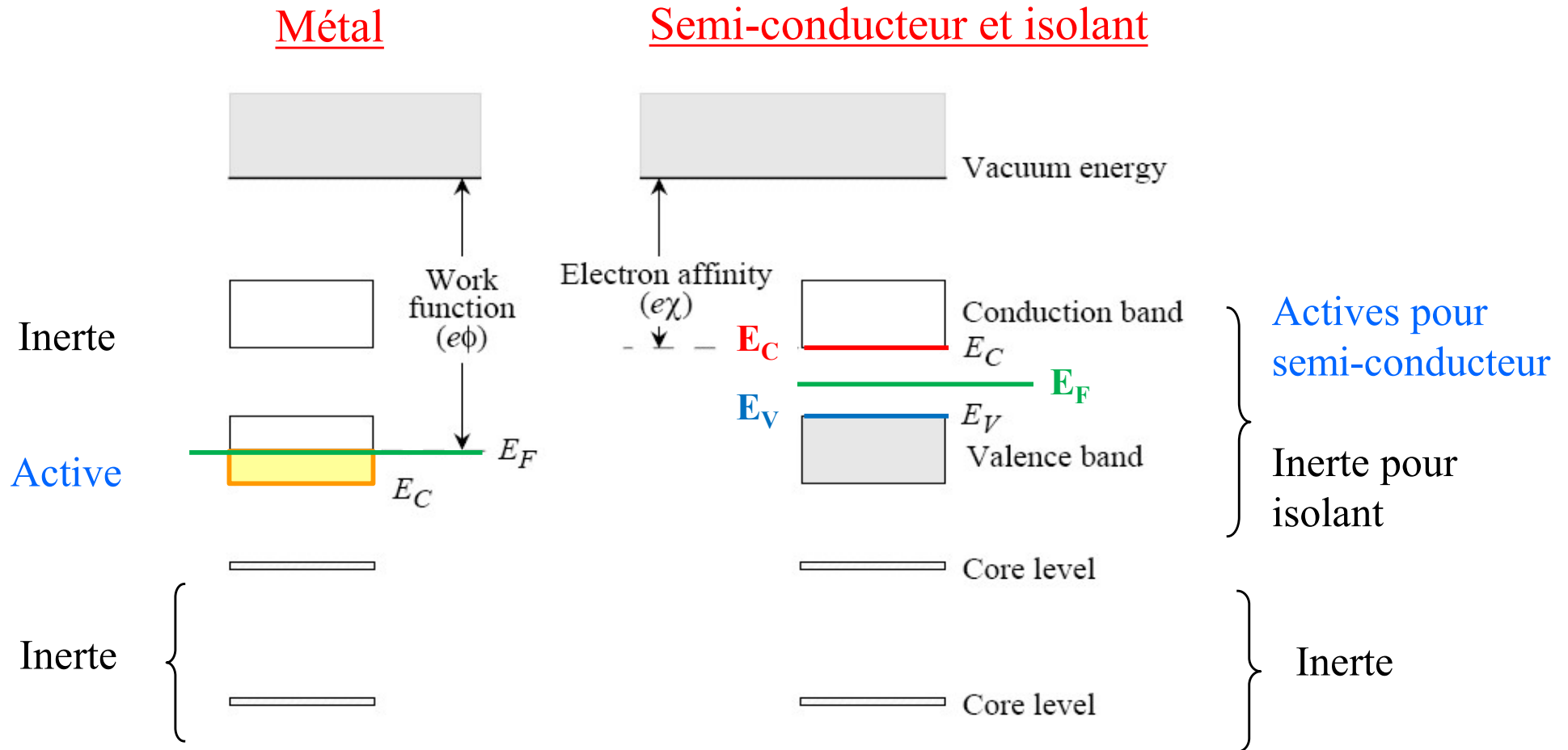
Puits périodiques: formation de bandes

$$K_n = n \cdot \frac{2\pi}{L}$$

$$n = -\frac{N}{2}, \dots, \frac{N-1}{2}$$

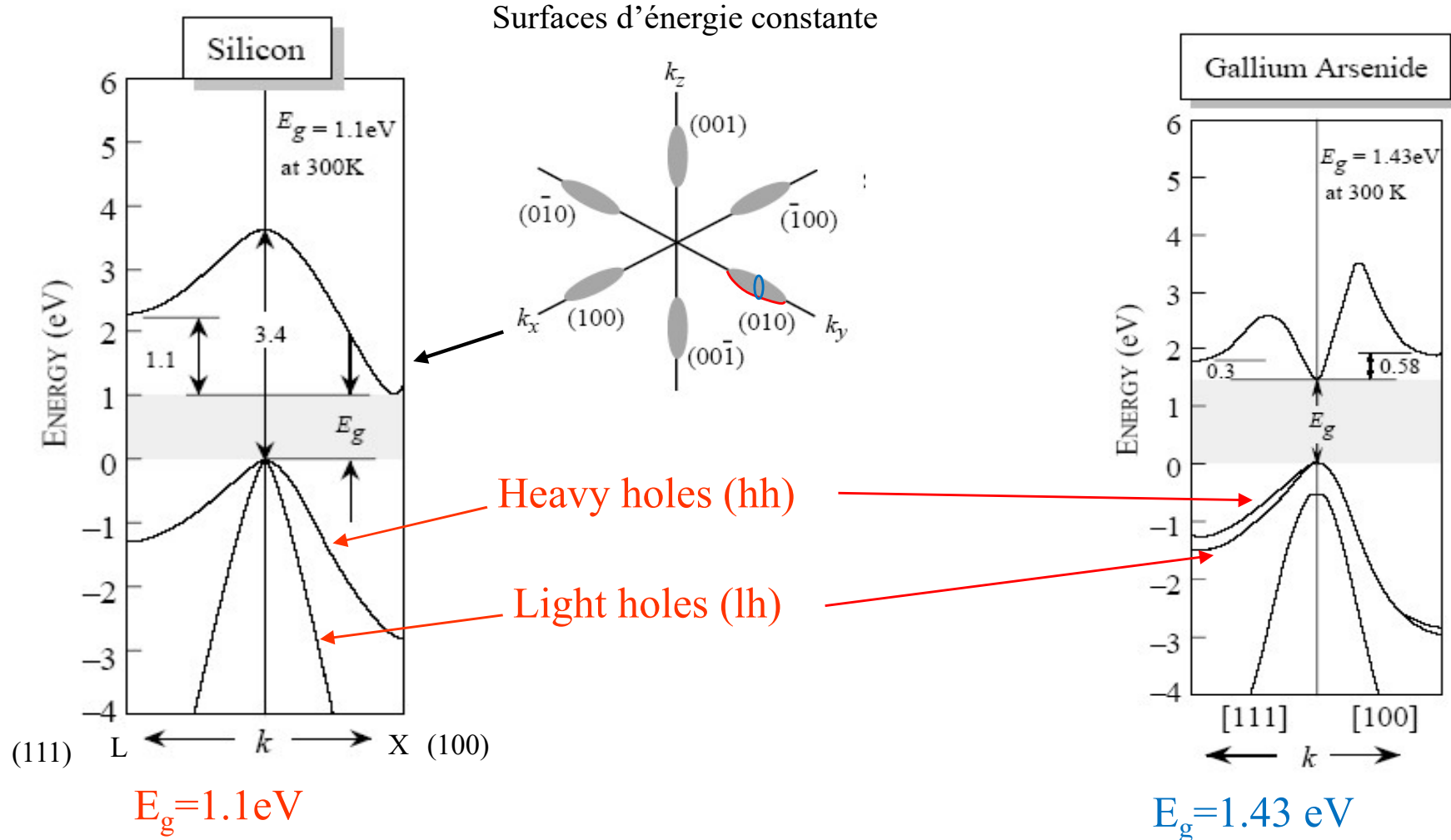


Métal, semi-conducteur, isolant

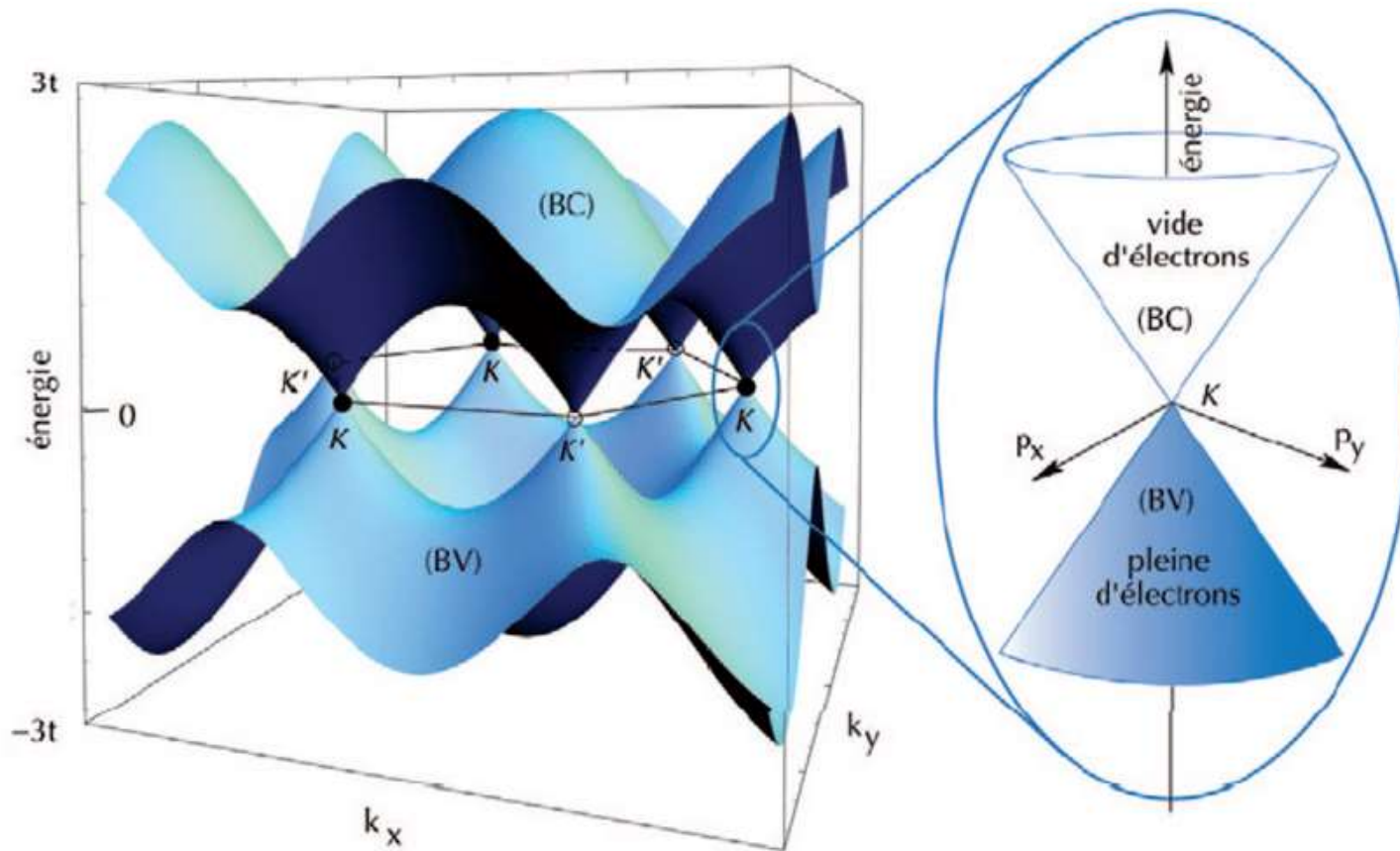


J. Singh "Semiconductor Devices"

Exemples: Si et GaAs



J. Singh "Semiconductor Devices"



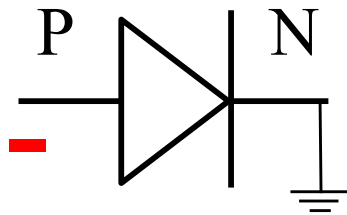
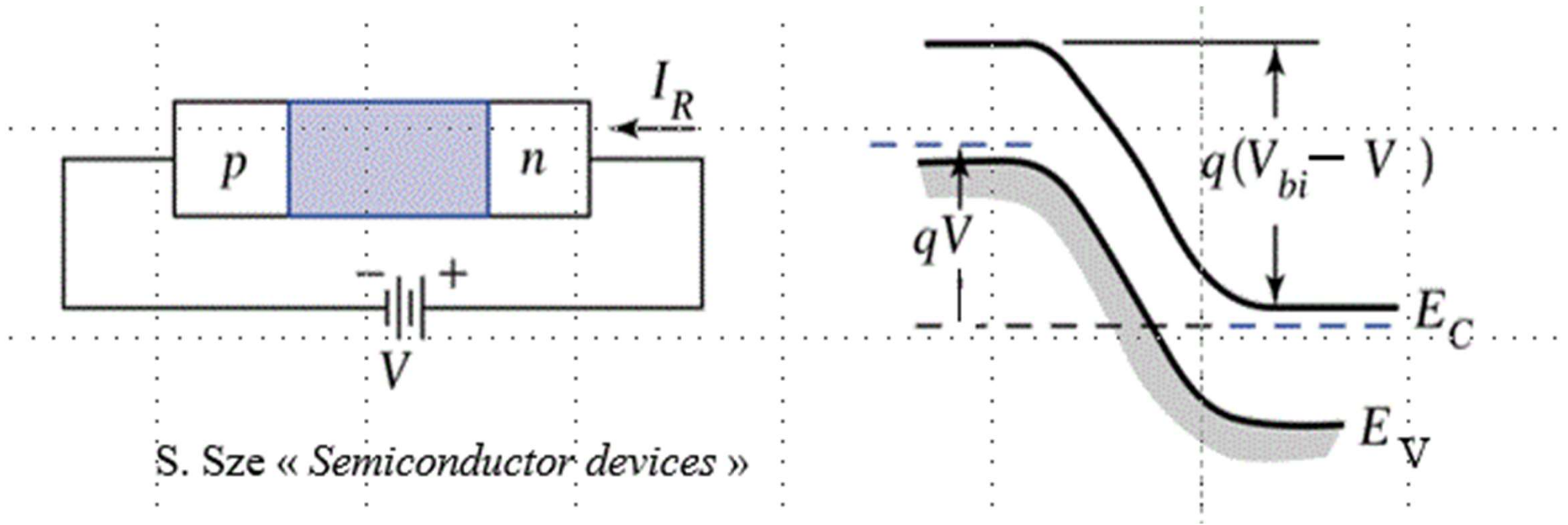
Fermion (électron) de masse nulle !

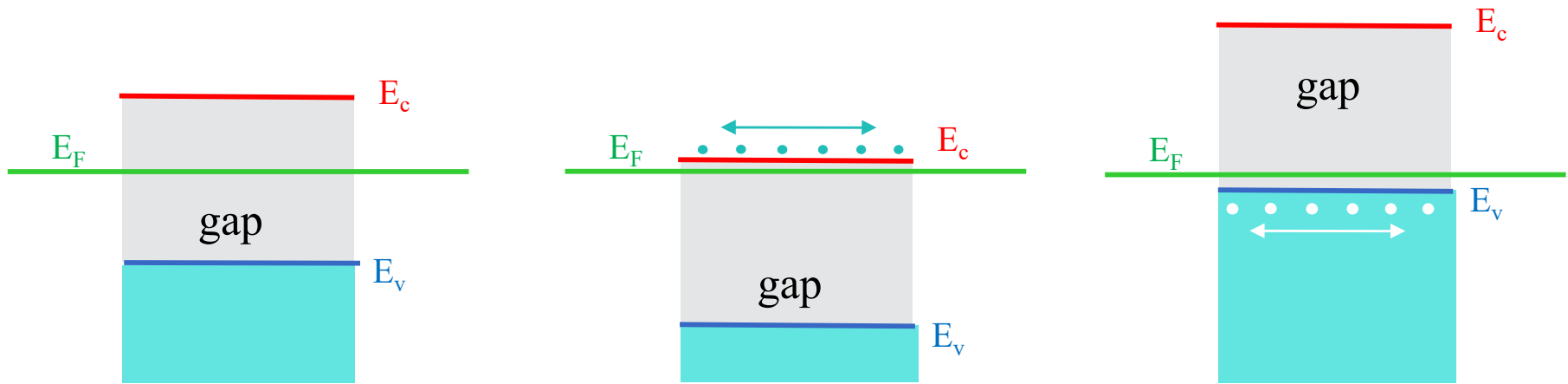
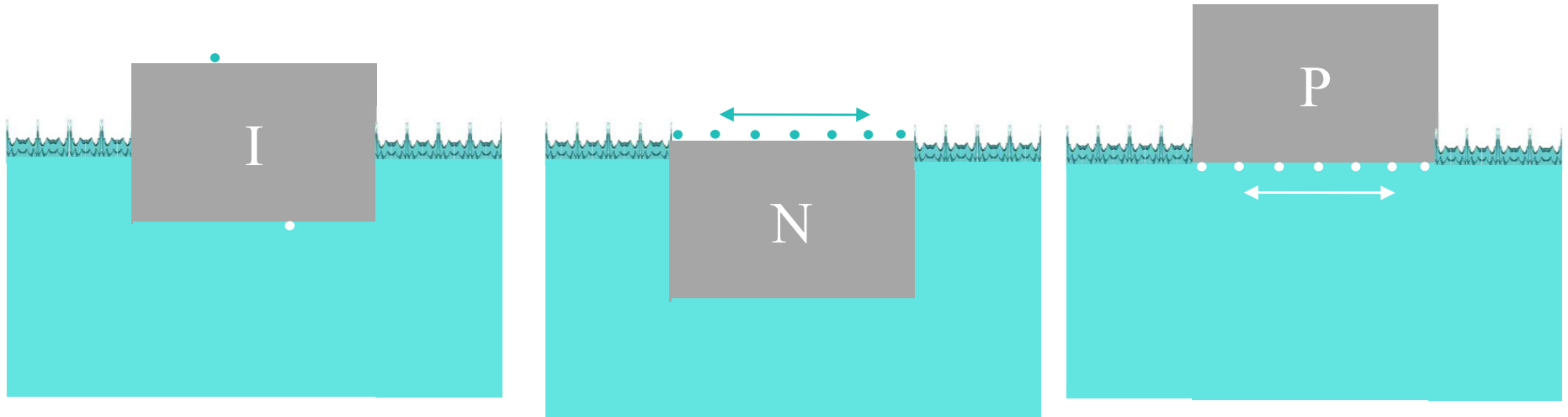
https://www.researchgate.net/figure/Structure-de-bande-electronique-du-graphene-dans-lapproximation-des-liaisons-fortes_fig5_279262409

Equations et inconnues:

Homostructures

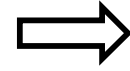
Exemple: jonction PN comment calculer son schéma de bandes ?





3 inconnues:

φ n p



E_{vac} $E_{F,n}$ $E_{F,p}$

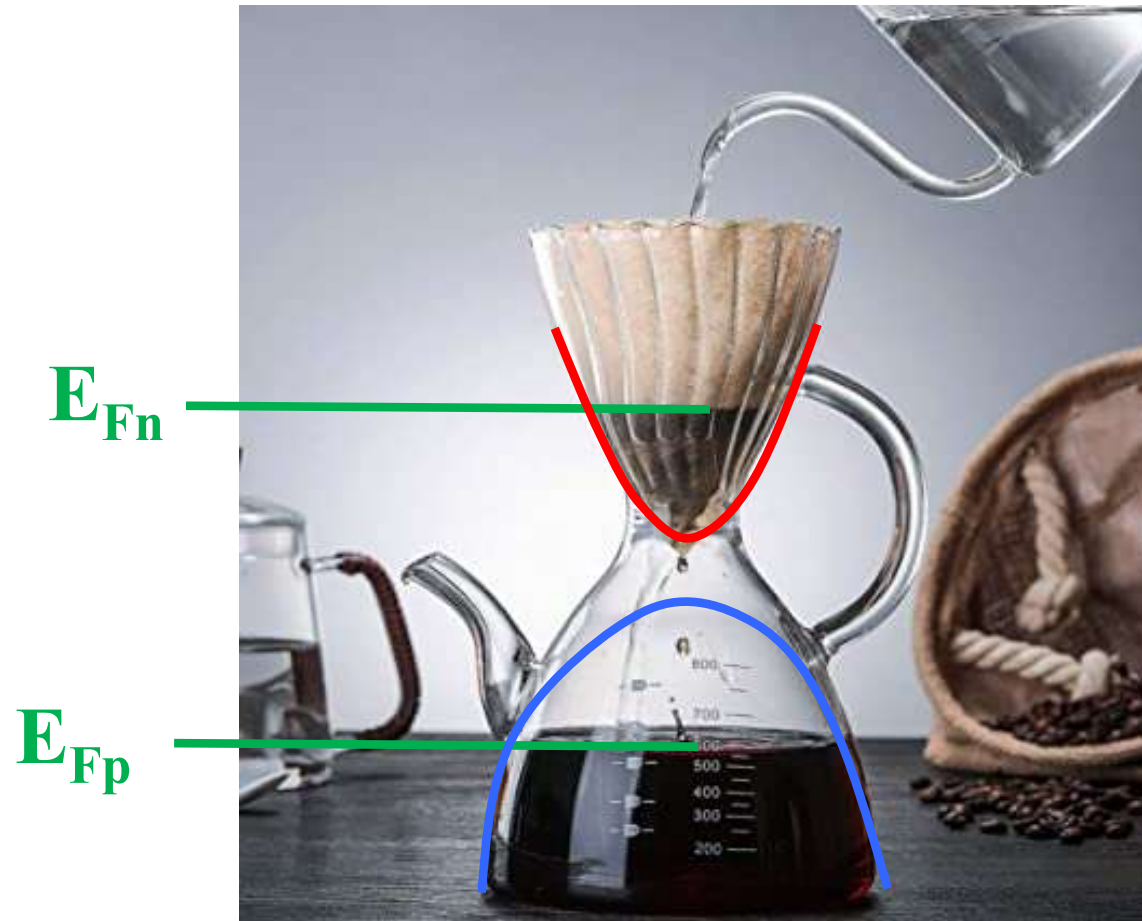
(1) $E_{vac} = -q \cdot \varphi$

(2) $n = N_c \cdot e^{-(E_{vac} - q\chi - E_{F,n})/kT}$

$\vec{j}_n = n\mu_n \cdot \vec{\nabla}(E_{F,n})$

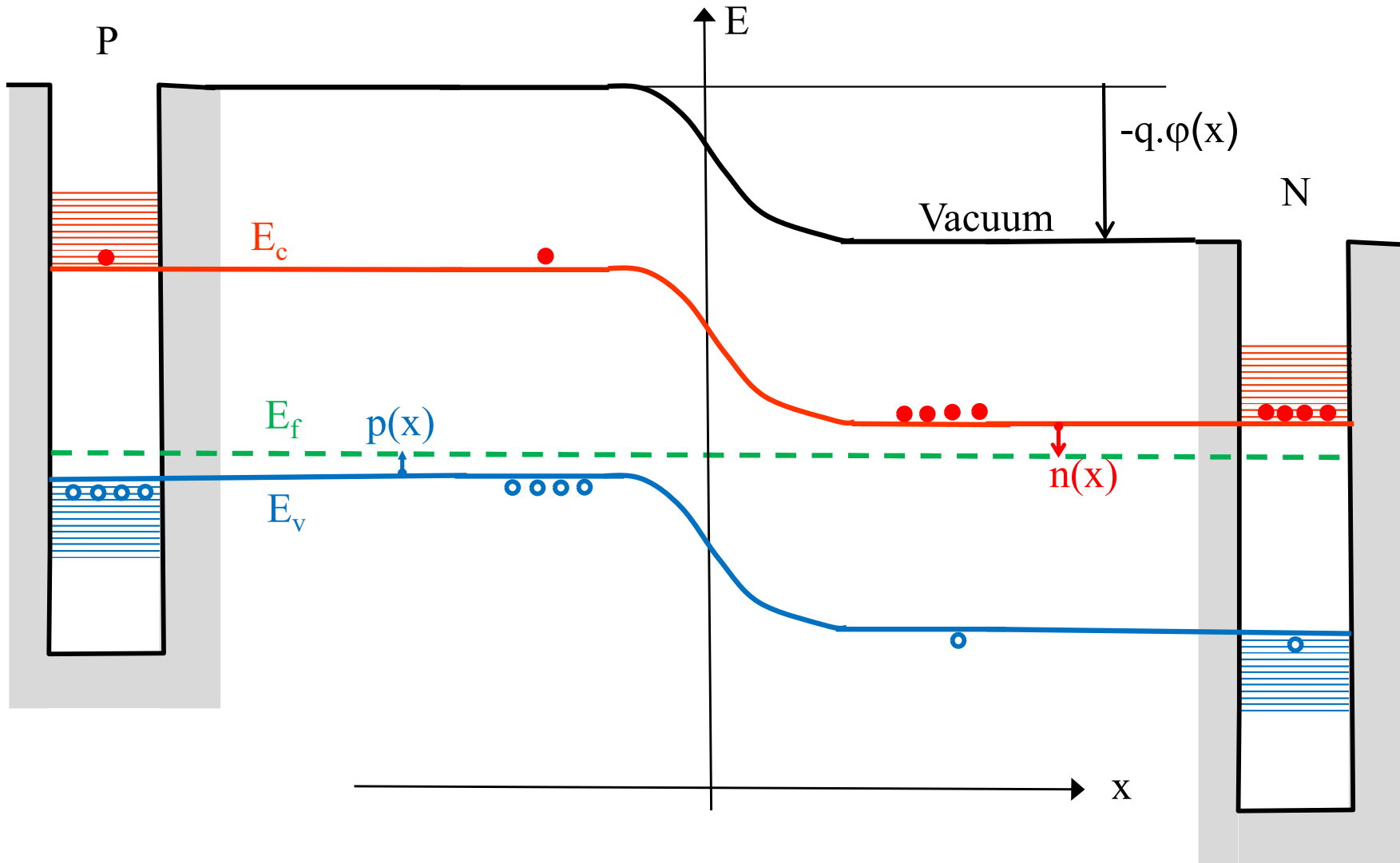
(3) $p = N_v \cdot e^{(E_{vac} - q\chi - E_g - E_{F,p})/kT}$

$\vec{j}_p = p\mu_p \cdot \vec{\nabla}(E_{F,p})$



Quasi-équilibre \rightarrow «quasi-niveaux de Fermi»

Exemple de structure de bandes



1) Energie potentielle

$$E_{pot} = E_{vac} = (-q) \cdot \varphi$$

L'énergie potentielle est l'énergie du vide

2) Maxwell :

$$\text{div}(\vec{E}) = \frac{\rho}{\epsilon_0 \epsilon} = \frac{q(p + N_d^+ - n - N_a^-)}{\epsilon_0 \epsilon}$$

1D \Rightarrow

$$E_x \sim + \int \rho \cdot dx$$

Le champ électrique est l'intégrale des charges nettes

3) Maxwell :

$$\text{rot}(\vec{E}) = -\frac{\partial \vec{B}}{\partial t} = 0 \quad \Rightarrow \quad \vec{E} = -\overrightarrow{\text{grad}}(\varphi) = \frac{1}{q} \overrightarrow{\text{grad}}(E_{vac})$$

1D \Rightarrow

$$E_x \sim + \frac{\partial E_{vac}}{\partial x}$$

Le champ électrique est la pente de l'énergie du vide

4) Equation de Poisson depuis 2) et 3)

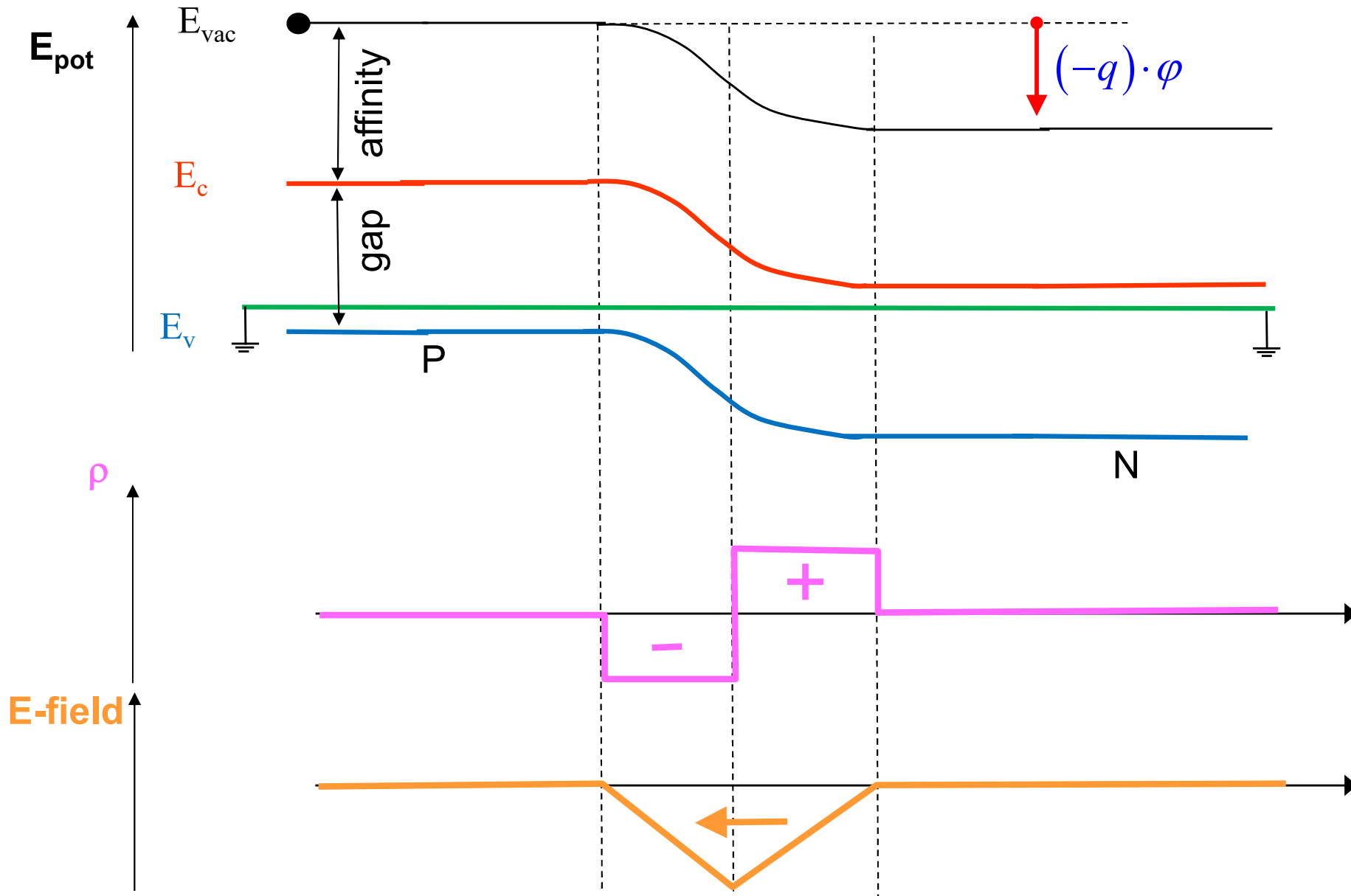
$$\Delta \varphi = -\frac{\rho}{\epsilon_0 \epsilon} = -\frac{q(p + N_d^+ - n - N_a^-)}{\epsilon_0 \epsilon} = -\frac{1}{q} \Delta E_{vac}$$

1D \Rightarrow

$$\rho \sim + \frac{\partial^2 E_{vac}}{\partial x^2}$$

La charge nette est la courbure de l'énergie du vide

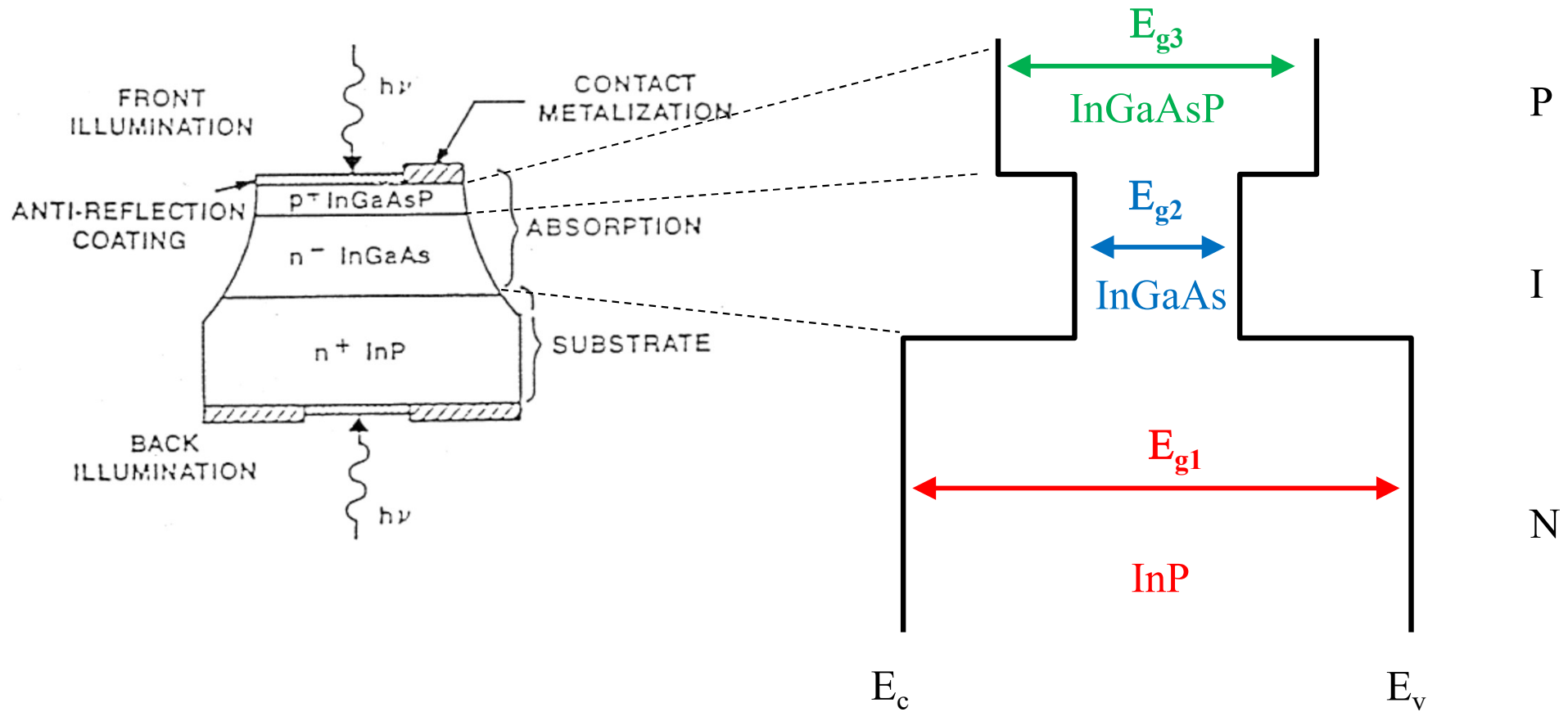
Schéma de bande



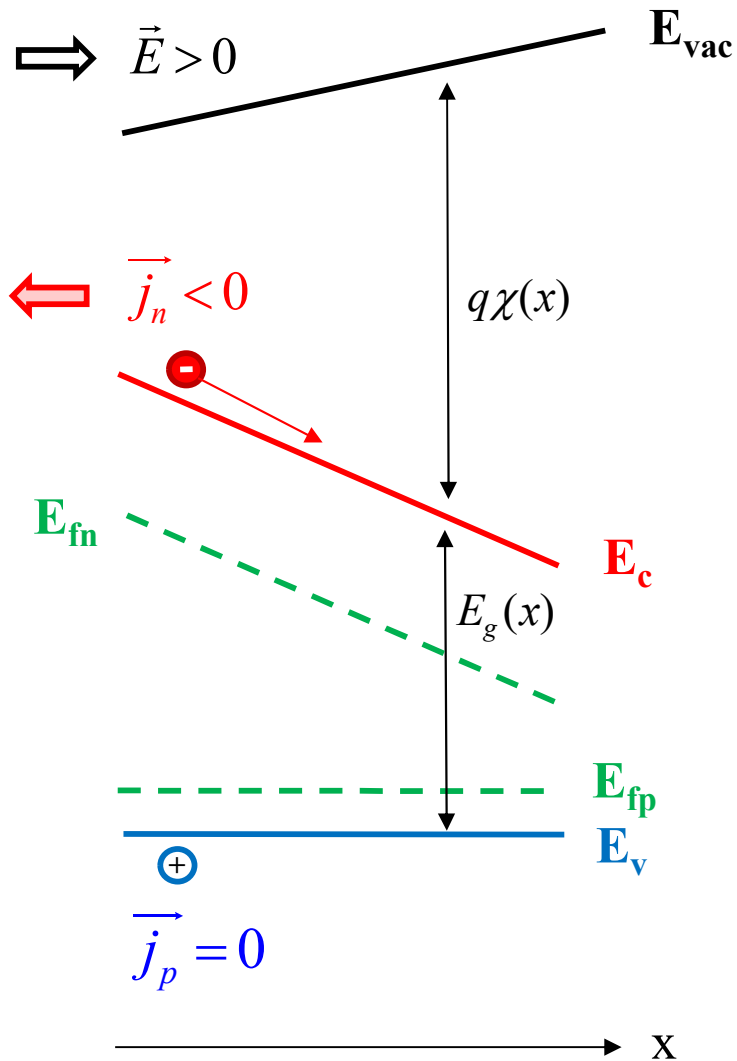
Equations et inconnues:

Hétéro-structures

Exemple: photodiode PIN



Exemple



Champ électrique

$$\vec{E} = -\vec{\nabla}\varphi = \frac{1}{q} \overrightarrow{grad}(E_{vac})$$

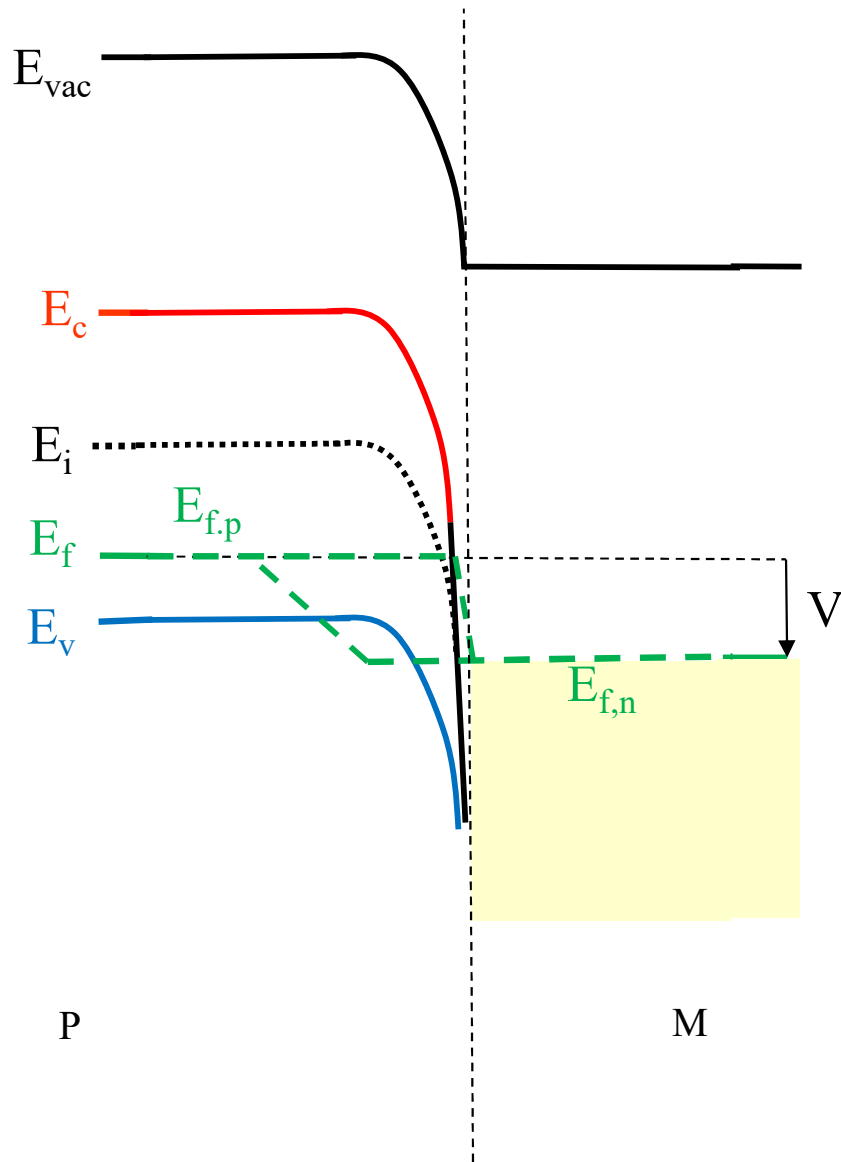
Courant d'électrons

$$\vec{j}_n = n \cdot \mu_n \cdot \overrightarrow{grad}(E_{fn})$$

Courant de trous

$$\vec{j}_p = p \cdot \mu_p \cdot \overrightarrow{grad}(E_{fp})$$

Exemple: p-semiconducteur - métal



- 1) Au point « left »:
- Décrire les bandes et déterminer E_f
- 2) Au point « right »:
- Trouver E_f à partir de la tension externe V
- Dessiner les bandes et trouver E_{vac}

3) Résoudre

$$\Delta E_{vac} + \frac{1}{\epsilon} \vec{\nabla} \epsilon \cdot \vec{\nabla} E_{vac} = \frac{q^2}{\epsilon_0 \epsilon} (p + N_d^+ - n - N_a^-)$$

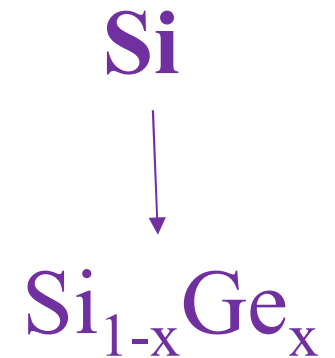
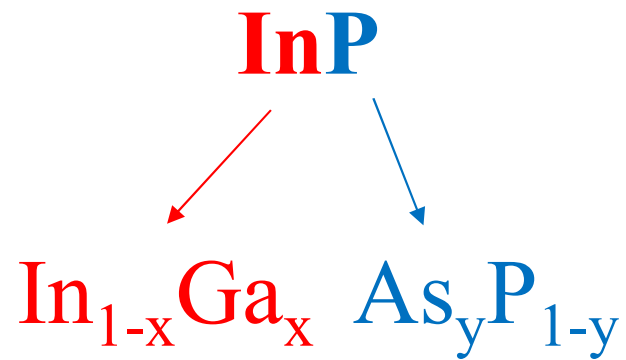
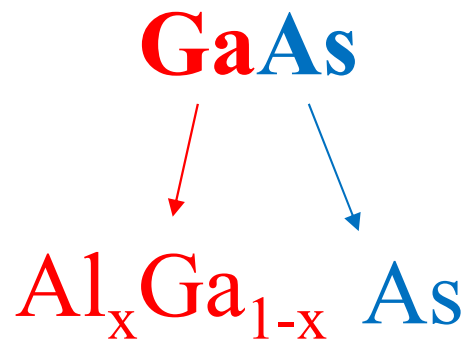
$$\frac{\partial n}{\partial t} = -U_{spec} - U_{th} + \frac{1}{q} \text{div}(\vec{j}_n) \quad \frac{\partial p}{\partial t} = -U_{spec} - U_{th} - \frac{1}{q} \text{div}(\vec{j}_p)$$

avec les conditions aux deux bords **modifiées**.
Les inconnues sont E_{vac} , $E_{F,n}$ et $E_{F,p}$

- 4) Tracer E_{vac} , $E_{F,n}$ et $E_{F,p}$
- 5) Tracer les bandes en tout point depuis E_{vac}

**Design des composants semiconducteurs
à hétérostructures:
Gap, indice de réfraction et
maille cristalline**

Variation et design du gap

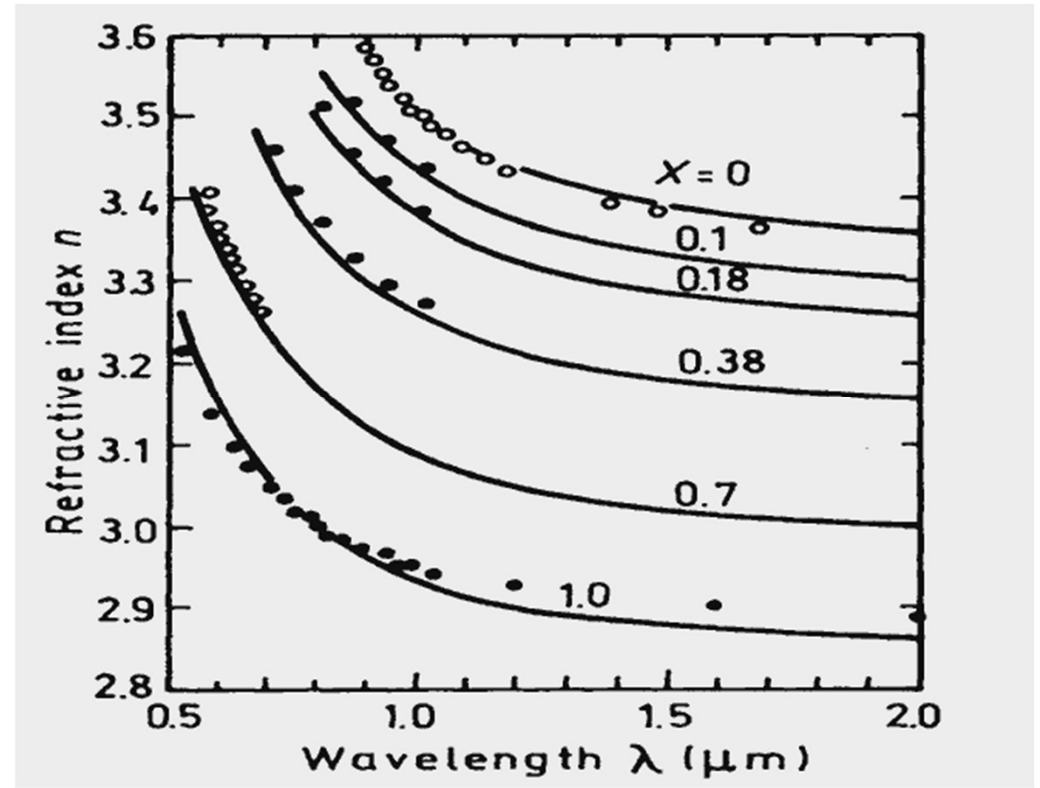
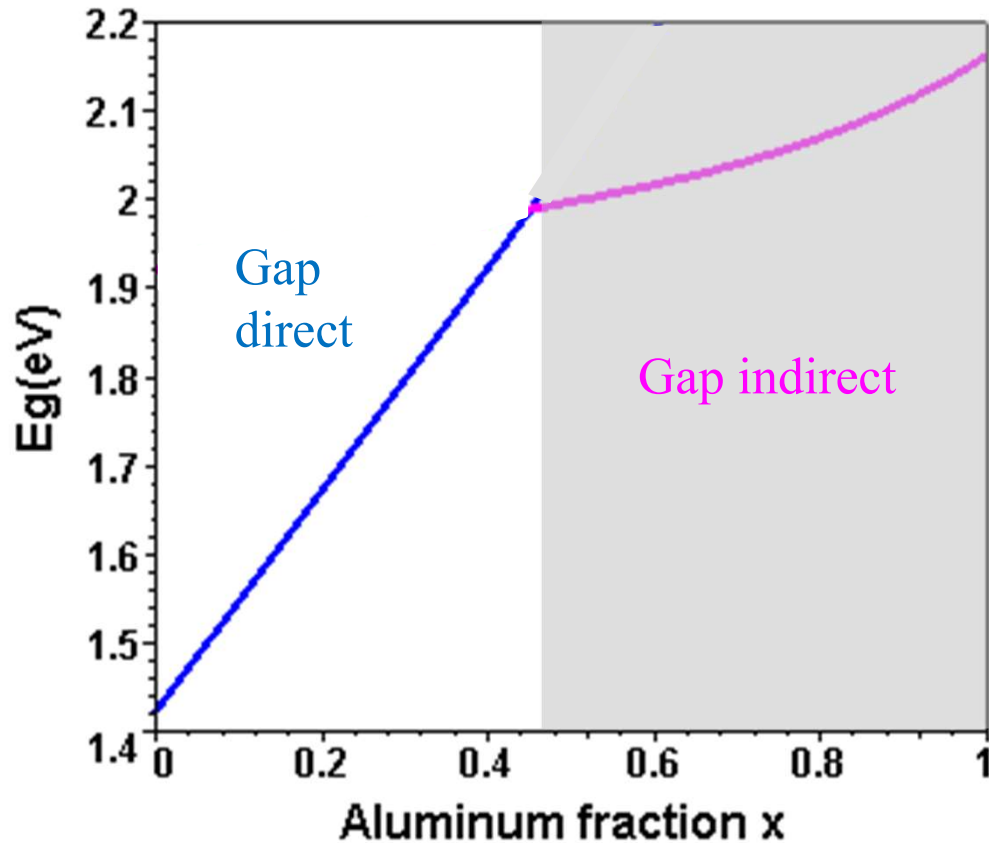


Al_xGa_{1-x}As Matched to GaAs

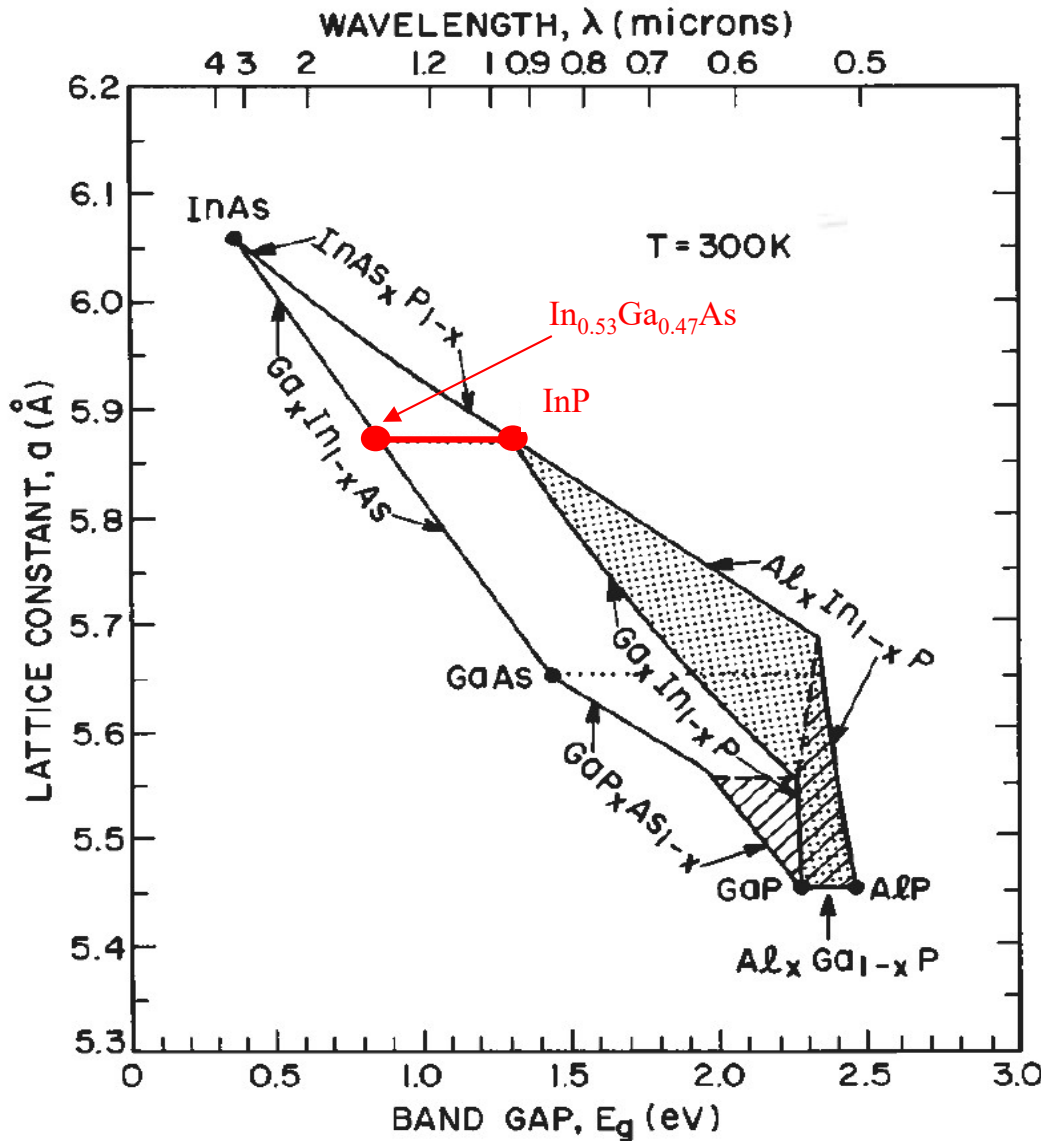
Bandgap direct (x < 0.45)

$$E_g(x) = 1.422 + 1.2475 \cdot x \quad [eV]$$

Energy gap of Al_xGa_{1-x}As



In_{1-x}Ga_xAs_yP_{1-y} Heterostructures



InGaAsP
matched to InP

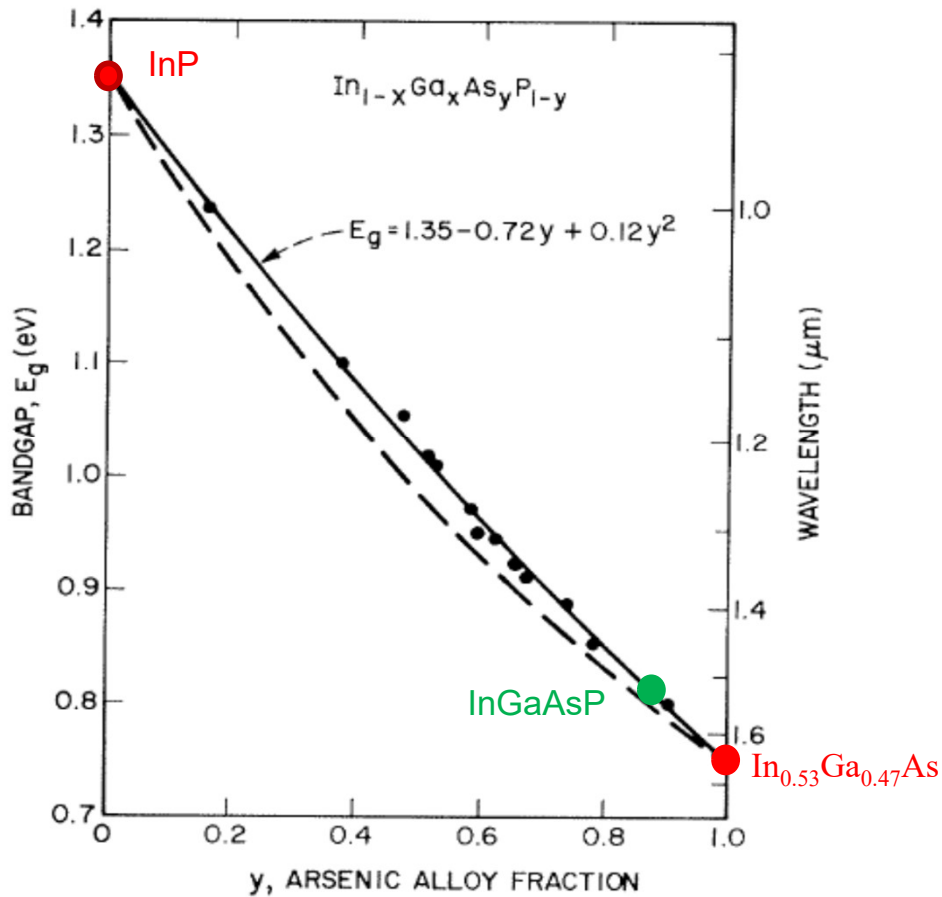
$$x = \frac{0.4562 \cdot y}{1 - 0.031 \cdot y} \cong 0.45 \cdot y$$

Agrawal, « long-wavelength semiconductor lasers », VNR

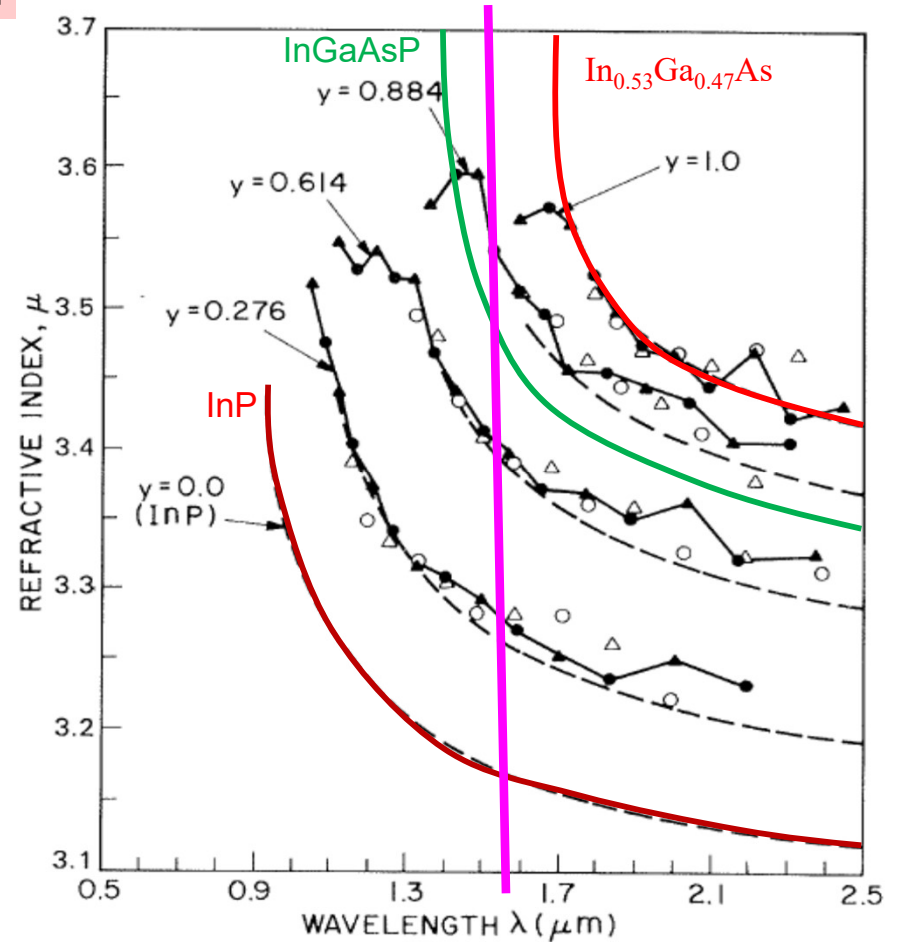
In_{1-x}Ga_xAs_yP_{1-y} Matched to InP (1)

Bandgap

$$E_g(y) = 1.35 - 0.72 \cdot y + 0.12 \cdot y^2 \quad [eV]$$



Refractive index

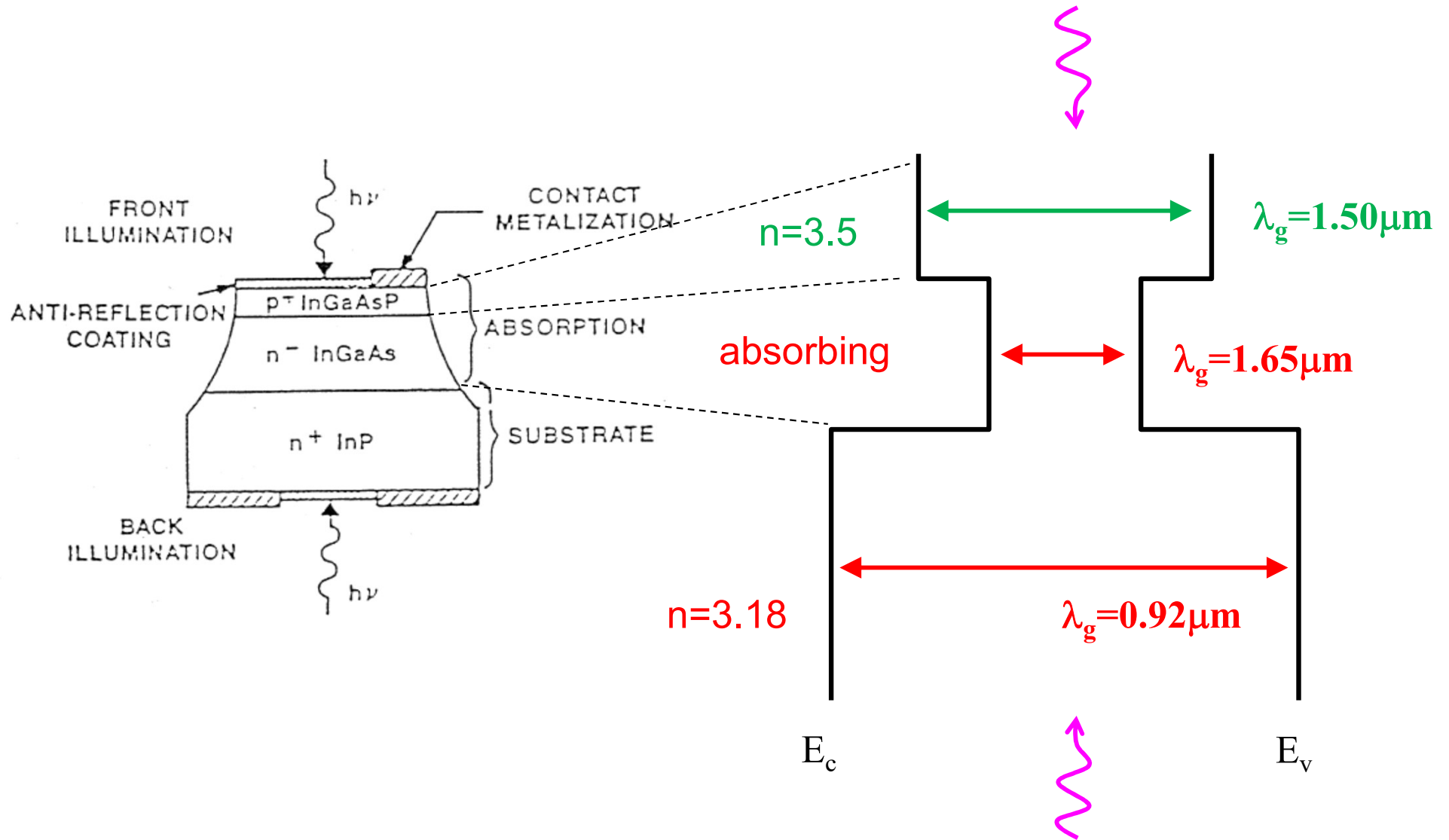


Agrawal, « long-wavelength semiconductor lasers », VNR

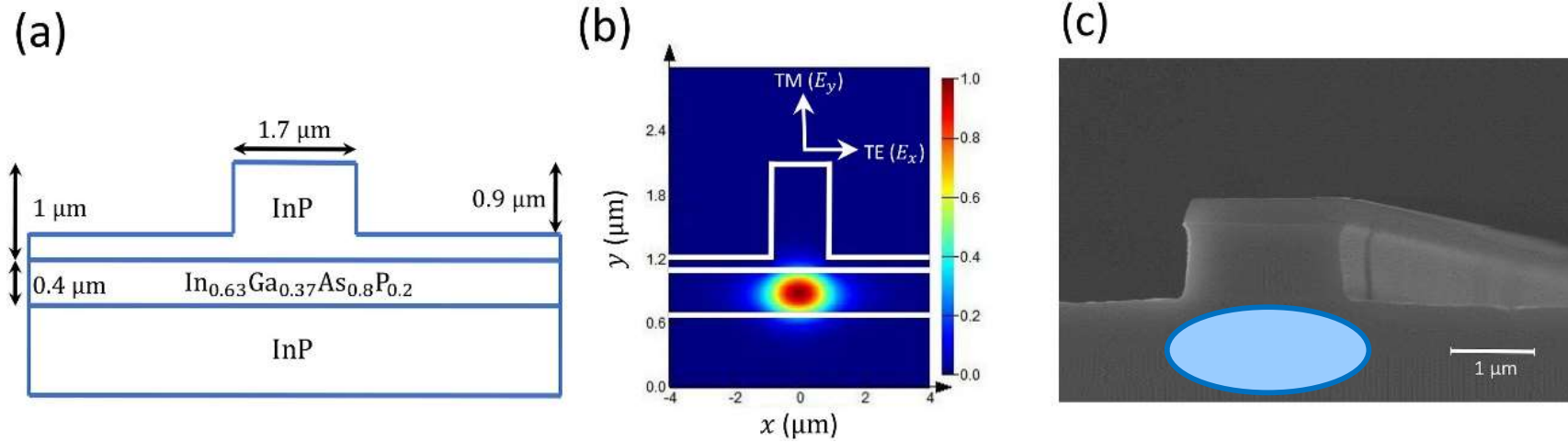
Loi de Kramer-Kronig

**Hétérostructures:
PIN, guides d'onde,
quantum wells, quantum wires
quantum dots**

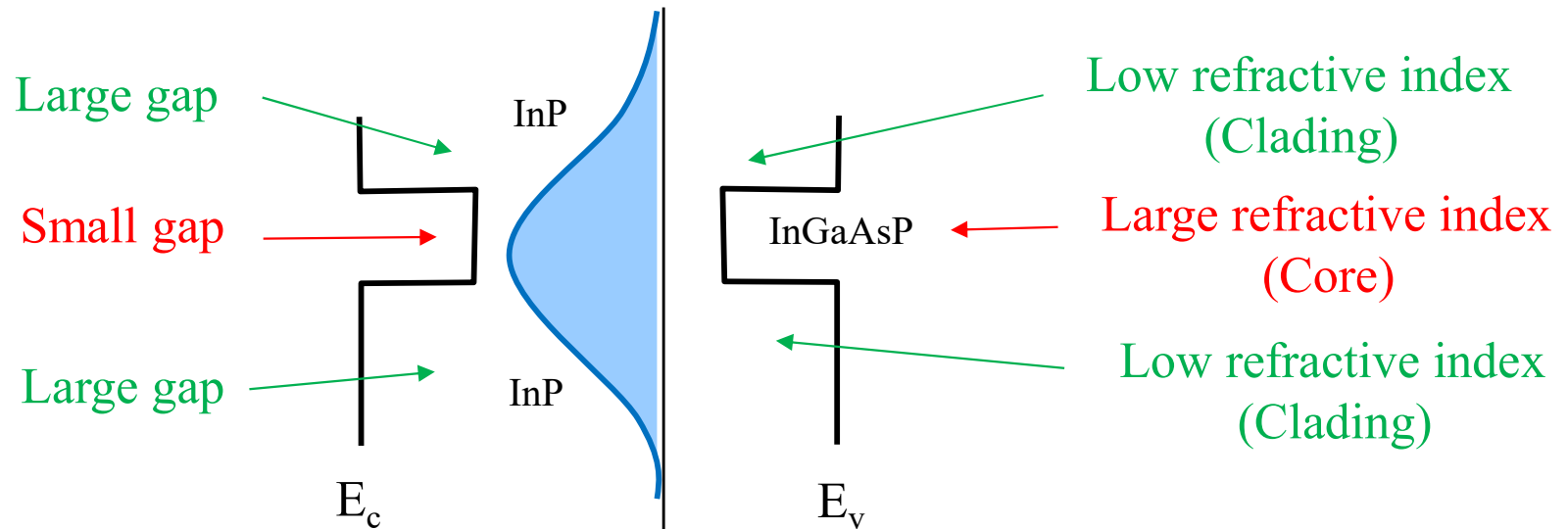
Exemple: photodiode PIN



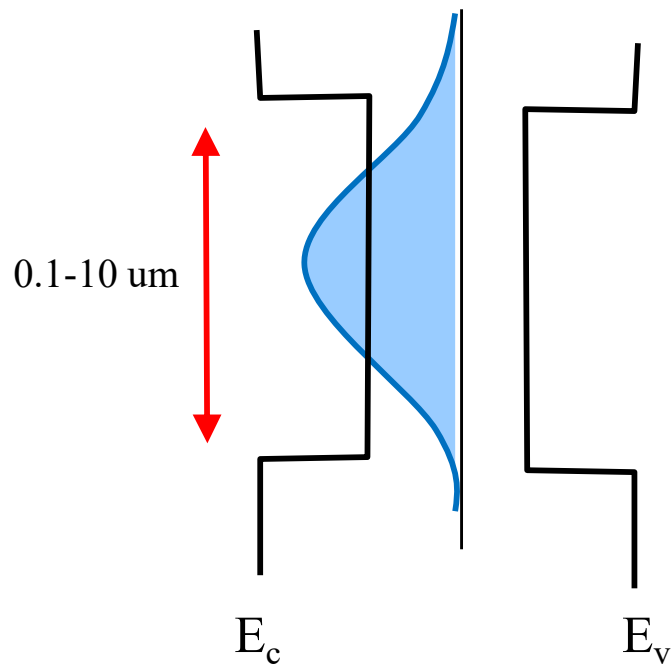
Guides d'onde, transparent, absorbant, ou émettant



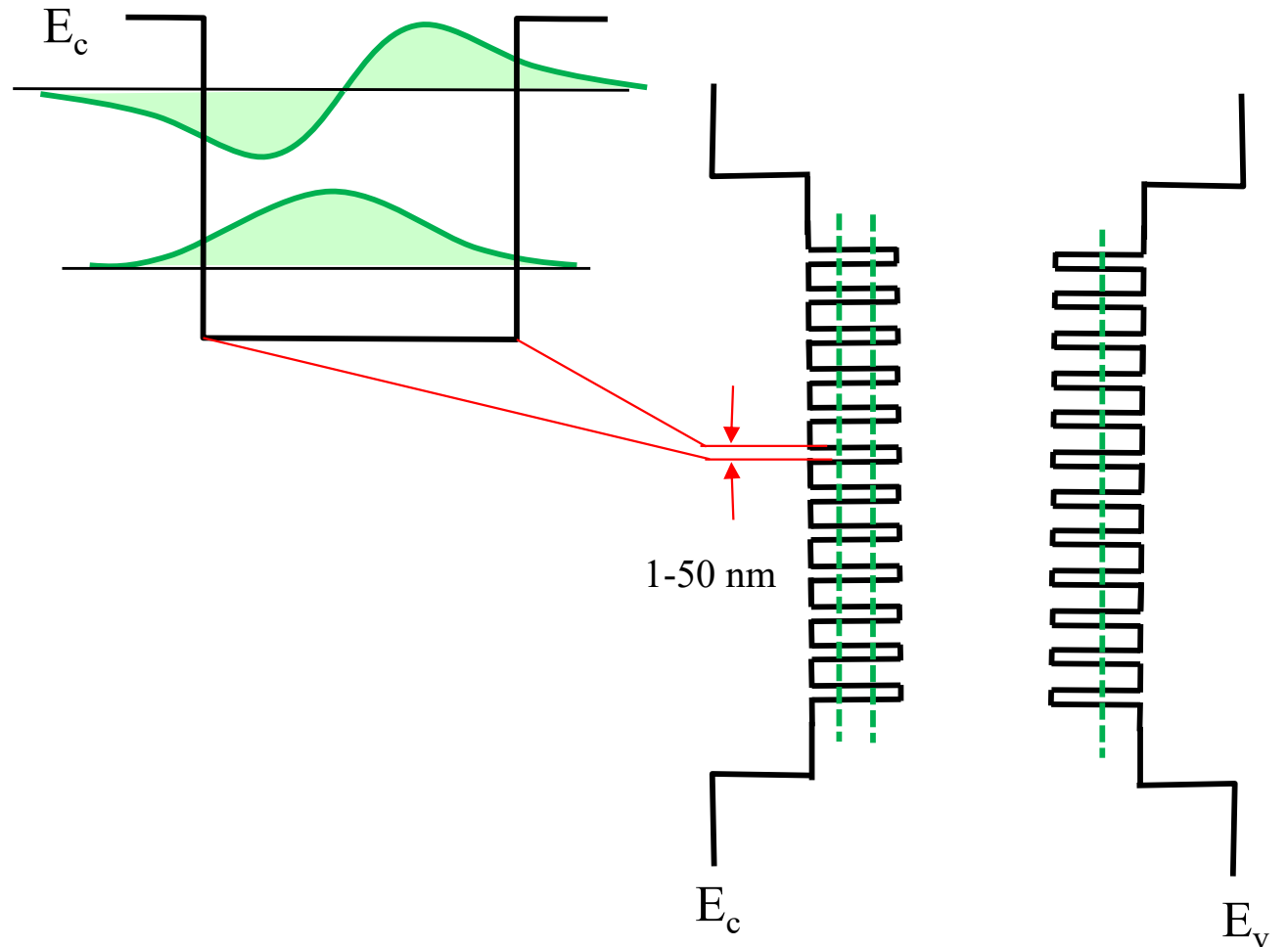
Optical Materials Volume 84, October 2018, Pages 524-530



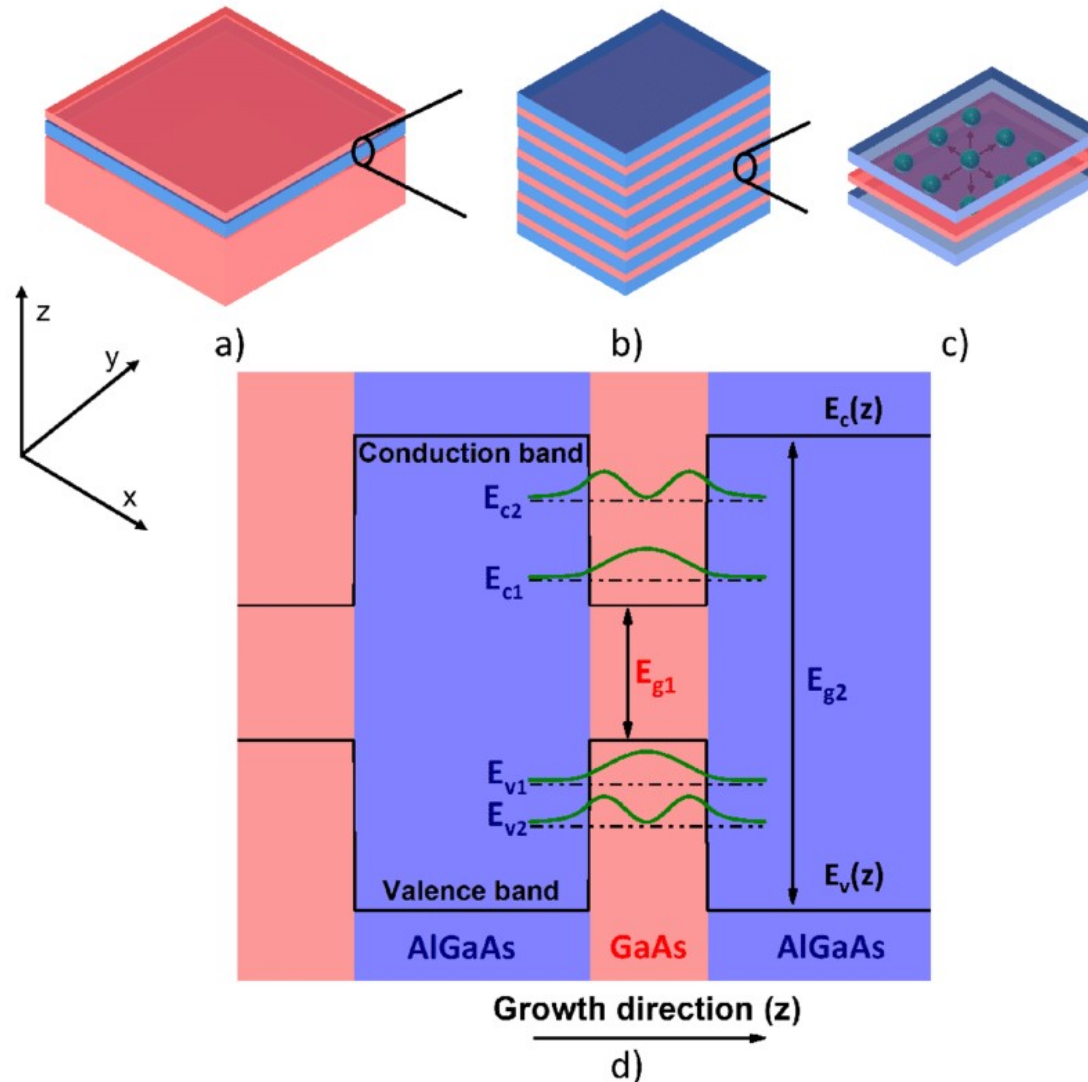
Etats optiques discrets
Continuum électronique



Etats électroniques discrets
Multi Quantum Wells (MQW)



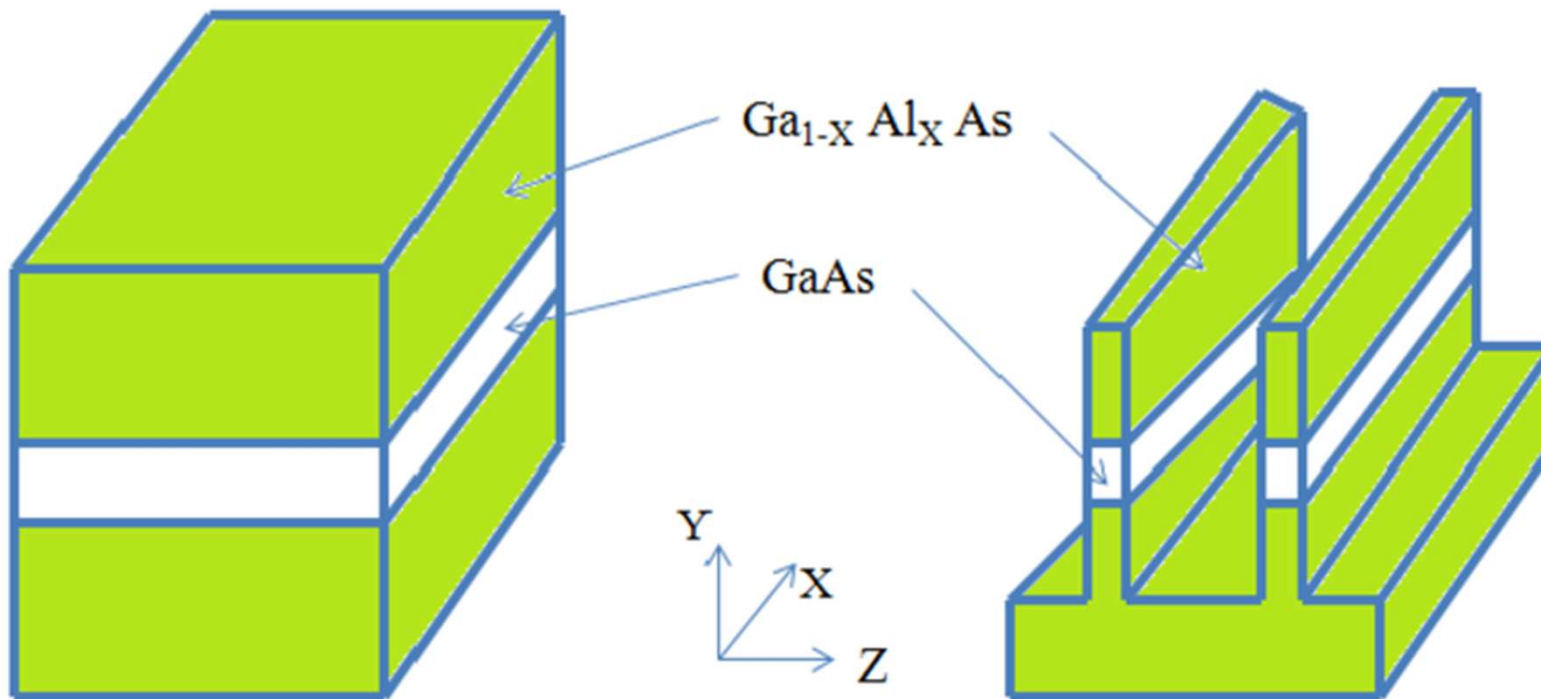
https://www.researchgate.net/publication/348894632_Mid-Infrared_Intersubband_Polaritonic_Devices



2D electron gas

- K_z discret
- K_x et K_y continus

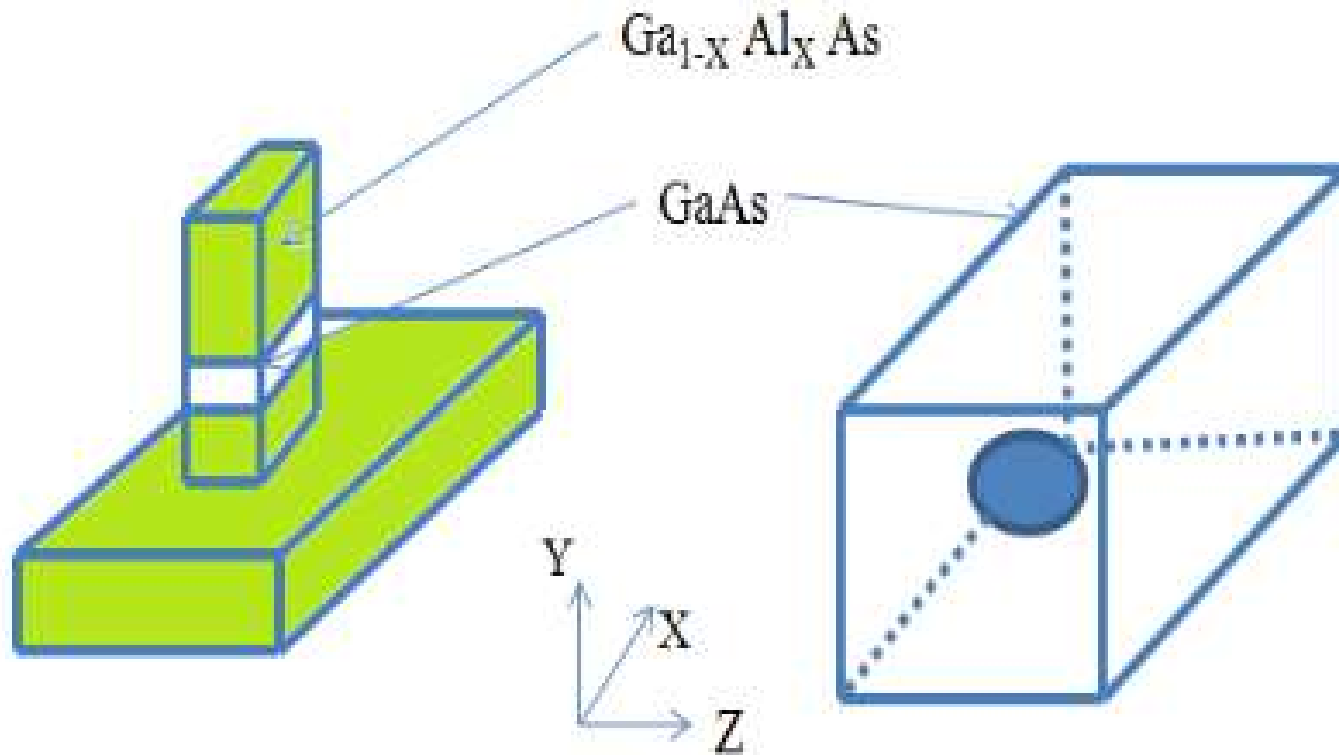
https://www.researchgate.net/publication/290582375_Characterization_and_Analysis_of_Quantum-Dot_PV_Solar-Cells



1D electron gas

- K_z et K_y discrets
- K_x continu

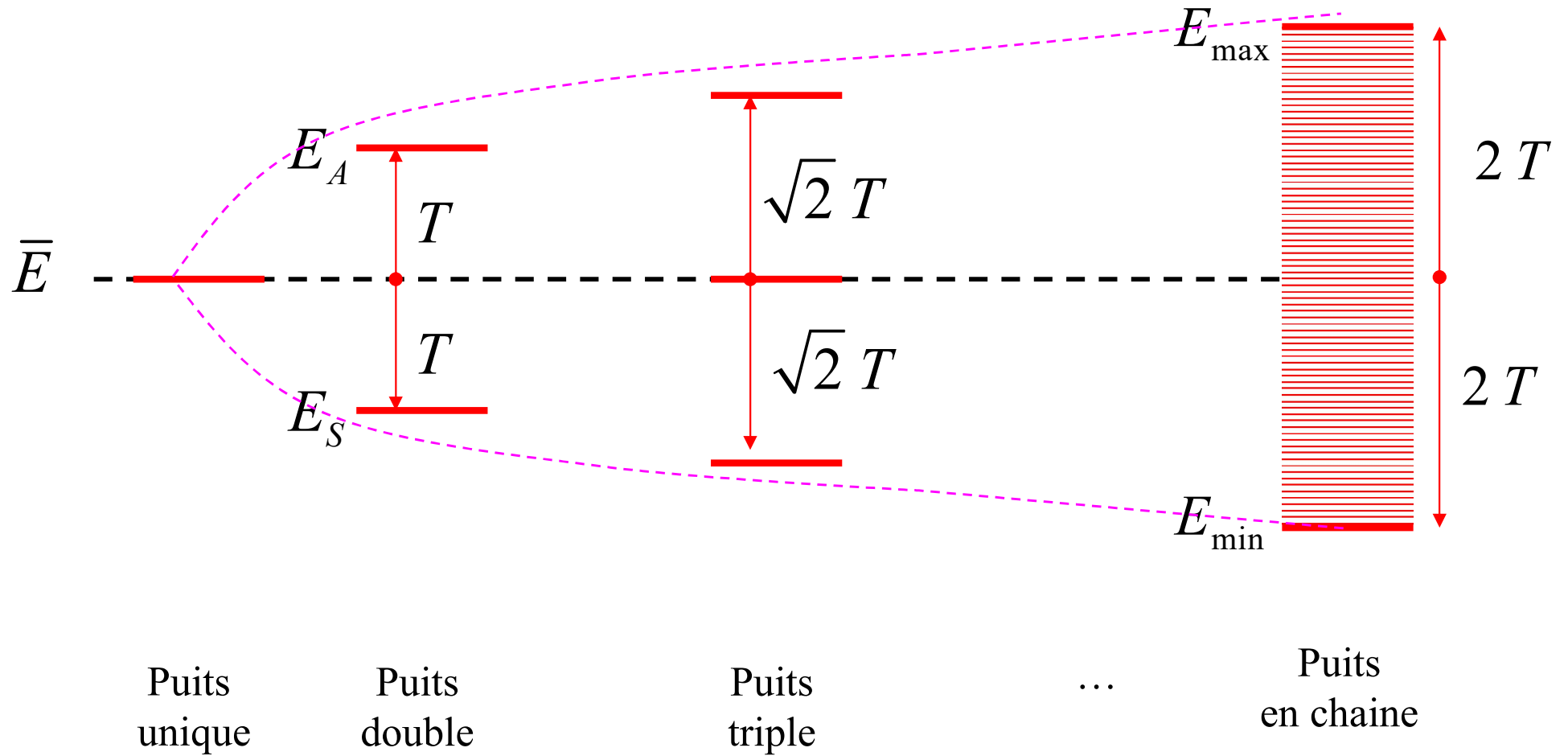
https://www.researchgate.net/publication/290582375_Characterization_and_Analysis_of_Quantum-Dot_PV_Solar-Cells



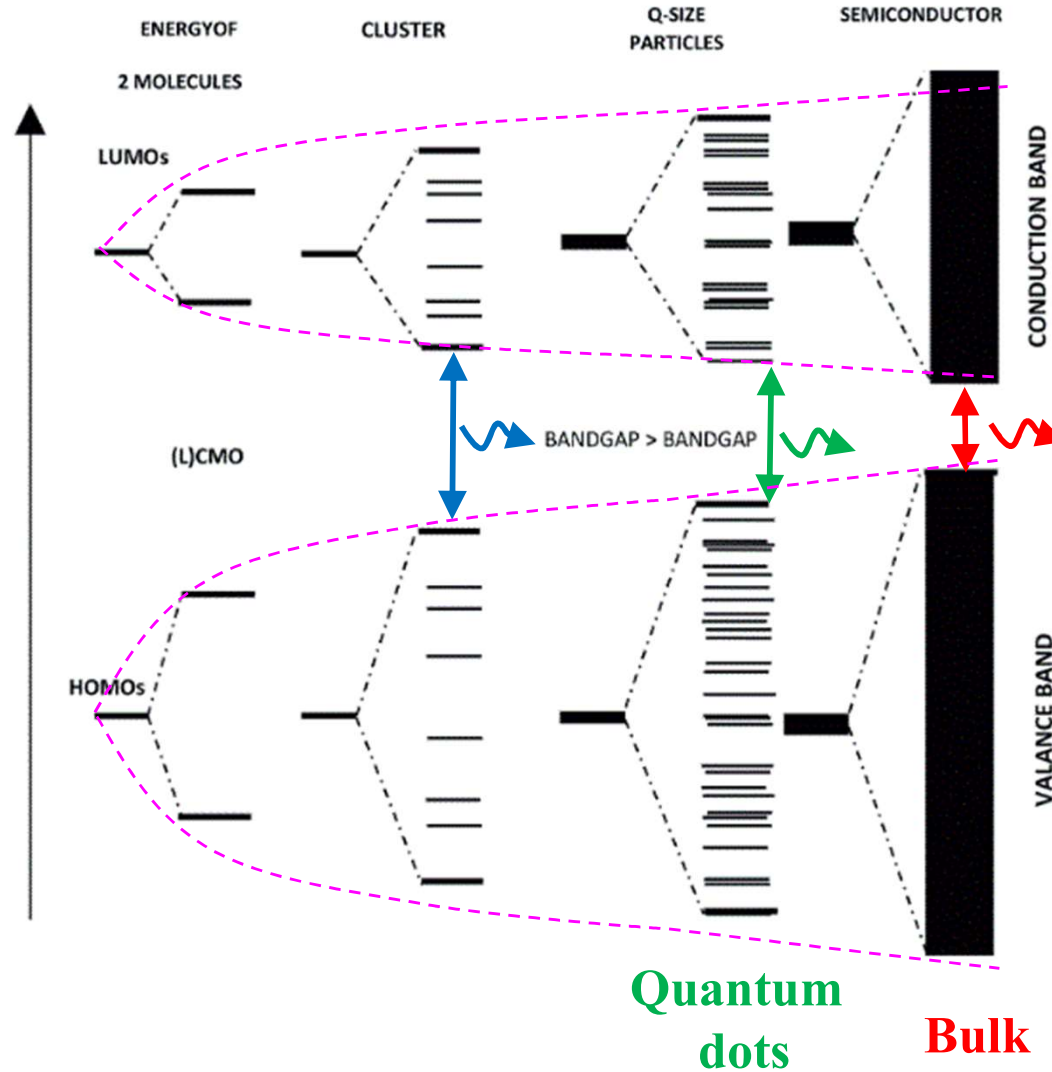
Traped electron

- K_z, K_y et K_x discrets

Chaine de puits couplés



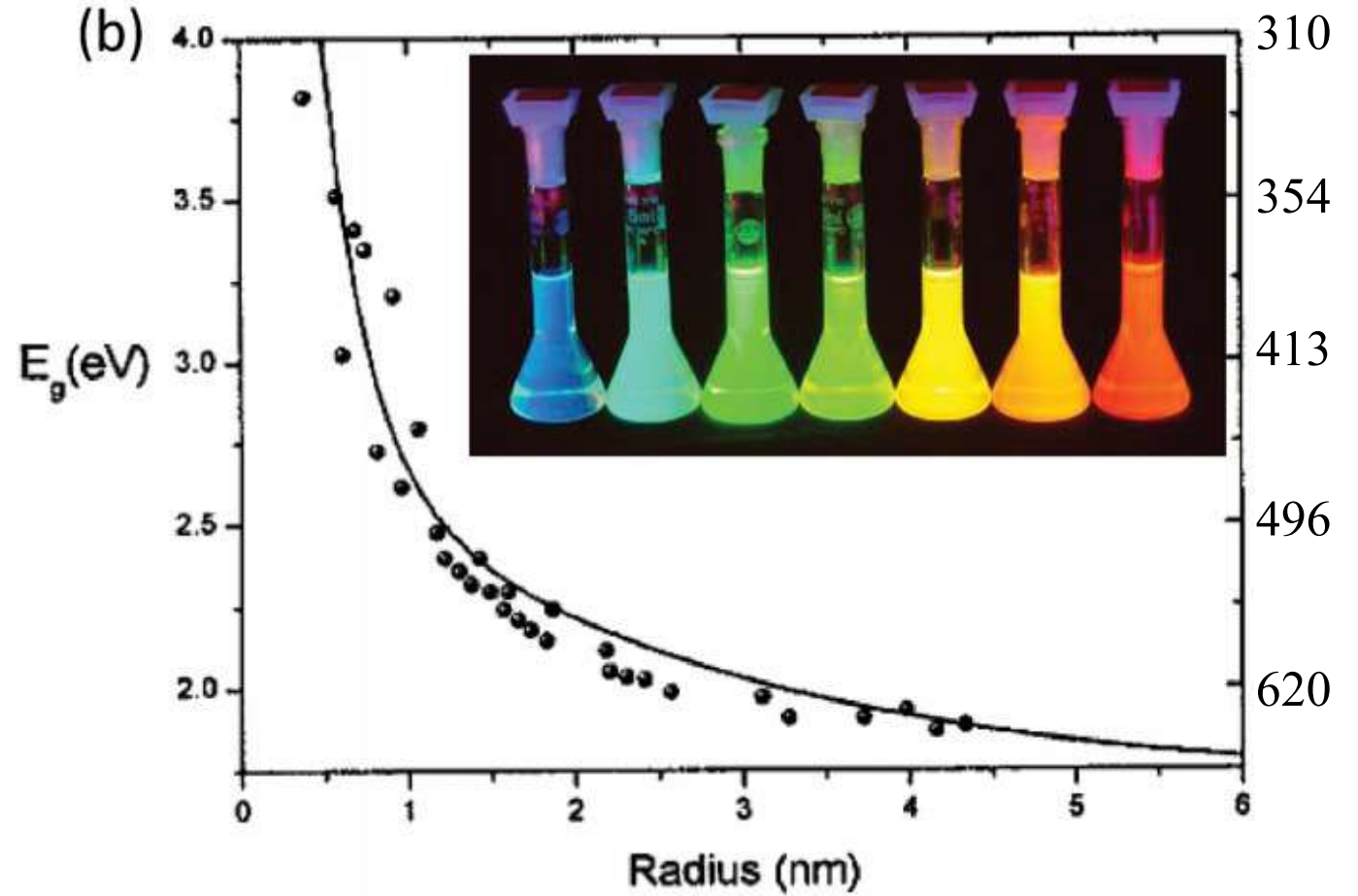
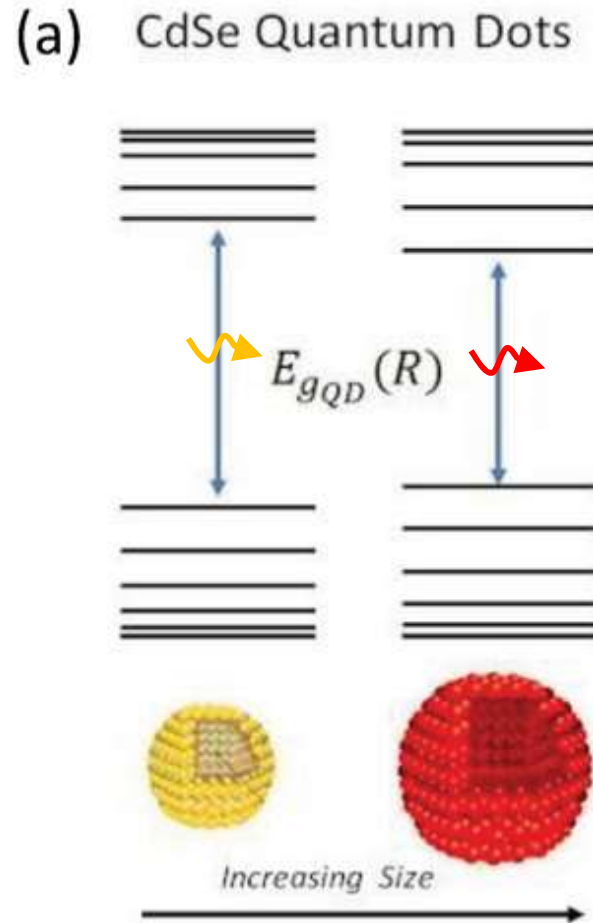
Quantum dots: formation de bandes





M. G. Bawendi, L. E. Brus and A. I. Ekimov
Nobel Prize (chemistry) 2023

Quantum dots: exemple d'application: marqueurs

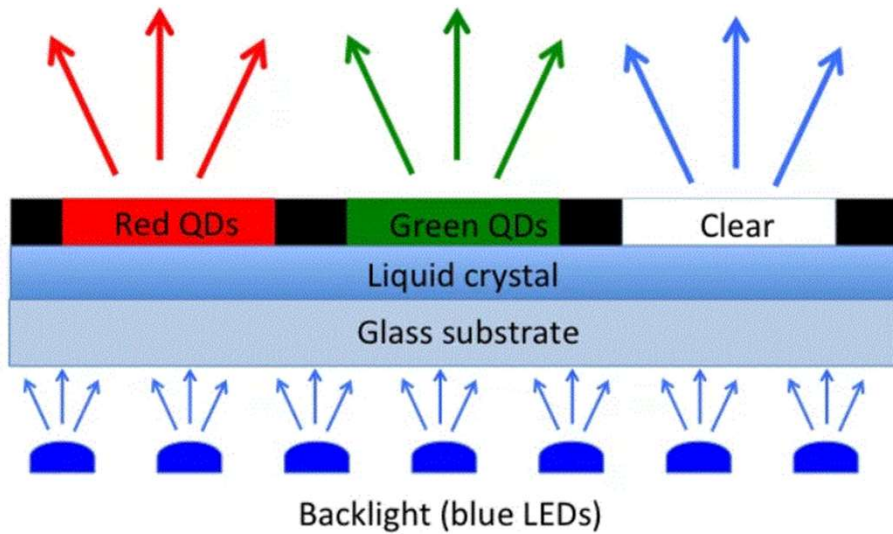


Nano-beads

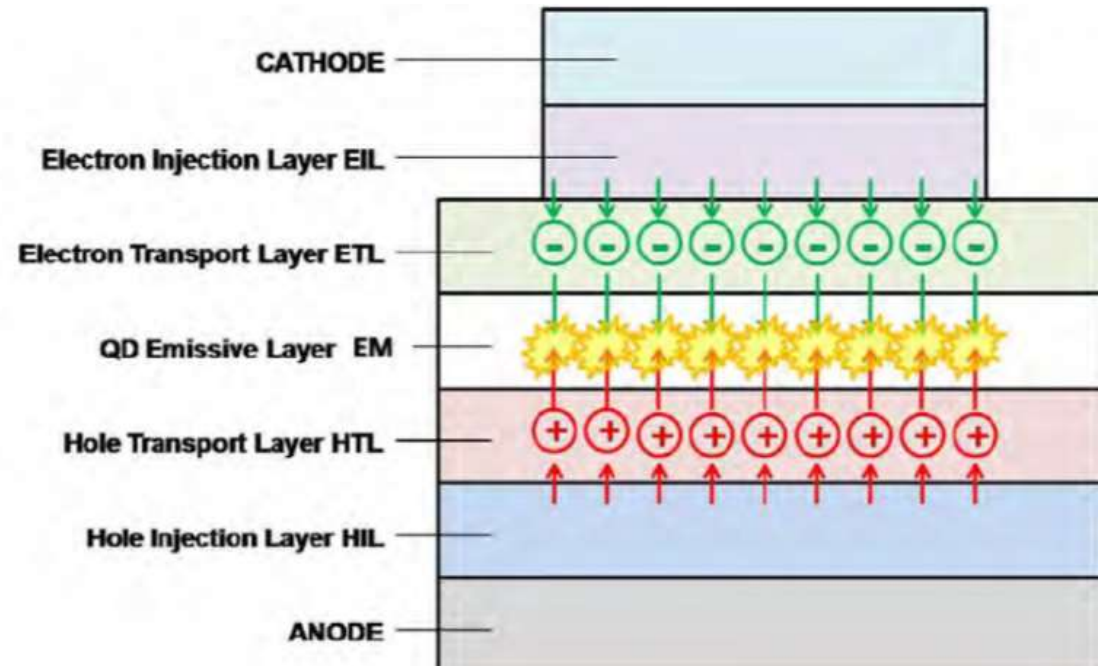
Advanced Science, Volume: 6, Issue: 22, First published: 11 October 2019, DOI: (10.1002/advs.201901345)



Quantum dots filters
(commercial)



Electro-luminescent QLED
(research)



<https://www.androidauthority.com/qled-vs-oled-3201810/>

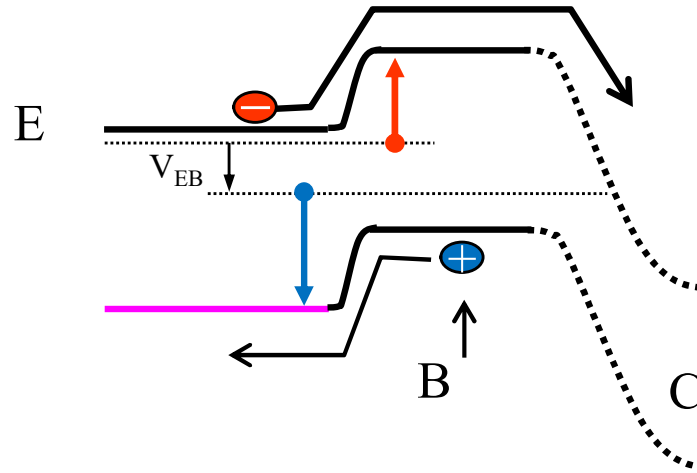
<https://onsitego.com/blog/everything-want-know-qled-tv/>

Hétérostructures: Transistors

Hetero Bipolar Transistors (HBT)

Homo-jonction

nnp

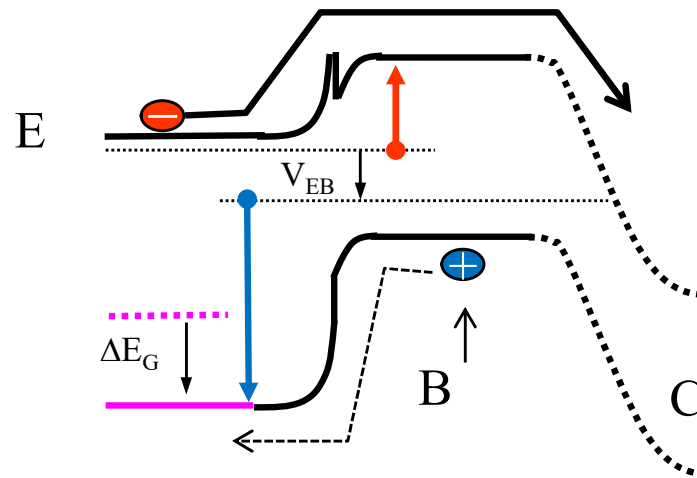


La barrière pour les électrons est plus petite que pour les trous uniquement à cause du dopage élevé dans l'émetteur.

→ β_F élevé mais pas optimal.

Hétéro-jonction

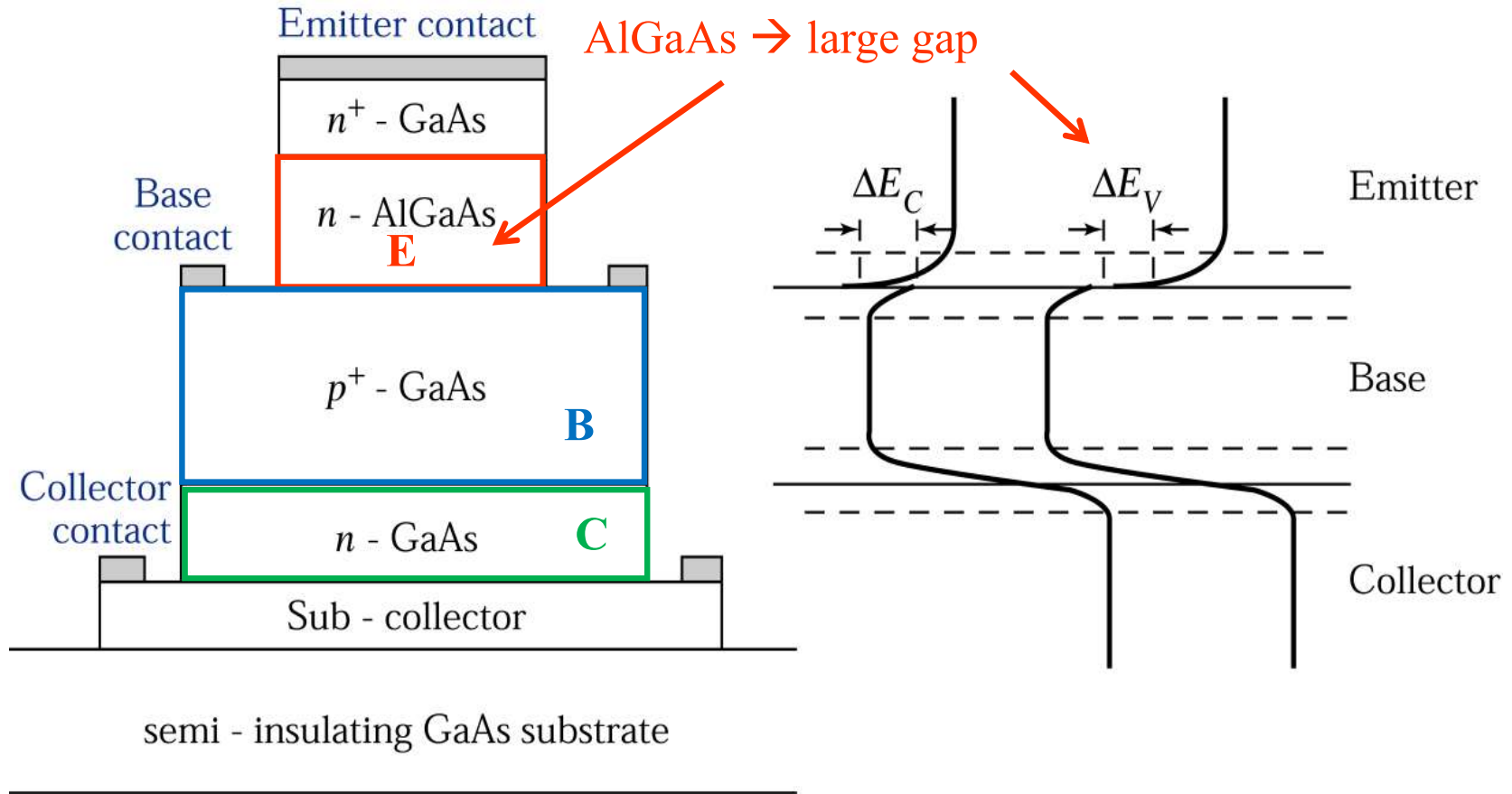
nnp



La barrière pour les trous est augmentée par l'agrandissement du gap ΔE_g dans l'émetteur.

→ β_F optimal et très élevé.

HBT: Exemple (1)



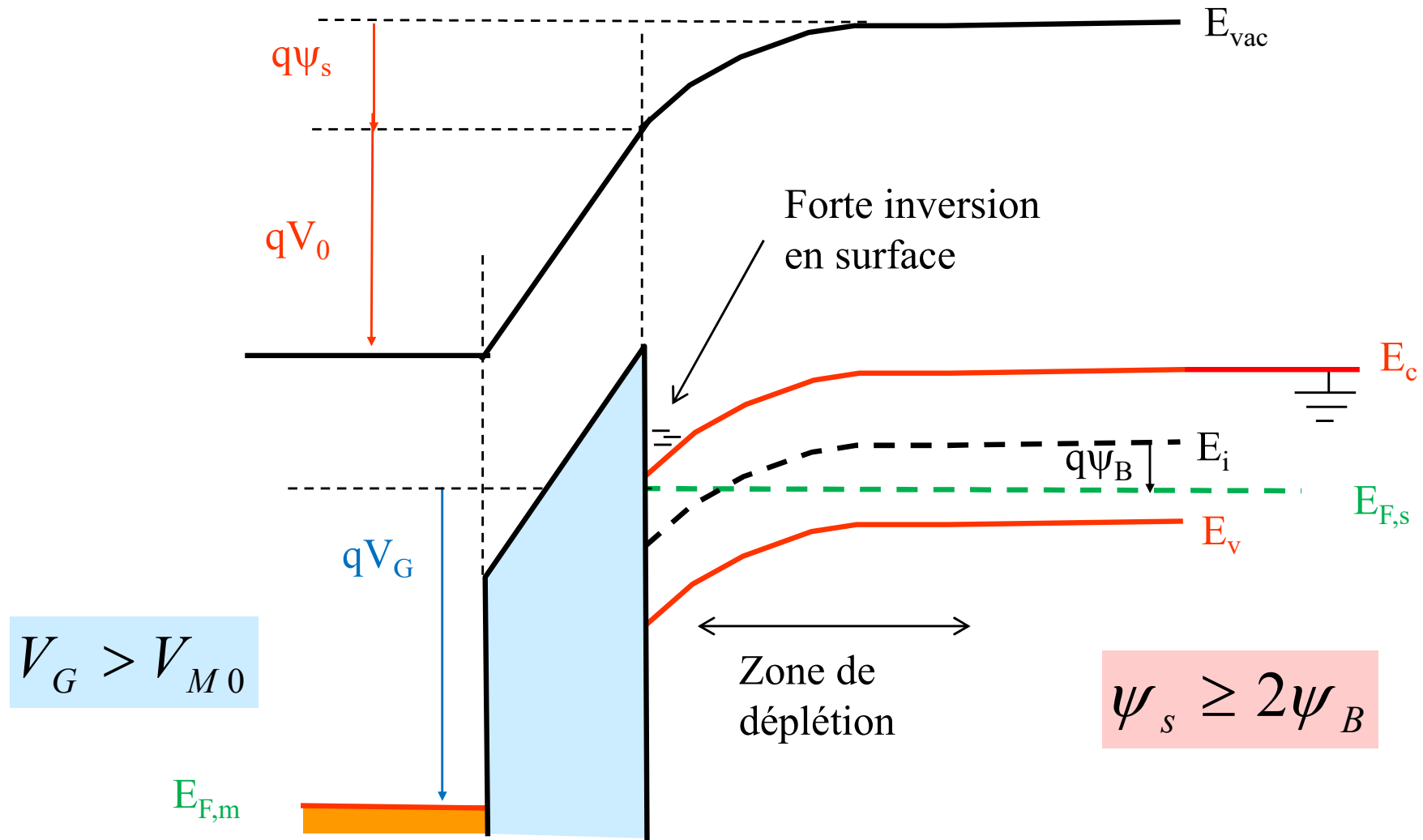
(a)

(b)

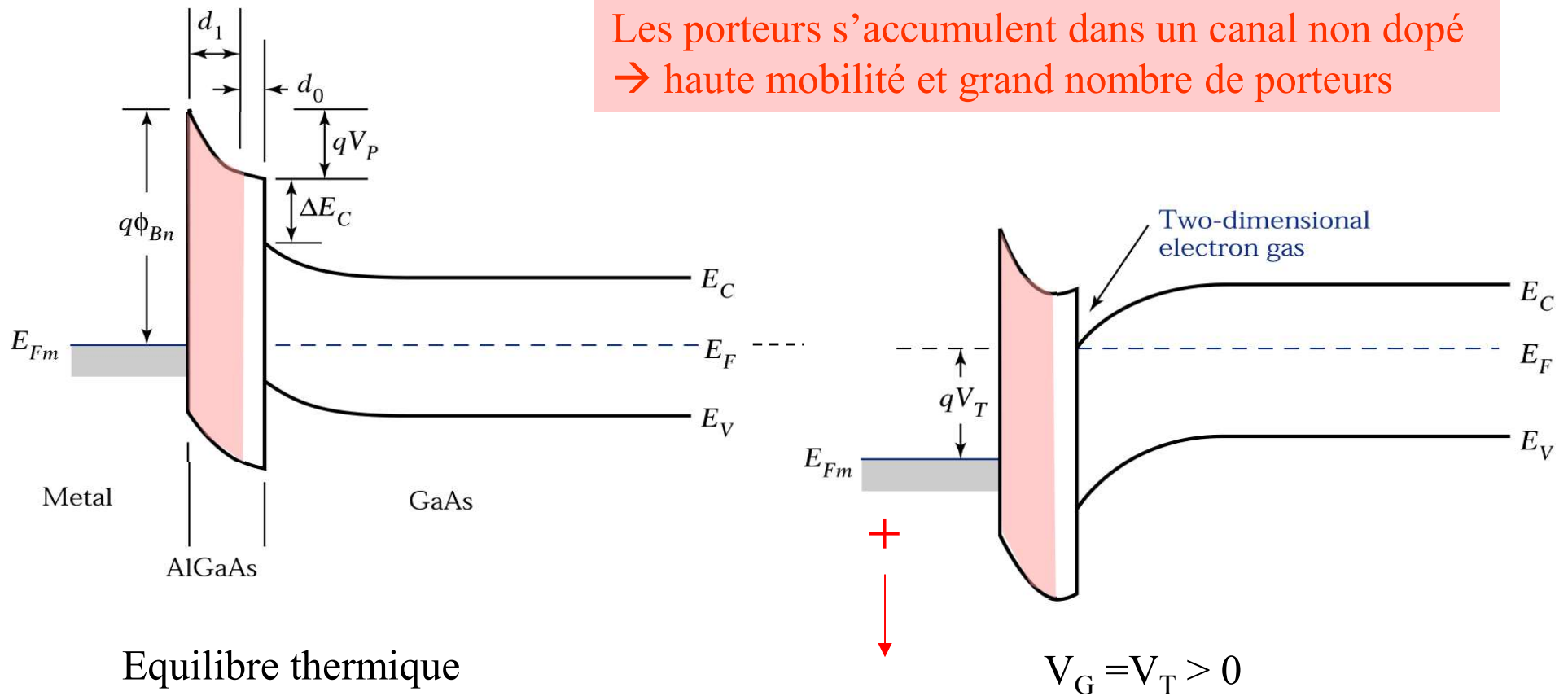
Semiconductor Devices,
2/E by S. M. Sze

Rappel: structure et canal dans NMOS

Inversion forte

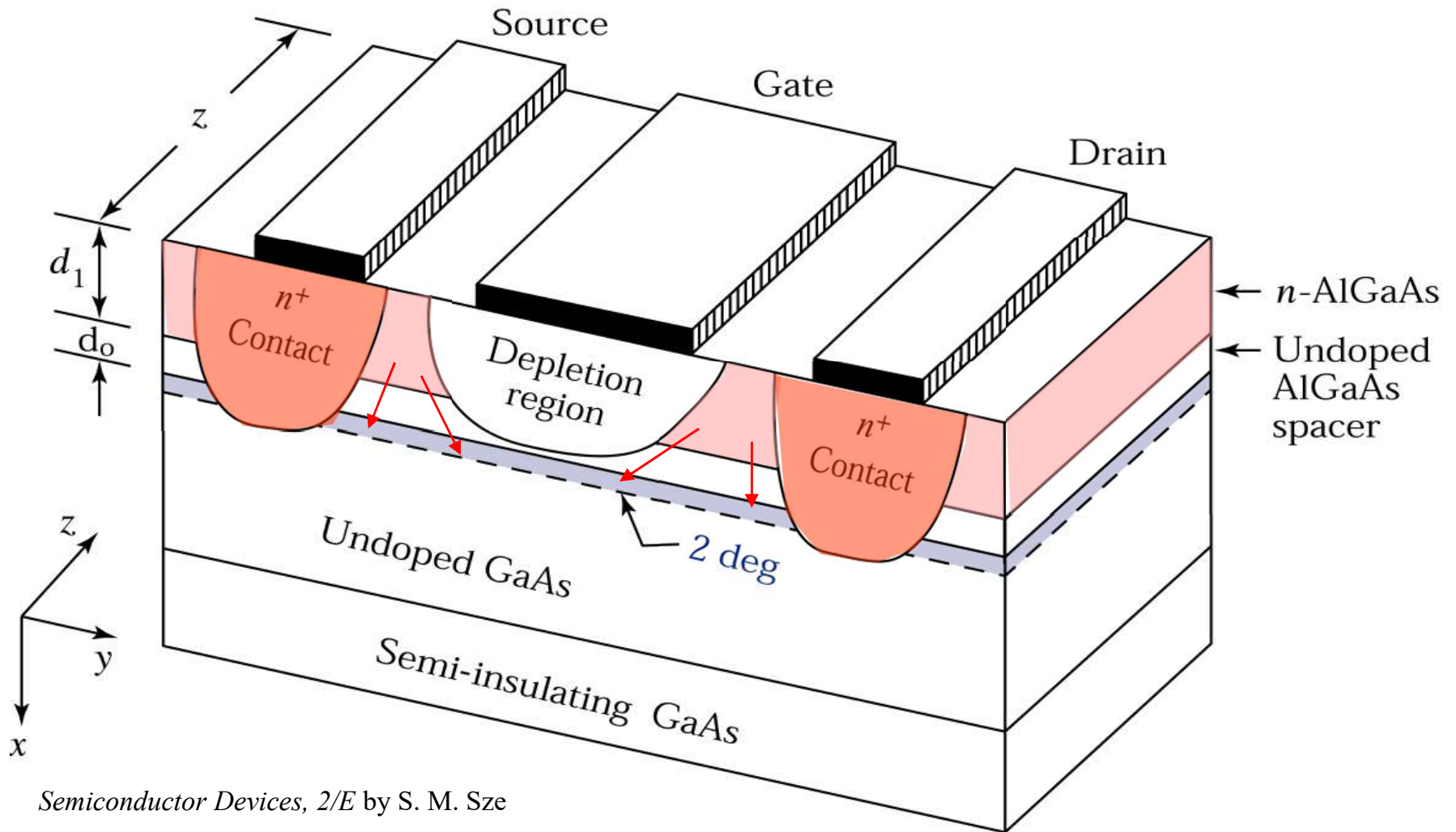


High Electron Mobility Transistors (HEMT)



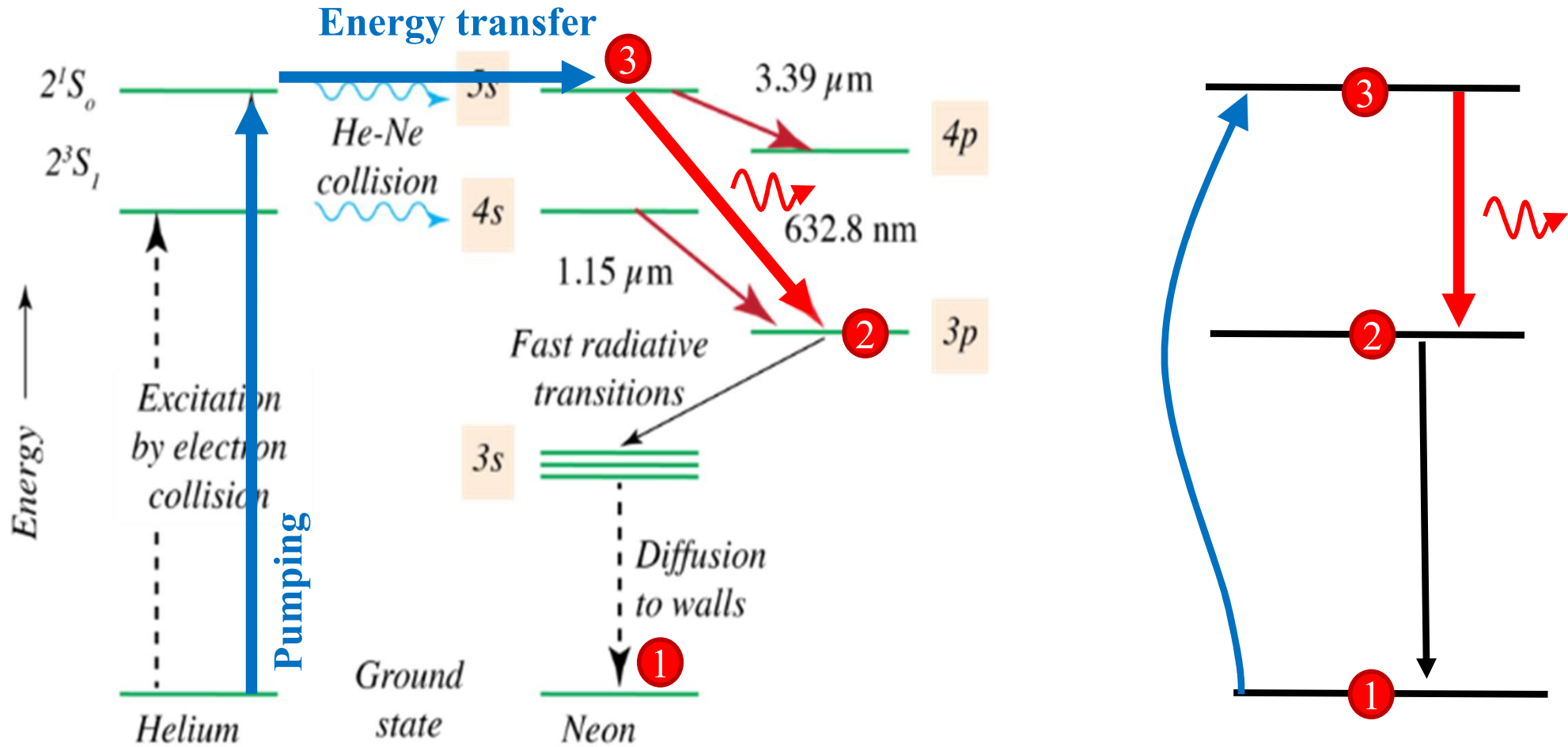
Semiconductor Devices, 2/E by S. M. Sze

High Electron Mobility Transistors (HEMT) canal d'électrons 2D



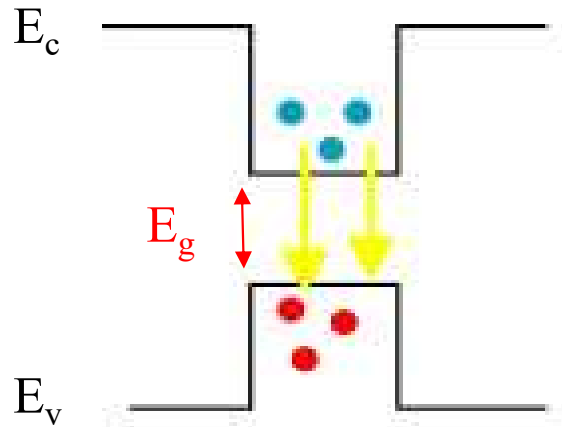
Semiconductor Devices, 2/E by S. M. Sze

Hétérostructures: QC Lasers et QWIP



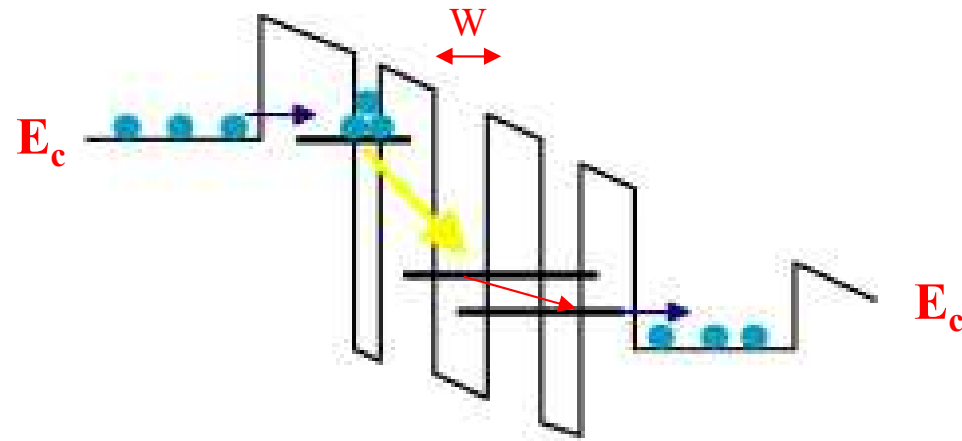
IR Source: Quantum Cascade Laser (QCL)

Classic Laser



Interband
Laser

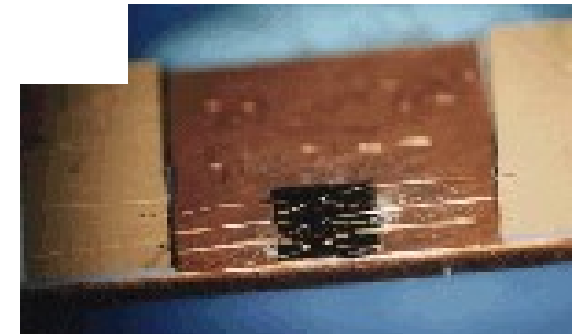
Quantum Cascade Laser



Intersubband
Laser

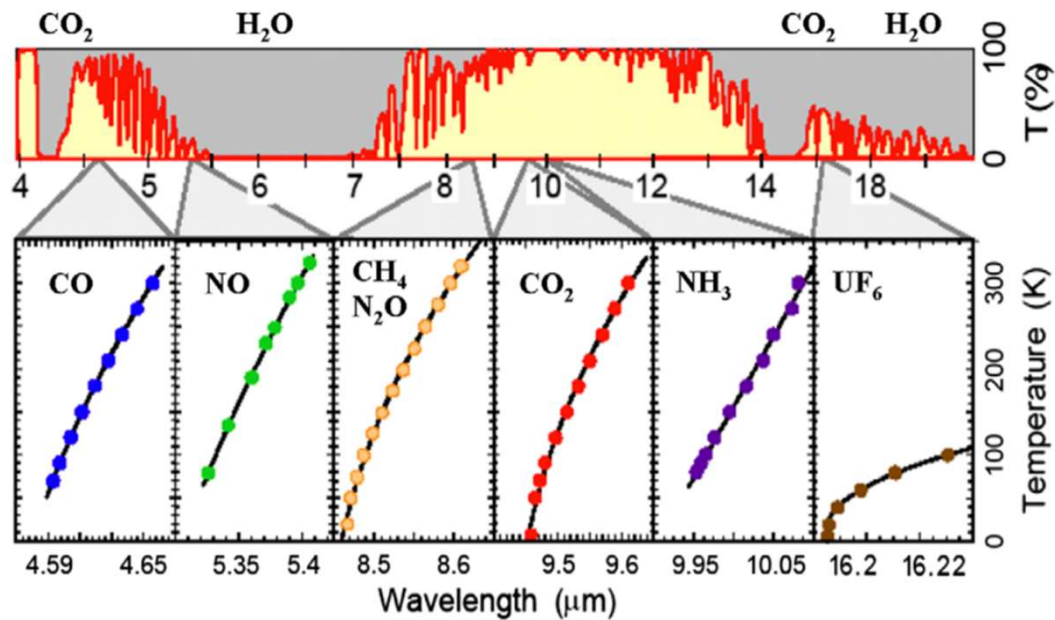
Prof. J. Faist
UniNe

<http://www.unine.ch/phys/meso/>

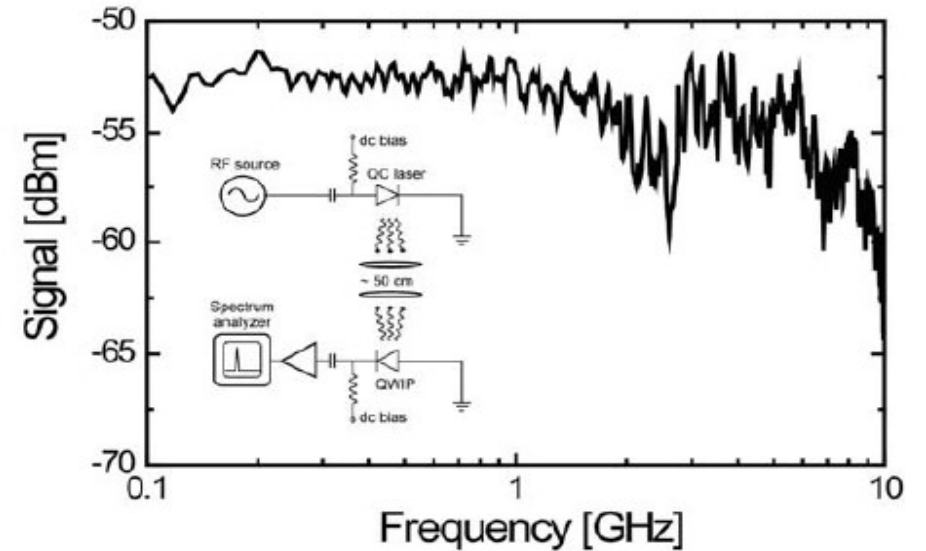


<https://www.edmundoptics.com/knowledge-center/application-notes/lasers/quantum-cascade-lasers/>

Optical spectrum



Electrical bandwidth

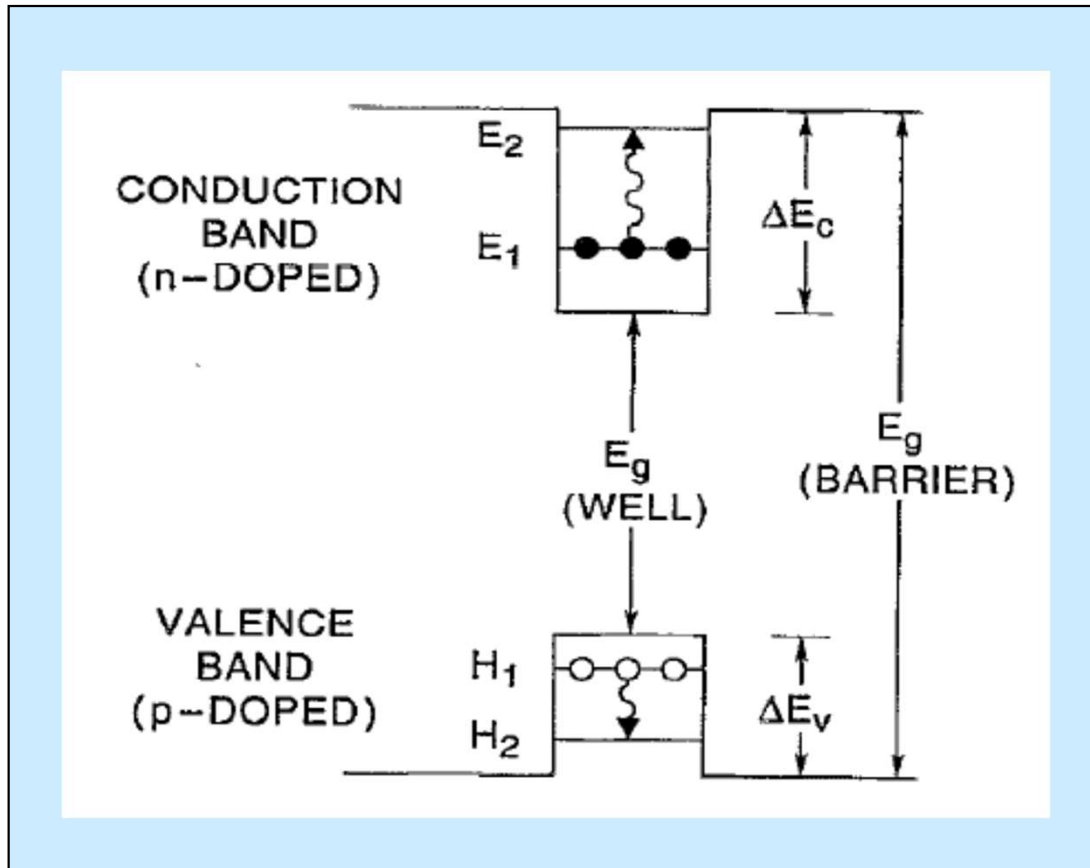


Free space data transmission

R. Martini, J. Opt. Fiber. Commun. Rep. 2, 279–292 (2005)

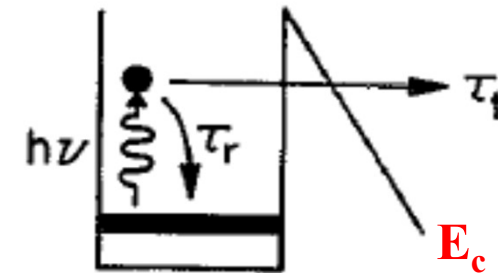
CW and room temperature operation possible

Absorption

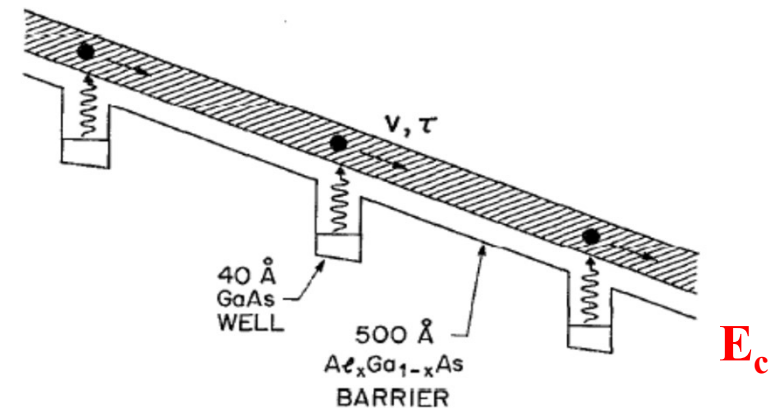


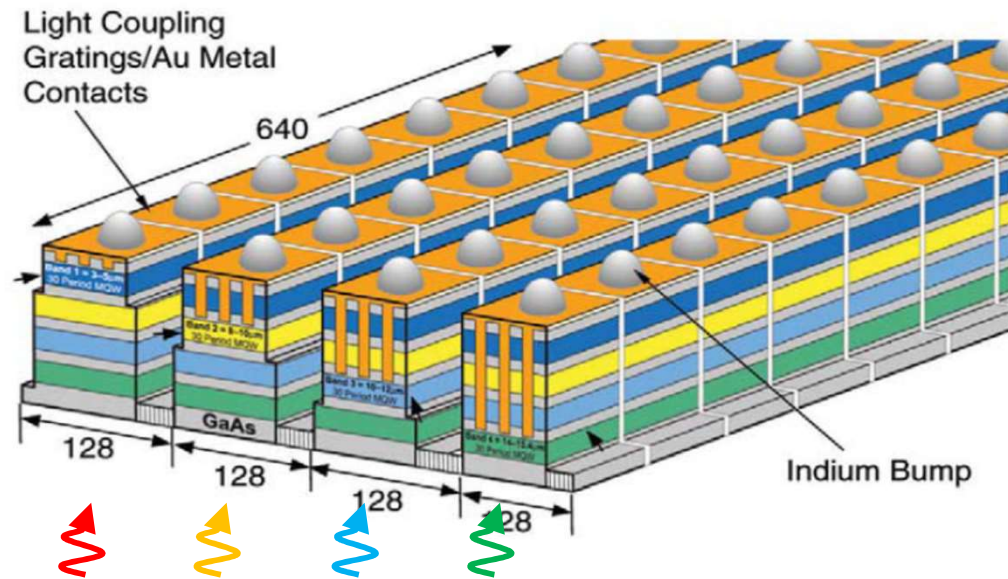
B.F. Lavine, J. Appl. Phys. 74 (8), 1993, pp. R1-R81

Bound to bound:
Tunneling escape

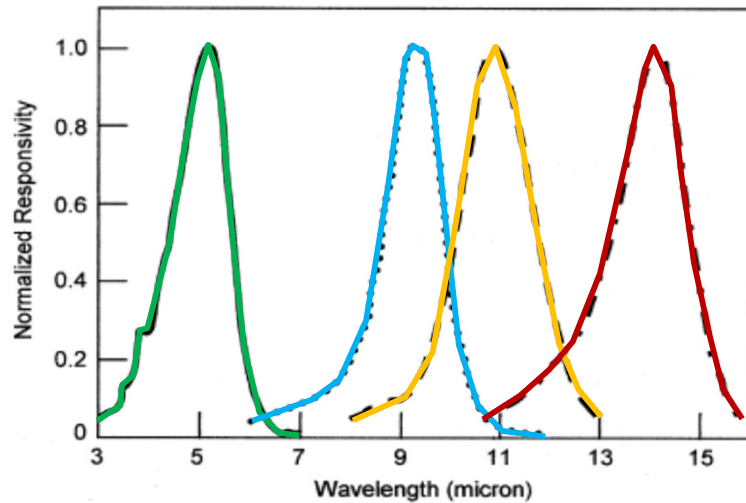


Bound to continuum





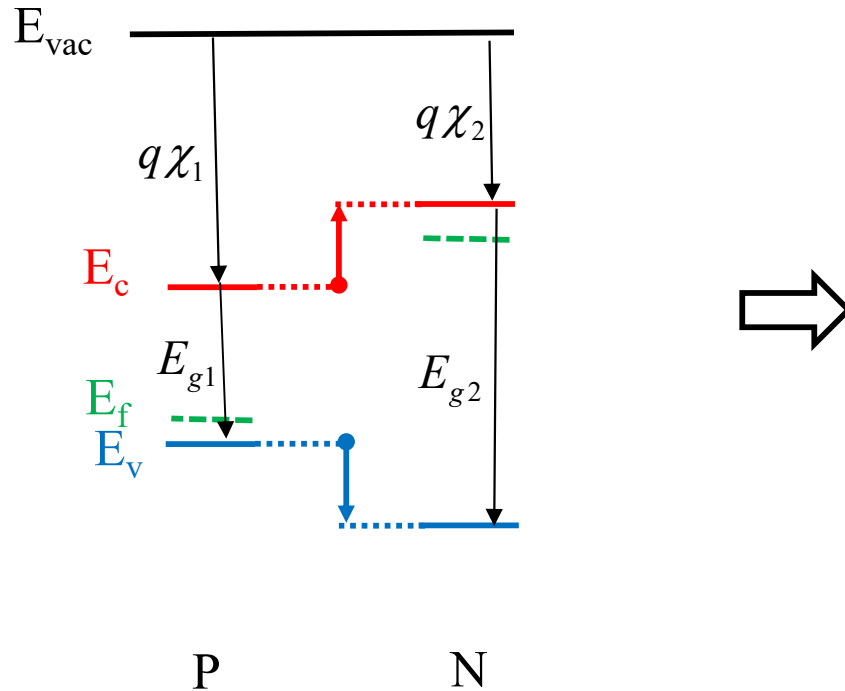
< 80°K



QWIP Phoenix™
640x520 pixels

S D Gunapala et al., *IEEE Trans. Electron. Devices* 50, 2000, pp.2353-60

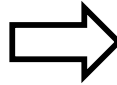
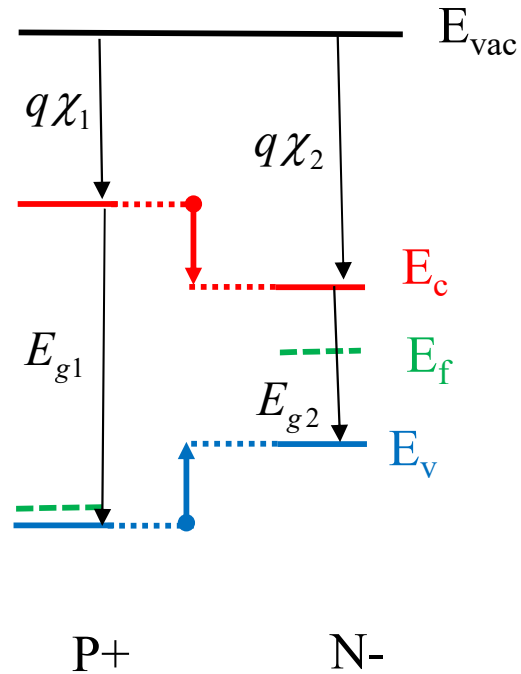
Exercice 5.3: PN hétérojonction



Construisez à l'équilibre

- le schéma de bande
- La charge nette
- Le champ électrique

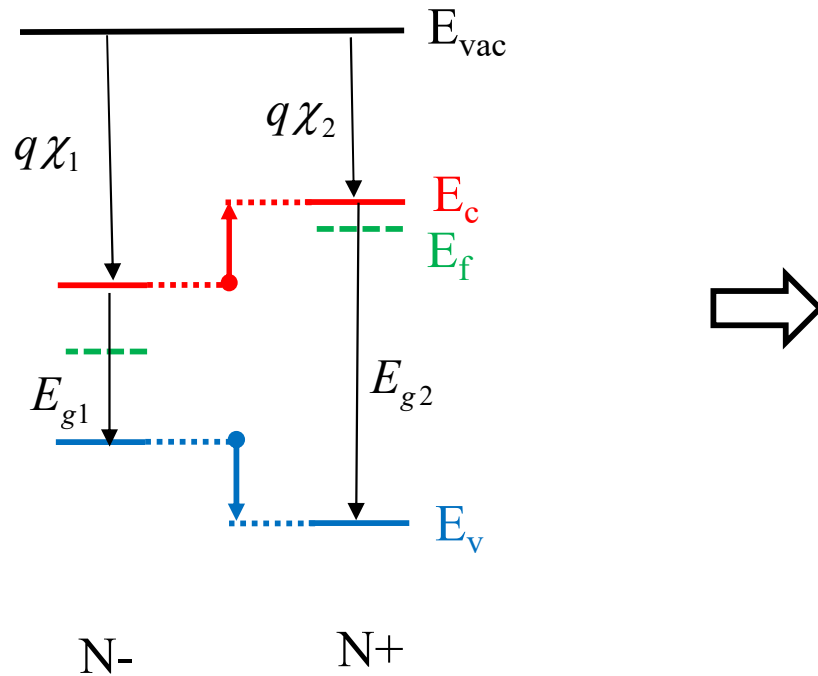
Exercice 5.4: P+N- hétérojonction



Construisez à l'équilibre

- **le schéma de bande**
- **La charge nette**
- **Le champ électrique**

Exercice 5.5: N-N+ hétérojonction



Construisez à l'équilibre

- **le schéma de bande**
- **La charge nette**
- **Le champ électrique**