# *Absorbtia luminii in dot-uri cuantice – spre celulele fotovoltaice de generatia a patra*

**V. Iancu[1], M. R. Mitroi[1], L. Fara[1]**

**A.-M. Lepadatu[2], I. Stavarache[2], M. L. Ciurea[2]**

[2] NATIONAL INSTITUTE OF MATERIALS PHYSICS
BUCHAREST-MAGURELE

[1] "POLITEHNICA" UNIVERSITY OF BUCHAREST

## Cuprins:

## Efecte de confinare in dot-uri cuantice

Groapa cuantica infinita: $V^{(\mathrm{I})}(r)=\begin{cases}0, & r<a,\\ \infty, & r>a,\end{cases}$

---

Functia de unda: $\psi^{(\mathrm{I})}_{n,l,m}(r,\theta,\varphi)=R^{(\mathrm{I})}_{n,l}(r/a)\cdot Y_{l,m}(\theta,\varphi)$

unde: $R^{(\mathrm{I})}_{n,l}(z)=a^{-3/2}N^{(\mathrm{I})}_{n,l}\begin{cases}j_l(x_{n+1,l}\cdot z), & z<1,\\ 0, & z>1,\end{cases}$

$x_{n+1,l}\neq 0$ - zero-ul n+1 al $j_l(x)$, $x_{0,l}\equiv 0$

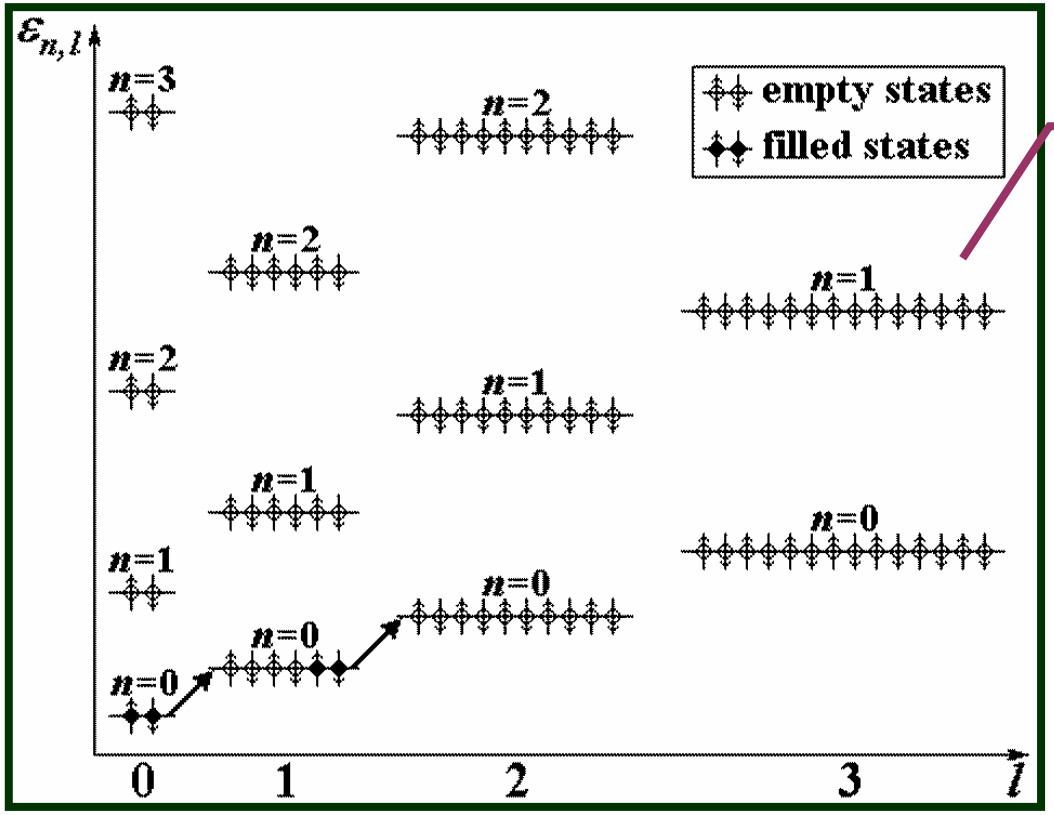
$$N^{(\mathrm{I})}_{n,l}=\left[\int_0^1 j_l^2(x_{n+1,l}z)z^2\mathrm{d}z\right]^{-1/2}$$

$Y_{l,m}(\theta,\varphi)$ - functia sferica

*n*, *l* si *m* ($|m|\le l$) sunt numerele cuantice radial, orbital si magnetic

$$\Rightarrow \boxed{\varepsilon^{(\mathrm{I})}_{n,l}=\left(\hbar^2 x^2_{n+1,l}\right)/2m_{\mathrm{e}}a^2}$$

## Efecte de confinare in dot-uri cuantice




Dependenta nivelelor de energie de numerele cuantice *n* si *l* (reprezentata la scara). Starile ocupate si libere sunt marcate per atom. Sagetile oblice reprezinta tranzitii de absorbtie a luminii.

## Efecte de confinare in dot-uri cuantice

Groapa cuantica finita: $V^{(\mathrm{F})}(r)=\begin{cases}0, & r<a,\\ V_0>0, & r>a.\end{cases}$

- Functia radiala se extinde si in afara dot-ului

$$\Rightarrow \qquad \varepsilon_{n,l}^{(F)}=\left(\hbar^2\alpha_{n+1,l}^2\right)/\left(2m_{\mathrm{e}}a^2\right)<V_0$$

unde $\alpha_{n,l}$ ( $x_{n,l}<\alpha_{n+1,l}<x_{n+1,l}$ , $\alpha_{n+1,l}<\gamma$ ) este solutia ecuatiei

$$\chi\frac{\mathrm{d}}{\mathrm{d}z}\ln j_l\left(\alpha_{n,l}z\right)\Big|_{z=1}+\sqrt{\chi\left(\gamma^2-\alpha_{n,l}^2\right)}+1=0$$

$$\chi=m_{\mathrm{a}}^*/m_{\mathrm{e}}\ ,\quad \gamma=\sqrt{2m_{\mathrm{e}}a^2V_0/\hbar^2}$$

## Absorbtia luminii pe nivele de confinare cuantica

Rata de absorbtie: $P_{i\to f} = (2\pi/\hbar)\left|H_{fi}\right|^2 f_i(T)\left[1 - f_f(T)\right]\delta(\Delta\varepsilon - hc/\lambda)$

Elementul de matrice: $\left|H_{n',l';n,l}\right|^2 = e^2E^2a^2F_l^{\pm}\Re_{n',l\pm1;n,l}\delta_{l',l\pm1}$

Coeficientul de absorbtie Einstein:

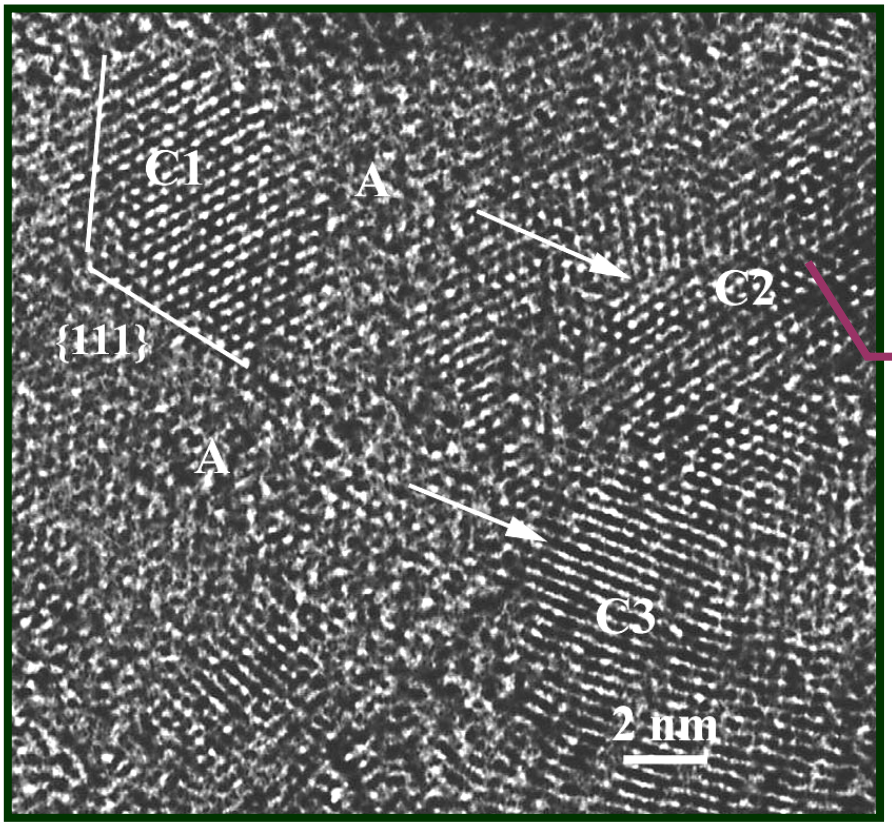
$$B_\lambda = \left[\left(2\pi a^2e^2\right)/\left(\hbar^2\varepsilon_0\varepsilon_r\right)\right]F_l^{\pm}\Re_{n',l\pm1;n,l}$$

Eficienta cuantica interna:

$$\eta_{\mathrm{Q,i}}^{\mathrm{dot}}(\lambda,T) = \frac{8\hbar}{ca^2}B_\lambda f_{n,l}(T)\left[1 - f_{n',l\pm1}(T)\right] = \frac{16\pi e^2}{\hbar c\varepsilon_0\varepsilon_r}F_l^{\pm}\Re_{n',l\pm1;n,l}f_{n,l}(T)\left[1 - f_{n',l\pm1}(T)\right]$$

**Eficienta cuantica nu depinde explicit de raza dot-ului**

# Aplicatie numerica – dot-uri de Si imersate in matrice de a-$SiO_2$




Imagine HRTEM pentru Si - $SiO_2$ (concentratie nc-Si: 75%).

## Aplicatie numerica – dot-uri de Si imersate in matrice de a-$SiO_2$

| $a = 2.5$ nm | Groapa infinita | Groapa finita |
|---|---|---|
| $\lvert 0,0\rangle \rightarrow \lvert 0,1\rangle$ | $\lambda \approx 19.7\ \mu\text{m}$<br>$\eta(\lambda,\ 300\ \text{K}) \approx 4.33\ \%$ | $\lambda \approx 21.2\ \mu\text{m}$<br>$\eta(\lambda,\ 300\ \text{K}) \approx 4.65\ \%$ |
| $\lvert 0,1\rangle \rightarrow \lvert 0,2\rangle$ | $\lambda \approx 15.6\ \mu\text{m}$<br>$\eta(\lambda,\ 300\ \text{K}) \approx 2.98\ \%$ | $\lambda \approx 16.8\ \mu\text{m}$<br>$\eta(\lambda,\ 300\ \text{K}) \approx 3.20\ \%$ |

## Concluzii

**S-a calculat eficienta cuantica interna a absorbtiei pe nivele de confinare:**

- S-a luat in considerare rolul factorilor de ocupare
- Eficienta cuantica nu depinde explicit de dimensiunea dot-ului
- Eficienta totala per dot este cu cel putin un ordin de marime mai mare decat eficienta spectrala
- Extinderea absorbtiei spre IR indepartat este utila pentru aplicatii spatiale

# Multumesc pentru atentie!!!