Partícula en una caja: Aplicaciones en ciencia de materiales

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Sistemas de baja dimensionalidad

Nanomateriales, sistemas confinados

- Ejemplos:
  - Nanoalambres
  - Puntos cuánticos
- Las propiedades ópticas de los puntos cuánticos son importantes en las aplicaciones tecnológicas:
  - Transistores
  - Celdas solares
- El modelo de la partícula en una caja permite analizar efectos cuánticos en nanomateriales cristalinos.

Pozo cuántico: Capa delgada de semiconductor entre dos capas de otro semiconductor.

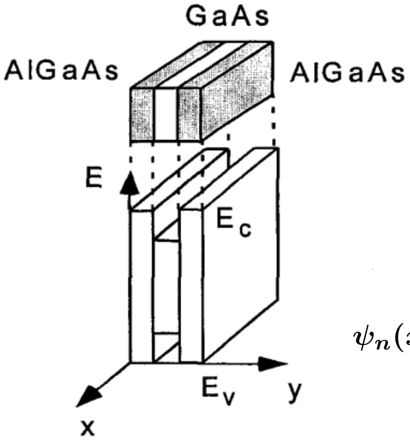

Fig. 4. AlGaAs/GaAs quantum well.

Movimiento electrónico:

- Plano xz: Partícula libre.
- Eje y: Caja de potencial infinito.

$$\psi_n(x,y,z) = \sqrt{\frac{2}{L}}\, e^{ik_x x + ik_z z} \operatorname{sen} \frac{n\pi y}{L}$$

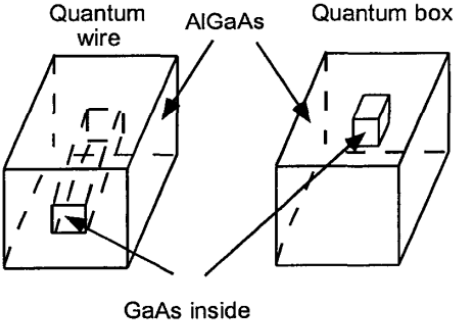

Fig. 7. Quantum wire and quantum box. (From [21])

Para el punto cuántico:

$$E_{n_x,n_y,n_z}(x,y,z) = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

E. Borovitskaya, M. S. Shur, "Low dimensional systems" *Int. J. High Speed Electronics and Systems*, **12**,1-14 (2002).

Puntos cuánticos

Simple Syntheses of CdSe Quantum Dots

Matthew L. Landry,† Thomas E. Morrell, Theodora K. Karagounis,† Chih-Hao Hsia, and Chia-Ying Wang*

J. Chem. Educ. 2014, 91, 274–279

Figure 2. Visible light illuminated (top) and short-wavelength UV light illuminated (bottom) CdSe QDs from procedure 1. The reaction time increases from left to right.

- Nanocristales semiconductores con propiedades ópticas importantes (fotoestabilidad, etc.)

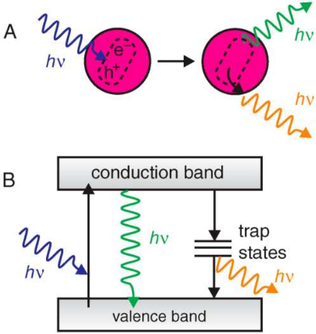

Figure 6. (A) Depiction of exciton formation in QDs after photoexcitation (blue), followed by the exciton emission (green) and/or the trap-state emission (orange). The black arrow inside the QD denotes radiationless relaxations. (B) Diagram of energy levels in QDs corrosponding to the transitions in (A). The black arrow pointing up shows the process of absorption. The black arrows pointing down represent two possible transitions due to the trap states. Originating from smaller energy-level spacings, the trap-state emission radiates at longer wavelengths than the exciton emission.

- A mayor tamaño de la nanopartícula, mayor la longitud de onda de emisión.

Quantum Dots in a Polymer Composite: A Convenient Particle-in-a-Box Laboratory Experiment

Charles V. Rice* and Guinevere A. Giffin

Journal of Chemical Education • Vol. 85 No. 6 June 2008

- En un punto cuántico, los niveles en las bandas de valencia y conducción son discretos.
- Al excitar un electrón a la banda de condución se crea un par electrón-agujero llamado excitón.
- La recombinación del excitón resulta en emisión de fluorescencia:

$$\boldsymbol{\Delta E(r) = \frac{hc}{\lambda} = E_{\mathrm{gap}} + \underbrace{\frac{h^2}{8r^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)}}$$

$\boldsymbol{\lambda}$ y $\boldsymbol{r}$ se relacionan

partícula en una caja esférica

$\boldsymbol{m_e^*}$: masa efectiva del electrón en el excitón.
$\boldsymbol{m_h^*}$: masa efectiva del agujero en el excitón.
$\boldsymbol{r}$: radio de la partícula.
$\boldsymbol{E_{\mathrm{gap}}}$: separación de bandas en el semiconductor extendido (bulto)

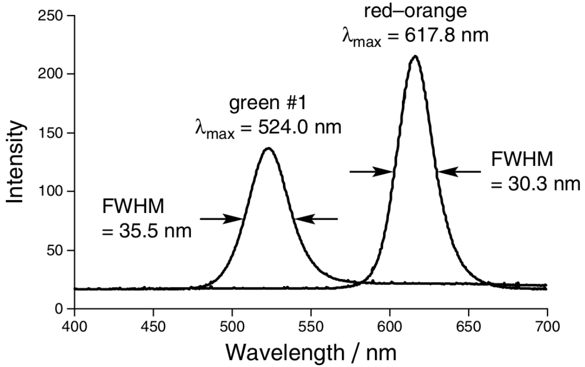

Figure 2. Photoluminescence spectrum of two core–shell CdSe/ZnS quantum dots. The nanocrystals are embedded in a matrix of polyurethane/acrylic acid. Peak maximum and line width are determined by the Ocean Optics software.

Table 1. Peak Frequency and Line Width Data for CdSe Quantum Dot Samples

Color	λ/(nm)	FWHM/(nm)	Diameter/(Å)
Blue	488.0	37.5	43
Green #1	524.0	35.5	48
Green #2	549.0	34.7	53
Yellow	565.9	32.0	57
Orange #1	586.5	31.2	63
Orange #2	600.8	30.8	67
Red–orange	617.8	30.3	74

NOTE: Dot samples were excited with the same wavelength. Data were calculated using eq 3.

- A partir de los valores de $\boldsymbol{\lambda}$, se obtuvieron los diámetros de las partículas.

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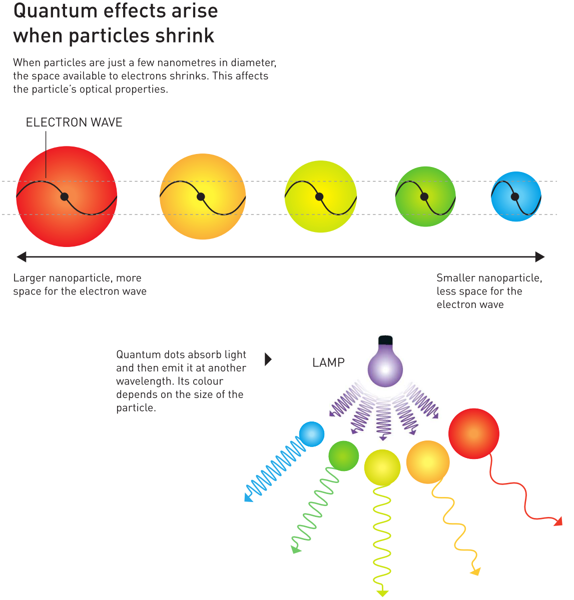
“Por el descubrimiento y síntesis de puntos cuánticos”



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https://www.nobelprize.org/prizes/chemistry/2023/press-release/

Puntos cuánticos: un área de investigación activa en ciencia de materiales.

Research briefing

It's time to shine for LEDs made using ecofriendly quantum dots

QLEDs – light-emitting diodes that rely on nanocrystals called quantum dots – are usually made with toxic heavy metals. A strategy has been developed to make QLEDs with a performance comparable to that of commercially available technologies but using a more environmentally friendly alloy of zinc, selenium, tellurium and sulfur, by improving the distribution of the tellurium atoms.

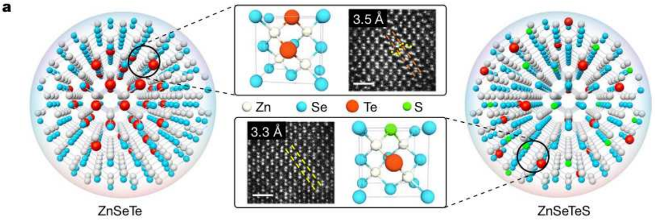

Figure 1 | Arrangement of alloy components in quantum-dot nanocrystals and performance of light-emitting diodes. a, Structural models (in colour) and transmission electron microscopy images corrected for spherical aberration (greyscale) of quantum-dot nanocrystals made using zinc, selenium and tellurium without (left; ZnSeTe) and with (right; ZnSeTeS) sulfur. Scale bars, 1 nanometre.

The performance of blue LEDs that use quantum dots as the electroluminescent component is approaching technologically relevant levels. But the best-performing materials typically include cadmium, an environmentally problematic heavy element. The appeal of this paper is that the authors have developed a strategy for preparing Cd-free quantum dots that suppresses compositional heterogeneities, enabling devices with efficiencies, lifetimes and spectral purities that rival the best Cd-based blue LEDs.

This is a summary of:
Wu, Q. *et al*. Homogeneous ZnSeTeS quantum dots for efficient and stable pure-blue LEDs. *Nature* https://doi.org/10.1038/s41586-025-08645-4 (2025).