



Optical measurements under high pressure in semiconductor nanostructures

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Outline of the talk

- Why do we study materials under high pressure?
- Experimental: high pressure techniques
- Optical properties of PbSe nanocrystals
- Optical properties InAs quantum wells and quantum wires
- Large metastability range of w- and rs-ZnO nanoparticles
- Conclusions



Why do we study materials under high pressure?

- High pressure is the only available tool to explore the interatomic potentials as a function of the interatomic distance.
- High pressure experiments are the most efficient tests of ab-initio electronic structure calculations.
- High pressure changes the band ordering in semiconductors (equivalence between chemical and mechanical pressure).











Diamond anvil cells











Transparency of diamond UV-VIS-IR



XR transmission of diamond







Microscopic optical bench







Optical properties of PbSe nanocrystals under high pressure

- Interest for solar cells: multiexciton processes
- Interest for LEDS: wide emission wavelength tuning (0.28–1 eV) and large emission efficiency



Recent results on PbSe NCs under presssure

No change of confinement energy under pressure!

Previous results on PbSe gap pressure coefficient: - (85 – 100) meV/GPa



PbSe nanocrystals: size effect











Effective mass model for size confinement in PbSe NCs

- Finite potential barriers for carrier confinement

$$x \cot(x) = 1 - \left(\frac{m^*}{m_0}\right) - \sqrt{\left(\frac{m^*}{m_0}\right)} \left(\frac{V_0}{\Delta} - x^2\right),$$

where $x = k_{in}r_0$.
$$\frac{1}{\Delta} = \frac{2m^*r_0^2}{\hbar^2} \quad k_{in}^2 = \frac{2m^*E}{\hbar^2} \text{ and } k_{out}^2 = \frac{2m_0|E - V_0|}{\hbar^2},$$

- Non parabolic effective masses
$$m^*_{e,h}(E, X) = \frac{m^*_{e,h}(0, X)}{\sqrt{1 - \frac{m^*_{e,h}(0, X)}{m_0} \frac{E}{E_{np}}}; \quad X = T, P$$

$$E_{np} = \frac{\hbar^2}{8m_0\gamma} = 0.05 \quad eV; \quad \gamma = 1.9 \times 10^{15} \text{ cm}^{-2}$$





PbSe (bulk and NCs) under high pressure



ICM UV



Confinement energy in PbSe NCs under high pressure







Temperature dependence of electronic transitions in PbSe NCs







Temperature dependence of the confinement energy in PbSe NCs

The increase of the effective mass with T makes the total confinement to decrease with higher rates for NCs with smaller diamters.







- Dimensions of QWires :average height (2.5 nm), average width (21 nm), and average length (185nm)
- QWires are randomly distributed
- QWires coexist with flat QWell islands of 1-2 ML high





✓ Four PL bands observed. The two bands with higher energy mainly arise from exciton recombination at the QW-like islands







Peak	E ₀ (eV)	a ₁ (meV/GPa)	a ₂ (meV/GPa²)
QWr-E _{1A}	0.786	99	-2.9
QWr-E _{2A}	0.828	98	-2.7
QW-E _{3A}	0.896	98	-2.5
QW-E _{4A}	0.964	103	-3.0

Pressure coefficient InP: 85 meV/GPa

Pressure coefficient InAs: 100 meV/GPa?

✓ QWrs and QWs pressure coefficients similar to those of InAs?

✓ Slightly larger pressure coefficients for the QW islands than for the QWrs?





Optical absorption in bulk InAs under pressure

Sample thickness: 14 µm FIR and MIR: FTIR spectrometer NIR: dispersive spectrometer





InAs direct bandgap pressure coefficient: 104 4 meV/GPa







InAs/InP	2 ML	3 ML	4 ML
E ₀ (eV)	1.055	0.975	0.898







InAs/InP	2 ML	3 ML	4 ML	
E ₀ (eV)	1.055	0.975	0.898	Similar PC to InP (85)
$lpha_1$ (meV/GPa)	89	83	78	



























Large metastability range of Zn_{1-x}Co_xO NCs under pressure

Effect of Co substitution on the optical properties of ZnO (thin films)







Structural phase transitions in Zn_{1-x}Co_xO thin films under pressure







Absorption edge of Zn_{1-x}Co_xO NCs under pressure







Absorption edge of $Zn_{1-x}Co_xO$ NCs under pressure (x=0.01)

Up-stroke

Down-stroke







Absorption edge of $Zn_{1-x}Co_xO$ NCs under pressure (x=0.20)

Up-stroke

Down-stroke







Conclusions

- 1) Optical absorption and photoluminescence experiments under pressure can be an useful tool to investigate the electronic structure of semiconductor nanostructures.
- 2) In some cases the interpretation of the results requires sophisticated theoretical methods beyond simple effective mass models.
- 3) High pressure is also an interesting tool in the preparation of new metastable nanostructures.
- 4) To improve the power of HP methods in nanoscience, by increasing the spatial resolution, new diamond anvil cells can be designed allowing for the use of shorter working distance objectives.



Acknowledgements



PbSe NCs

R. Abargues, J.L. Valdés, E. Pedrueza

ICMUV, Universidad de Valencia

InAs QWrs and QWs

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ZnCoO NCs

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DCITIMAC, Universidad de Cantabria,