Excitons in self-assembled type-II quantum dots and coupled dots

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Self-assembled quantum dots

Necessary ingredients:

2 semiconductor materials with a substantially different lattice parameter, e.g.

InP : $a \sim 5.869 \text{ Å}$ and GaInP : $a \sim 5.653 \text{ Å}$ (mismatch $\sim 3.8\%$)

MBE growth

Result

lattice mismatch strain fields formation of islands

self-assembled quantum dots
Different type-II systems

electron in the dot, hole outside
  e.g. InP/GaInP dots

hole in the dot, electron outside
  e.g. GaSb/GaAs dots

InGaP

InP

InAs/Si dots

InAs

Si

GaAs

GaSb

Si

CB (Γ)

CB (X)

VB

h ≈

e

h ≈

h ≈

h ≈

h ≈
Theoretical approach


\[
\varepsilon_{ij}(\vec{r}) = \varepsilon_0 \delta_{ij} - \frac{\varepsilon_0}{4\pi(1-\nu)} \int dS' \frac{r_i - r_i'}{|\vec{r} - \vec{r}'|^3}
\]

- **Band structure**: effective ‘anisotropic’ mass (following the ideas of L.R. Wilson *et al.*, Phys. Rev. B *57*, R2073 (1998) – which was successfully applied to InAs/GaAs SAQD’s).

- **Exciton energy**: Hartree-Fock approximation

→ advantages: much faster numerical program + magnetic field can easily be included
No strain

Only Coulomb interaction
Single dots

the hole can sit: - at the radial boundary of the dot - above/below the disk

- Study of the influence of the disk parameters $d$ and $R$ (at $B = 0T$)
  \[ P_{side} = 2\pi \int_{-\infty}^{\infty} dz_h \int_{R_h}^{\infty} r_h |\psi_h (r_h, z_h)|^2 dr_h \]

Distinguish between 2 regimes:
- \textbf{disk-like} regime: $d \ll 2R$ \hspace{1cm} (3)
- \textbf{pillar-like} regime: $d \gg 2R$ \hspace{1cm} (1)
the hole is sitting at the radial boundary of the quantum disk
appearance of angular momentum transitions
Vertically coupled quantum dots

- Two vertically coupled dots
  Result for: $R = 6\text{nm}$, $d = 6\text{nm}$ and $d_d = 3.6\text{nm}$

- Extra parameter to vary: interdot-distance $d_d$
- Easier realization of the pillar-like system
Spontaneous symmetry breaking

- enhancement of the Coulomb attraction
- magnetic field induces a permanent dipole moment
Stark effect

Single and coupled type-II dots

- Single type-II disk

\[ R = 10\text{nm}, \ d = 8\text{nm} \]

- non-parabolic Stark shift (cfr. coupled type I disks)

- creation of a strong dipole moment for \( F \neq 0 \)

- linear contribution is more important

\[ E(F) = E(F_0) - p(F - F_0) - \beta(F - F_0)^2 \]
Two coupled type II-disks

- $R = 12\, \text{nm}$, $d = 3\, \text{nm}$, $d_d = 3\, \text{nm}$

- Hysteresis due to spontaneous symmetry breaking

- System is trapped in the energy minimum

- Permanent dipole moment
Effects due to strain

Hole band engineering
Pseudomorphic quantum wells: case of compressive strain

Hydrostatic strain splits the HH and LH bands

Tetrahedral strain splits the HH and LH bands
The effective potentials: for different SAQD’s height

InP/In$_{0.49}$Ga$_{0.51}$P

Conduction band

Heavy hole band

Light hole band
Effective potentials

- Unstrained VB offset
- Light hole
- Heavy hole

Parameters:
- $R = 8\text{nm}$
- $d = 4\text{nm}$

Axes:
- $z$ (nm)
- $r$ (nm)
- Potential (meV)
Heavy hole: type I → type II

- Potential (meV) vs. z (nm) for different R (nm) and d (nm) values.
- 50% type II-like behavior at specific d (nm) and R (nm) values.
Heavy – light hole transition

| Mass (m_o) | z    | || |
|------------|------|----|
| hh         | 0.61 | 0.15 |
| lh         | 0.12 | 0.30 |

![Graph showing the transition between heavy and light hole ground states](image-url)
Comparison with experiment

Diamagnetic shift: $\Delta E = E(B) - E(B = 0T)$

![Graph showing comparison with experiment and fitted masses](image)

- Influence of radius?
- Influence of masses?

Fitted masses:

- $m_e = 0.15m_0 \leftrightarrow 0.077m_0$
- $m_{hh,□} = 0.5m_0 \leftrightarrow 0.1515m_0$
- $m_{lh,□} = 1.5m_0 \leftrightarrow 0.269m_0$

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Start with a positive unstrained VB offset\(^1\)
\[ \Rightarrow \text{Still discrepancy between theory and experiment} \]
\[ \Rightarrow \text{increase of the masses needed to obtain good fit} \]
\[ m_e = 0.15m_0; \ m_{hh, \square} = 0.5m_0; \ m_{lh, \square} = 1.5m_0 \]

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Coupled cylindrical SAQD’s

Two-dot stack

Three-dot stack
Energy levels in vertically coupled quantum dots

Electron
Heavy hole
Light hole

R = 8 nm
h = 2 nm
Effective potentials in two vertically coupled quantum dots

Conduction band

Heavy hole band

Light hole band
Hole states

\[ F_z = J_z + L_z = f\hbar : \text{total angular momentum} \]

\[ J_z = j\hbar : \text{Bloch part} \]

\[ L_z = l\hbar : \text{envelope part} \]

| \(|f| = 3/2 : \) | | \(|f| = 1/2 : \) |
|----------------|----------------|
| Heavy hole \((j=3/2), l=0,-3\) | Heavy hole \((j=3/2), l=-1,-2\) |
| Light hole \((j=1/2), l=-1,-2\) | Light hole \((j=1/2), l=0,-1\) |
Probability density of the odd $S_{3/2}$ state in the two-dot stack (ground state for $d > 2$ nm)
Ground

$S_{1/2}^+$

Second

$S_{1/2}^+$

Ground

$S_{1/2}^-$
Energy levels in a three-dot stack
Probability density of the even $S_{3/2}$ state in the three-dot stack (ground state for $d>2$ nm)
Excitons in the two-dot stack

Dependence of the ground states for $F_{\text{exc}}=-1$ and $F_{\text{exc}}=0$ on the spacer thickness ($h=2\text{nm}; r=8\text{nm}$).

$F_{\text{exc}}=-1$ (heavy-hole-like exciton)

$F_{\text{exc}}=0$ (light-hole-like exciton).

There appears substantial overshoots in the exciton energies.
Conclusions (1/2)

- **Exciton in a type II quantum dot: pillar – disk systems**
- **Magnetic field effect:**
  - disk-like system: parabolic -> linear increase of energy with B (Cfr. Type I)
  - pillar-like system: angular momentum transitions
    - vertically coupled dots with small interdot distance
    - spontaneous symmetry breaking -> magnetic field induced dipole moment
- **Electric field effect:** **Stark shift**
  - Parabolic field dependence only for single type-I disk
  - Strongly linear dependence for coupled type-I and single and coupled type II disks -> creation of dipole moment
Conclusions (2/2)

- Strain effect: hole band engineering (light – heavy hole).

- The total angular momentum of the ground state of holes changes with the thickness of the quantum dot.

- In coupled quantum dots: strain acts opposite to quantum mechanical coupling. It increases the electron ground state above the single quantum dot value.
  - Electron coupling is effective only for spacers thinner than the coupling length.
  - Holes exhibit ‘electronic’ coupling only for very thin spacers.

- Strain predominantly influences the “holes”. Therefore, our simple model calculation will be more appropriate for e.g. GaSb/GaAs and InAs/Si dots.
The end
For details see: http://cmt.uia.ac.be

- **Magnetoexcitons in planar type-II quantum dots in a perpendicular magnetic field**

- **Single and vertically coupled type-II quantum dots in a perpendicular magnetic field: exciton groundstate properties**

- **Stark shift in single and vertically coupled type-I and type-II quantum dots**

- **Effect of isotropic versus anisotropic elasticity on the electronic structure of cylindrical InP/In_{0.49}Ga_{0.51}P self-assembled quantum dots**

- **Strain and band edges in single and coupled cylindrical InAs/GaAs and InP/InGaP self-assembled quantum dots**

- **Electronic structure of the valence band in cylindrical strained InP/InGaP quantum dots in an external magnetic field**

- **Electron and hole localization in coupled InP/InGaP self-assembled quantum dots**