Strained Quantum Dot: Examples

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Network for Computational Nanotechnology (NCN) Electrical and Computer Engineering
• Schroedinger Solver
  - Example1: InAs cuboid Quantum Dot (QD)
  - Example2: InAs dome-shape QD
  - Example3: InAs pyramid QD

• Strain+Schroedinger Solver
  - Example1: InAs strained cuboid QD
  - Example2: InAs strained dome-shape QD
  - Example3: InAs strained pyramid QD

• Realistic QD examples
How to obtain eigen-states?

Atomistic Construction

Hamiltonian Construction

Single Particle States

\[ H \Psi = E \Psi \]

Ground State

Excited States

Ground State
Example 1: Cuboid QD

Structure

Band Diagram along the red line

InAs

GaAs

1.43eV

E_c

GaAs

InAs

0.36eV

E_v
Material
{
    name     = GaAs
    tag      = substrate
    crystal_structure = zincblende
    regions   = (1)
    Bands:TB:sp3d5sstar_SO:param_set = param_Klimeck
}

Material
{
    name     = InAs
    tag      = dot
    crystal_structure = zincblende
    regions   = (2)
    Bands:TB:sp3d5sstar_SO:param_set = param_Klimeck
}

Define Material:
- GaAs (substrate) in region(1)
- InAs (dot) in region(2)

Define Tight Binding parameter set:
sp3d5sstar_SO (Klimeck)
Domain
{
    name               = atomic_structure
    type                 = pseudomorphic
    base_material = substrate

    dimension       = (18,18,18)
    periodic           = (false,false,false)

    crystal_direction1 = (1,0,0)
    crystal_direction2 = (0,1,0)
    crystal_direction3 = (0,0,1)

    space_orientation_dir1 = (1, 0, 0)
    space_orientation_dir2 = (0, 1, 0)

    passivate = true
    origin  = (0,0,0)
    regions = (1,2)
}

GaAs

18x18x18 unit cells

Non-periodic in all three directions (x,y,z)

Passivate the system
Geometry
{
  Region
  {
    shape = cuboid
    region_number = 1
    priority = 1
    min = (-0.1,-0.1,-0.1)
    max = (12,12,12)
  }
  Region
  {
    shape = cuboid
    region_number = 2
    priority = 2
    min = (2,2,2)
    max = (8,8,8)
  }
}
Input deck: Schroedinger solver

```plaintext
solver
{
  name = schroedi
  type = Schroedinger
  domain = atomic_structure
  active_regions = (1,2)

  tb_basis = sp3d5sstar_SO

  k_space_basis = cartesian
  k_points = [(0,0,0)]
  number_of_nodes = (1)

  eigen_values_solver = krylovshur
  number_of_eigenvalues = 8
  shift = 0.9
  solver_transformation_type = shift

  Tight Binding Model we use:
  sp3d5s* with spin orbital

  Only one k-point (Γ point)

  Find 8 eigen-states around this value
```
Input deck: Schroedinger solver

```plaintext
job_list = (assemble_H, passivate_H, calculate_band_structure)
output = (energies,eigenfunctions_Silo)

max_number_iterations = 80000
convergence_limit = 1e-6
monitor_convergence = true
ncv = 60
```

Change these options to get convergence

```plaintext
Global
{
    solve = (schroedi)
    logfile = qd.log
    messaging_level = 3
    database = ../all.mat
}
```

Solve for Schroedinger
**Schroedi\_energies.dat:**

- **Ground State (eV):** 0.921589896316
- **1st Excited State (eV):** 1.13047133425
- **2nd Excited State (eV):** 1.13478442955
- **3rd Excited State (eV):** 1.28909697824
Example 2: dome shape QD

Geometry
{
  Region
  {
    shape = cuboid
    region_number = 1
    priority = 1
    min = (-0.1, -0.1, -0.1)
    max = (12, 12, 12)
  }
  Region
  {
    shape = dome
    region_number = 2
    priority = 2
    min = (2, 2, 4)
    max = (8, 8, 7)
  }
}
Schroedi_energies.dat:

1.12307899109  1.35429143635  1.52322593363  1.58783804964

Ground State (eV)  1st Excited State (eV)  2nd Excited State (eV)  3rd Excited State (eV)
Example 3: pyramid QD

Geometry
{
    Region
    {
        shape = cuboid
        region_number = 1
        priority = 1
        min = (-0.1,-0.1,-0.1)
        max = (12,12,12)
    }
    Region
    {
        shape = pyramid
        region_number = 2
        priority = 2
        min = (2,2,4)
        max = (8,8,7)
    }
}
Schroedi\_energies.dat:

<table>
<thead>
<tr>
<th>Ground State(eV)</th>
<th>1\textsuperscript{st} Excited State (eV)</th>
<th>2\textsuperscript{nd} Excited State(eV)</th>
<th>3\textsuperscript{rd} Excited State(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.15123980388</td>
<td>1.39629873796</td>
<td>1.40380755409</td>
<td>1.50972569902</td>
</tr>
</tbody>
</table>
Strain + Schroedinger Simulation

- Geometry Construction
- Atomistic Relaxation
- Strain
- Piezoelectric Potential
- Hamiltonian Construction
- Single Particle States

Diagram showing the process of strain and Schroedinger simulation with materials such as GaAs and InAs.
Input deck change: Schroedinger solver

```
solver
{
  name               = schroedi
  type               = Schroedinger
  domain            = atomic_structure
  active_regions    = (1,2)

  tb_basis           = sp3d5sstar_SO

  ...  

  job_list        = (assemble_H, passivate_H, include_strain_H,
                      calculate_band_structure)

  ...
}

Global
{
  solve = (keating, schroedi)

  ...
}
```

Include strain effect in the Hamiltonian
What does include_strain_H do?

When the system is strained, atom position varies, distance to neighboring atoms (d) changes.

**Harrison’s scaling law:**

\[ H_{\text{off}} = H_{0,\text{off}} \left( \frac{d_0}{d} \right)^n \]

\[ H_{\text{on}} = H_{0,\text{on}} \]

**Boykin’s model:**

\[ H_{\text{off}} = H_{0,\text{off}} \left( \frac{d_0}{d} \right)^n \]

\[ H_{\text{on}} = H_{0,\text{on}} + \text{strain dependent terms} \]

---

**Include_strain_H:** include strain effects in the diagonal elements of the Hamiltonian.

Timothy B. Boykin et al., PRB, 66, 125207(2002)
Example 1: cuboid QD

Displacement:

Compare eigen-states:

<table>
<thead>
<tr>
<th></th>
<th>Ground State(eV)</th>
<th>1st Excited State(eV)</th>
<th>2nd Excited State(eV)</th>
<th>3rd Excited State(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unstrained</td>
<td>0.921589</td>
<td>1.130471</td>
<td>1.134784</td>
<td>1.289096</td>
</tr>
<tr>
<td>Strained</td>
<td>1.433982</td>
<td>1.567295</td>
<td>1.567715</td>
<td>1.570308</td>
</tr>
</tbody>
</table>
Wave functions

**Unstrained:**

**Strained:**
Example 2: dome shape QD

Displacement:

Compare eigen-states:

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<th>3\textsuperscript{rd} Excited State (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unstrained</td>
<td>1.123078</td>
<td>1.354291</td>
<td>1.523225</td>
<td>1.587838</td>
</tr>
<tr>
<td>Strained</td>
<td>1.442144</td>
<td>1.567384</td>
<td>1.599155</td>
<td>1.684464</td>
</tr>
</tbody>
</table>
Wave functions

Unstrained:

Strained:
Example 3: pyramid QD

Displacement:

Compare eigen-states:

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<th>3&lt;sup&gt;rd&lt;/sup&gt; Excited State(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unstrained</td>
<td>1.151239</td>
<td>1.396298</td>
<td>1.403807</td>
<td>1.509725</td>
</tr>
<tr>
<td>Strained</td>
<td>1.446310</td>
<td>1.571351</td>
<td>1.579728</td>
<td>1.592485</td>
</tr>
</tbody>
</table>
Wave functions

Unstrained:

Strained:
Realistic QD example

**Structure**

- GaAs
- InAs
- 3nm height
- 10nm width
- 30nm length

**Displacement**

Boundary Condition: Bottom fixed, sides periodic, top open

**Eigen-values**

- GS(strained)
- ES1(strained)
- GS(unstrained)
- ES1(unstrained)

**Wave functions (with strain):**
Realistic QD example 2

Structure

Contains 10 million atoms!

Displacement

Boundary Condition:
Bottom fixed, sides periodic, top open

Eigen-values

Wave functions (with strain):

ES1(strained)
GS(strained)

ES1(unstrained)
GS(unstrained)
Thank You