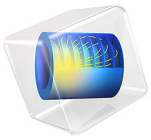
Created in COMSOL Multiphysics 6.2



Superlattice Band Gap Tool

The Superlattice Band Gap Tool model helps the design of periodic structures made of two alternating semiconductor materials (superlattices). The model uses the effective mass Schrödinger equation to estimate the electron and hole ground state energy levels in a given superlattice structure. Device engineers can use the model to quickly compute the effective band gap for a given periodic structure and iterate the design parameters until they reach a desired band gap value.

Introduction

A superlattice is constructed from multiple thin layers of alternating material compositions. It finds applications in HEMTs, LEDs, lasers, and photodetectors. (Ref. 1)

The superlattice in the model is composed of layers of GaAs and AlGaAs. The envelope function approximation (Chap. 1, Sec. 1.7 in Ref. 2) can be employed to justify the use of the single-particle Schrödinger equation. Note that not only the electron potential energy, but also the effective mass, is a function of material composition. To properly take care of the discontinuity in the effective mass, the **Schrödinger Equation** physics interface applies the BenDaniel–Duke boundary condition (Chap. 2, Sec. 2.6 in Ref. 2) by default.

Model Definition

The band gap energies of the well and the barrier materials are 1.424 and 2.168 eV, respectively. The conduction band offset is 0.283 eV. The electron effective masses of the well and the barrier materials are 0.063 and 0.71, respectively. The hole effective masses of the well and the barrier materials are 0.51 and 0.76, respectively. The widths of the well and the barrier are both 5 nm. The modeling domain consists of one unit cell.

Two Schrödinger Equation physics interfaces are set up to solve for the electron and hole ground state wave functions and energy levels, in two separate studies, respectively. Periodic boundary condition of the Continuity type is used at the two ends of the unit cell. The solutions from the two studies are combined to compute the effective band gap and to generate the plot of electron and hole wave functions. The Array 1D dataset is used to extend the solutions from one to three unit cells for plotting.

Results and Discussion

Figure 1 summarizes the result by plotting the conduction and valence band edges, and the real and imaginary parts of the electron and hole ground state wave functions. The wave functions are shifted to the corresponding ground state energy levels.

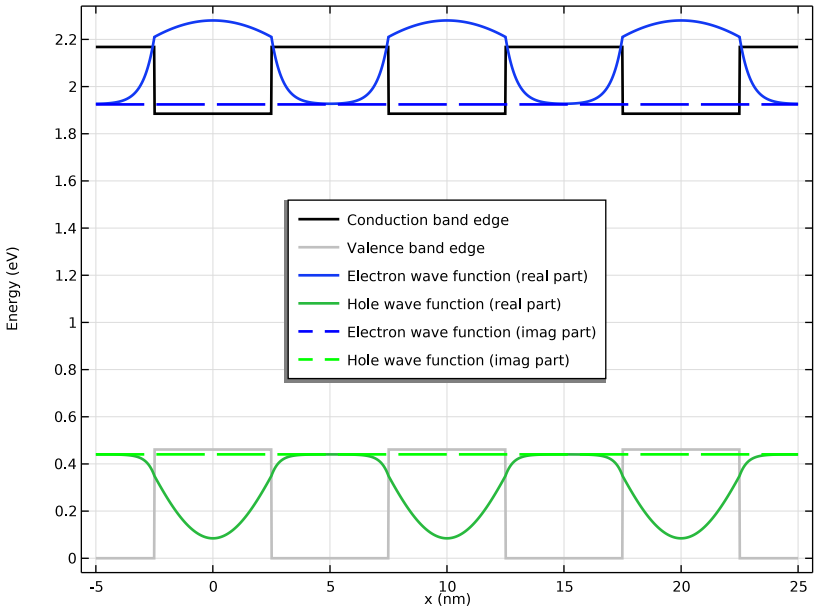


Figure 1: Summary plot for the superlattice, including the conduction and valence band edges, and the real and imaginary parts of the electron and hole ground state wave functions.

The Global Evaluations show that the electron ground state energy level is 0.039 eV from the conduction band edge, and the one for the hole is 0.021 eV. This leads to the effective band gap of 1.484 eV for the superlattice structure.

References

1. S. M. Sze and K.K. Ng, *Physics of Semiconductor Devices*, 3rd ed., John Wiley & Sons, Inc., 2007.

2. P. Harrison, *Quantum Wells, Wires and Dots*, 3rd ed., John Wiley & Sons, Inc., 2009.

Application Library path: `Semiconductor_Module/Quantum_Systems/superlattice_band_gap_tool`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

2 In the **Select Physics** tree, select **Semiconductor>Schrödinger Equation (schr)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Eigenvalue**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard exits and starts the COMSOL Desktop at the Geometry node. We can set the length scale here right away. Then import some model parameters from a text file.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **nm**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `superlattice_band_gap_tool.txt`.

Create the geometry for one unit cell of the superlattice.

GEOMETRY 1

Interval 1 (i1)

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.
2. In the **Settings** window for **Interval**, locate the **Interval** section.
3. From the **Specify** list, choose **Interval lengths**.
4. In the **Left endpoint** text field, type `-lw/2-lb/2`.
5. In the table, enter the following settings:

Lengths (nm)
lb/2
lw
lb/2

6. Click **Build All Objects**.

Add physics for the electrons in the conduction band. Use two separate nodes for the different potential energy and effective mass values in the well and barrier regions. Since we are only interested in the ground state, use the default Continuity option for the Periodic Condition at the exterior boundaries of the unit cell.

SCHRÖDINGER EQUATION E-

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.
2. In the **Settings** window for **Schrödinger Equation**, type `Schrödinger Equation e-` in the **Label** text field.
3. In the **Name** text field, type `schre`.
4. Click to expand the **Dependent Variables** section. In the **Wave functions (1)** table, enter the following settings:

psie

Effective Mass 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation e- (schre)** click **Effective Mass 1**.
2. In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

3 In the $\mathbf{m}_{\text{eff,e,11}}$ text field, type `meb*me_const`.

Electron Potential Energy 1

1 In the **Model Builder** window, click **Electron Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

3 From the V_e list, choose **User defined**. In the associated text field, type `Egb*e_const`.

Effective Mass 2

1 In the **Physics** toolbar, click **Domains** and choose **Effective Mass**.

2 Select Domain 2 only.

3 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

4 In the $\mathbf{m}_{\text{eff,e,11}}$ text field, type `mew*me_const`.

Electron Potential Energy 2

1 In the **Physics** toolbar, click **Domains** and choose **Electron Potential Energy**.

2 Select Domain 2 only.

3 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

4 From the V_e list, choose **User defined**. In the associated text field, type `-CBO*e_const`.

Periodic Condition 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

2 In the **Settings** window for **Periodic Condition**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

Add physics for the holes in the valence band in a similar way.

ADD PHYSICS

1 In the **Physics** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Recently Used>Schrödinger Equation (schr)**.

4 Click **Add to Component 1** in the window toolbar.

5 In the **Physics** toolbar, click **Add Physics** to close the **Add Physics** window.

SCHRÖDINGER EQUATION HOLE

1 In the **Settings** window for **Schrödinger Equation**, type `Schrödinger Equation hole` in the **Label** text field.

2 In the **Name** text field, type `schrh`.

3 Locate the **Model Properties** section. From the **Particle type** list, choose **Holes**.

4 Locate the **Dependent Variables** section. In the **Wave functions (1)** table, enter the following settings:

`psih`

Effective Mass 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Schrödinger Equation hole (schrh)** click **Effective Mass 1**.

2 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

3 In the $\mathbf{m}_{\text{eff,h,11}}$ text field, type `mhb*me_const`.

Electron Potential Energy 1

1 In the **Model Builder** window, click **Electron Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

3 From the V_h list, choose **User defined**. In the associated text field, type `0`.

Effective Mass 2

1 In the **Physics** toolbar, click **Domains** and choose **Effective Mass**.

2 Select Domain 2 only.

3 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

4 In the $\mathbf{m}_{\text{eff,h,11}}$ text field, type `mhw*me_const`.

Electron Potential Energy 2

1 In the **Physics** toolbar, click **Domains** and choose **Electron Potential Energy**.

2 Select Domain 2 only.

3 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

4 From the V_h list, choose **User defined**. In the associated text field, type `VBO*e_const`.

Periodic Condition 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

2 In the **Settings** window for **Periodic Condition**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

Create the mesh.

MESH 1

Edge 1

In the **Mesh** toolbar, click **Edge**.

Size

1 In the **Model Builder** window, click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `hmax`.

5 Click **Build All**.

STUDY 1

Step 1: Eigenvalue

1 In the **Model Builder** window, under **Study 1** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

3 In the **Desired number of eigenvalues** text field, type `1`.

4 In the **Search for eigenvalues around shift** text field, type `(Egb-CBO)[1/V]`.

5 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Schrödinger Equation hole (schrh)**.

Use two studies, one for each carrier type. Then combine the solutions to inspect the result.

6 In the **Model Builder** window, click **Study 1**.

7 In the **Settings** window for **Study**, locate the **Study Settings** section.

8 Clear the **Generate default plots** check box.

9 In the **Home** toolbar, click **Compute**.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Eigenvalue**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Schrödinger Equation e- (schre)**.

5 Click **Add Study** in the window toolbar.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

1 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

2 In the **Desired number of eigenvalues** text field, type `1`.

3 In the **Search for eigenvalues around shift** text field, type `-VBO[1/V]`.

4 In the **Model Builder** window, click **Study 2**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** check box.

7 In the **Home** toolbar, click **Compute**.

RESULTS

In the **Model Builder** window, expand the **Results** node.

Join 1

1 In the **Model Builder** window, expand the **Results>Datasets** node.

2 Right-click **Results>Datasets** and choose **Join**.

3 In the **Settings** window for **Join**, locate the **Data 1** section.

4 From the **Data** list, choose **Study 1/Solution 1 (sol1)**.

5 From the **Solutions** list, choose **One**.

6 Locate the **Data 2** section. From the **Data** list, choose **Study 2/Solution 2 (sol2)**.

7 From the **Solutions** list, choose **One**.

8 Locate the **Combination** section. From the **Method** list, choose **Explicit**.

Array 1D 1

1 In the **Results** toolbar, click **More Datasets** and choose **Array 1D**.

2 In the **Settings** window for **Array 1D**, locate the **Data** section.

3 From the **Dataset** list, choose **Join 1**.

4 Locate the **Array Size** section. In the **X size** text field, type `3`.

5 Click to expand the **Advanced** section. Select the **Define variables** check box.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Join 1**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`data1(schre.Ei)/e_const-(Egb-CBO)`	`V`	`Conduction band edge shift`

5 Click **Evaluate**.

Global Evaluation 2

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Join 1**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`data2(schrh.Ei)/e_const+VBO`	`V`	`Valence band edge shift`

5 Click **Evaluate**.

Global Evaluation 3

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Join 1**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
`(data1(schre.Ei)+data2(schrh.Ei))/e_const`	`V`	`Effective band gap`

5 Click **Evaluate**.

1D Plot Group 1

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Array 1D 1**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `x (nm)`.

7 Select the **y-axis label** check box. In the associated text field, type `Energy (eV)`.

8 Locate the **Legend** section. From the **Position** list, choose **Center**.

Ve

1 Right-click **1D Plot Group 1** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Ve` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data1(schre.V)/e_const`.

4 Select the **Description** check box. In the associated text field, type `Conduction band edge`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `arr1x`.

7 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Black**.

8 From the **Width** list, choose **2**.

9 Click to expand the **Quality** section. From the **Smoothing** list, choose **Everywhere**.

10 From the **Resolution** list, choose **Extra fine**.

11 Click to expand the **Legends** section. Select the **Show legends** check box.

12 From the **Legends** list, choose **Manual**.

13 In the table, enter the following settings:

Legends
`Conduction band edge`

14 Right-click **Ve** and choose **Duplicate**.

Vh

1 In the **Model Builder** window, under **Results>1D Plot Group 1** click **Ve 1**.

2 In the **Settings** window for **Line Graph**, type `Vh` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data2(-schrh.V)/e_const`.

4 In the **Description** text field, type `Valence band edge`.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Gray**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Valence band edge`

7 Right-click **Vh** and choose **Duplicate**.

psie

1 In the **Model Builder** window, under **Results>1D Plot Group 1** click **Vh 1**.

2 In the **Settings** window for **Line Graph**, type `psie` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data1(schre.Psi*Egw/4/schre.plot_fac+schre.Ei/e_const)`.

4 In the **Description** text field, type `e- wave function`.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
Electron wave function (real part)

7 Right-click **psie** and choose **Duplicate**.

psih

1 In the **Model Builder** window, under **Results>1D Plot Group 1** click **psie 1**.

2 In the **Settings** window for **Line Graph**, type `psih` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data2(-schrh.Psi*Egw/4/schrh.plot_fac-schrh.Ei/e_const)`.

4 In the **Description** text field, type `hole wave function`.

5 Locate the **Legends** section. In the table, enter the following settings:

Legends
Hole wave function (real part)

psie

In the **Model Builder** window, right-click **psie** and choose **Duplicate**.

Im(psie)

1 In the **Model Builder** window, under **Results>1D Plot Group 1** click **psie 1**.

2 In the **Settings** window for **Line Graph**, type `Im(psie)` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data1(imag(schre.Psi)*Egw/4/schre.plot_fac+schre.Ei/e_const)`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Blue**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Electron wave function (imag part)`

psih

In the **Model Builder** window, right-click **psih** and choose **Duplicate**.

Im(psih)

1 In the **Model Builder** window, under **Results>1D Plot Group 1** click **psih 1**.

2 In the **Settings** window for **Line Graph**, type `Im(psih)` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `data2(-imag(schrh.Psi)*Egw/4/schrh.plot_fac-schrh.Ei/e_const)`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Green**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Hole wave function (imag part)`

7 In the **1D Plot Group 1** toolbar, click **Plot**.