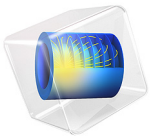
Created in COMSOL Multiphysics 5.6



Heterojunction 1D

This benchmark model simulates three different heterojunction configurations under forward and reverse bias. It shows the difference in using the continuous quasi-Fermi level formulation versus the thermionic emission formulation for the charge transfer across the heterojunction. The simulated energy levels are compared between each configuration in order to illustrate the origin of the charge transfer, that is, whether it is primarily from holes in the valence band or from electrons in the conduction band. The computed I-V curves for each configuration are compared with results from the literature. Several methods for better convergence are demonstrated in the setup of the various study steps.

Introduction

Semiconductor heterojunctions are interfaces where two different semiconducting materials are in contact. There are two types of heterojunctions:

- Isotypes: same type of majority carrier on both side of the junction, for example, n-n or p-p.
- Anisotypes: the majority carrier are electrons on one side and hole on the other, for example, n-p or p-n.

Depending on the configuration, heterojunctions show different behaviors depending on the material band-gap difference and doping type.

TABLE 1: HETEROJUNCTION CONFIGURATIONS.

DOPING MATERIAL 1	DOPING MATERIAL 2	BAND-GAP DIFFERENCE EG2-EG1	ANODE CONTACT SIDE	CATHODE CONTACT SIDE	CURRENT MOSTLY CARRIED BY
n-doped	n-doped	>0	material 1	material 2	electrons
p-doped	p-doped	>0	material 2	material 1	holes
n-doped	n-doped	<0	material 2	material 1	electrons
p-doped	p-doped	<0	material 1	material 2	holes
p-doped	n-doped	>0	material 1	material 2	electrons
n-doped	p-doped	>0	material 2	material 1	holes
p-doped	n-doped	<0	material 1	material 2	holes
n-doped	p-doped	<0	material 2	material 1	electrons

Heterojunctions are characterized by a discontinuous conduction (and/or valence) band at the interface. In the Semiconductor Module, one can choose between two models to define the heterojunction. The continuous quasi-Fermi level model and the thermionic emission model.

The continuous quasi-Fermi level model defines the current continuity at the interface by setting the quasi-Fermi level to be continuous on each side of the junction.

The thermionic emission model defines the current continuity through a thermionic current density generated at the potential barrier.

Model Definition

This model simulates the behavior of an heterojunction under reverse and forward bias for three different configurations: isotype n-n, anisotype p-n, and anisotype n-p. The modeled junction is composed of two different materials, GaAs and $Al_{0.25}Ga_{0.75}As$, respectively located on the left and right side of the junction. As displayed on Figure 1, the junction has a length of 10 µm and a net doping concentration of: $1{\cdot}10^{15}$ cm^{-3} for the GaAs and $1{\cdot}10^{16}$ cm^{-3} for the $Al_{0.25}Ga_{0.75}As$. A Shockley-Read-Hall recombination feature is also added to the model for the sake of comparison with the reference model reported in Ref. 1.

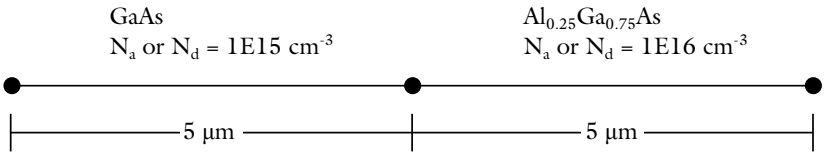


Figure 1: Schematic of the geometry. The GaAs and $Al_{0.25}Ga_{0.75}As$ are, respectively, located on the left and on the right side of the junction (center). Depending on the configuration (n-n, p-n or n-p), the doping might be of donor type (N_d) or acceptor type (N_a) for both materials. Note that the impurity concentration stays the same for each material for all three configurations, that is, $1{\cdot}10^{15}$ cm^{-3} for GaAs and $1{\cdot}10^{16}$ cm^{-3} for $Al_{0.25}Ga_{0.75}As$.

The equation system for heterojunctions is highly nonlinear and numerically challenging. In this tutorial we show a few different ways to achieve better convergence. See the section Modeling Instructions for details.

Results and Discussion

Figure 2 shows a comparison between the continuous quasi-Fermi level model and the thermionic emission model for the n-n isotype junction under forward and reverse bias. The figure also compares our results with the ones obtained in Ref. 1. Figure 2 shows that

the thermionic current model is in good agreement with the reference. The continuous quasi-Fermi level model is a little larger than the reference model in the reverse case.

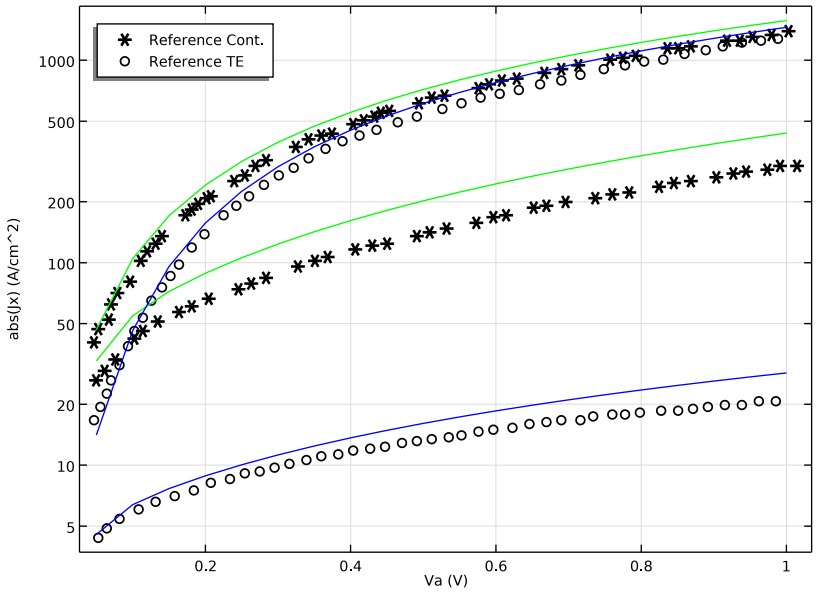


Figure 2: Comparison of the current densities obtained using the continuous quasi-Fermi level model (green) and the thermionic emission model (blue) with the results obtained in Ref. 1 *for the n-n isotype junction under forward and reverse bias.*

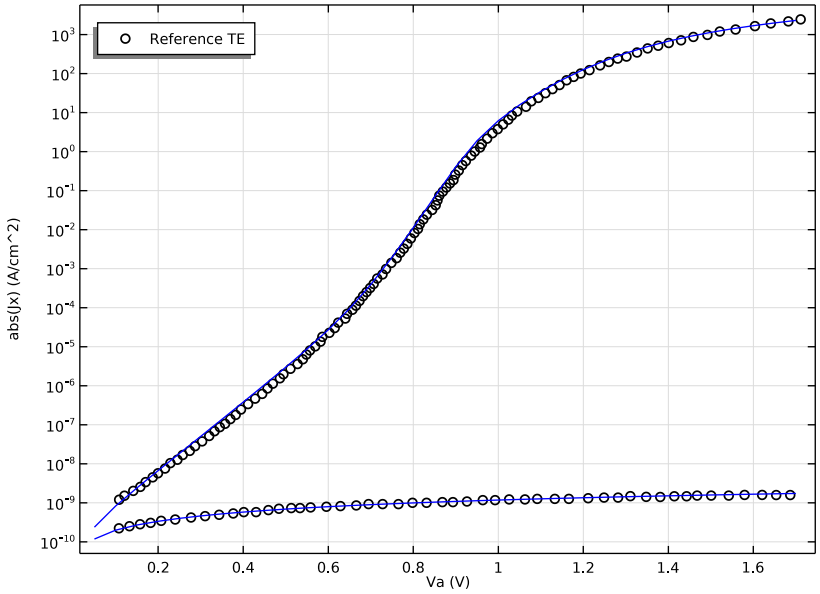


Figure 3: Comparison of the current densities obtained using the thermionic emission model (blue) with the results obtained in Ref. 1 for the p-n anisotype junction under forward and reverse bias.

Figure 3 shows a comparison between the thermionic emission current density obtained with the model and the reference under forward and reverse bias for the p-n junction. A very good agreement is observed between the two models. Figure 4 shows the same kind of agreement for the n-p junction.

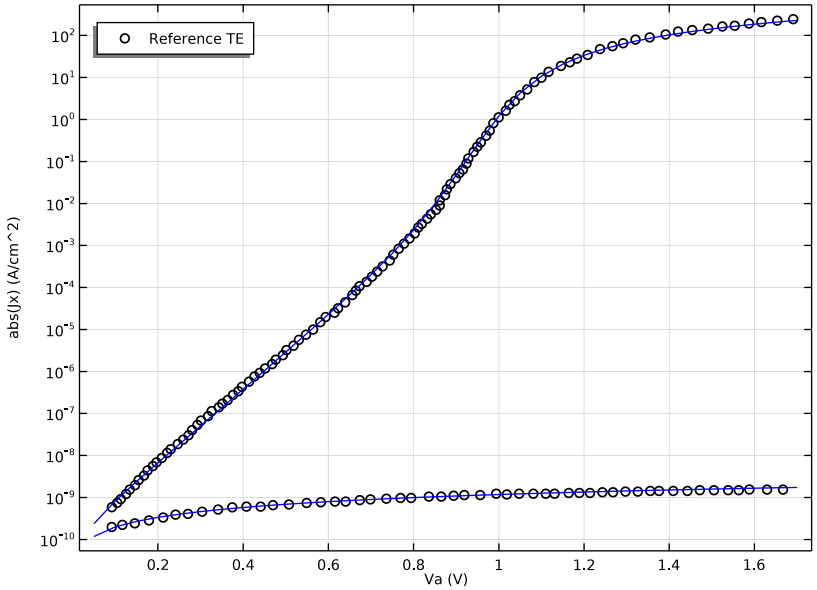


Figure 4: Comparison of the current densities obtained using the thermionic emission model (blue) with the results obtained in Ref. 1 *for the n-p anisotype junction under forward and reverse bias*

The thermionic current at the junction can come from the electrons in the conduction band or the holes in the valence band. Depending on the configuration, the current is primarily due to one of the two carriers. This is the result of the existence (or nonexistence) of a potential barrier generated by the bending of one of the bands (conduction or valence). Figure 5 displays the energy diagram for the n-n junction under forward bias at Va = 0.05 V. The figure shows that, for this configuration, it is the conduction band that forms the barrier (spike) over which electrons can transit. The current for the isotype heterojunction is then mainly due to electrons. A similar observation can be made on Figure 6 and Figure 7. The latter figures show that the current is mainly produced by electrons for the p-n heterojunction and by holes for the n-p heterojunction. Note that for the n-p junction, the forward bias appears when the applied potential is negative.

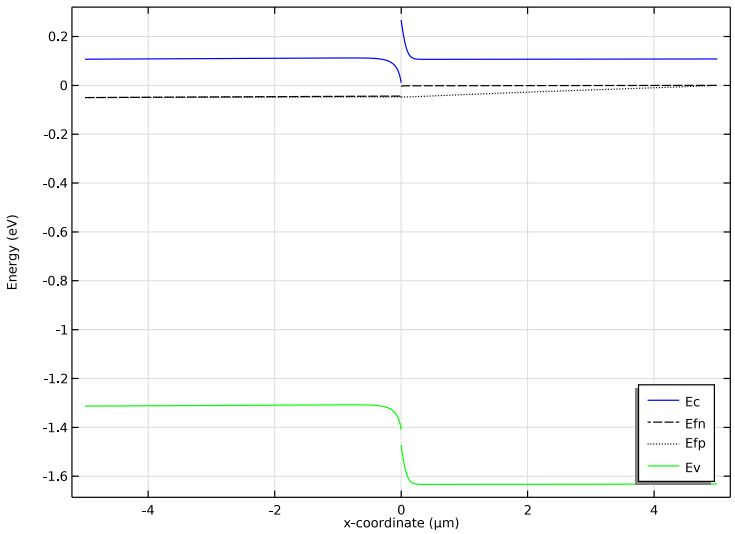


Figure 5: Energy diagram for the n-n heterojunction using the thermionic emission model.

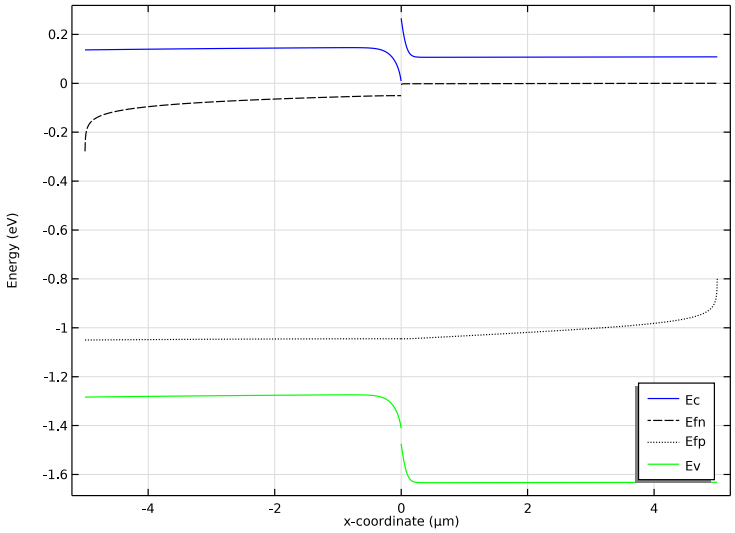


Figure 6: Energy diagram for the p-n heterojunction using the thermionic emission model.

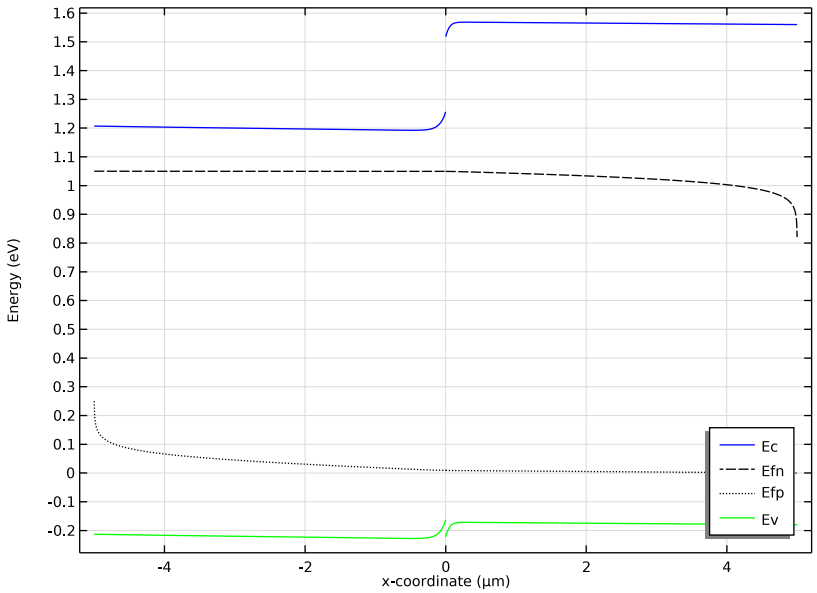


Figure 7: Energy diagram for the n-p heterojunction using the thermionic emission model.

Reference

1. K. Horio and H. Yanai, "Numerical Modeling of Heterojunctions Including the Thermionic Emission Mechanism at the Heterojunction Interface," *IEEE Transaction on Electron Devices*, vol. 37, no. 4, pp. 1093–1098, 1990.

Application Library path: `Semiconductor_Module/Verification_Examples/heterojunction_1d`

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>Semiconductor (semi)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Click **Done**.

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 In the table, enter the following settings:

Name	Expression	Value	Description
sign	1	1	Sign of applied voltage
Va	0[V]	0 V	Voltage
ramp	1	1	Continuation parameter
L	5[um]	5E-6 m	Length
T0	300[K]	300 K	Temperature

Create the geometry, the junction is located at $x = 0$.

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 In the table, enter the following settings:

Coordinates (m)
-L
0

Interval 2 (i2)

1 Right-click **Interval 1 (i1)** and choose **Duplicate**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
L

Choose um as the default length units.

4 In the **Model Builder** window, click **Geometry 1**.

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

6 From the **Length unit** list, choose **µm**.

Load the material properties for GaAs and Al_0.25Ga_0.75As. The properties will be respectively assigned to the left and right side of the junction.

DEFINITIONS

GaAs

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, type `GaAs` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `heterojunction_1d_gaas.txt`.

Al_0.25Ga_0.75As

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, type `Al_0.25Ga_0.75As` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 2 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `heterojunction_1d_algaas.txt`.

Set the reference temperature to T0.

7 Click the **Show More Options** button in the **Model Builder** toolbar.

8 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.

9 Click **OK**.

SEMICONDUCTOR (SEMI)

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

2 In the **Settings** window for **Semiconductor**, click to expand the **Reference Temperature** section.

3 In the T_0 text field, type `T0`.

Set the lattice temperature to T0.

Semiconductor Material Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)** click **Semiconductor Material Model 1**.

2 In the **Settings** window for **Semiconductor Material Model**, locate the **Model Input** section.

3 In the T text field, type `T0`.

Add a Shockley-Read-Hall recombination feature to all domains.

Trap-Assisted Recombination 1

1 In the **Physics** toolbar, click **Domains** and choose **Trap-Assisted Recombination**.

2 In the **Settings** window for **Trap-Assisted Recombination**, locate the **Domain Selection** section.

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

The voltage is applied on the left side of the junction (GaAs). The sign variable is used by the study steps to sweep the applied voltages from reverse to forward.

Metal Contact 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Metal Contact**, locate the **Terminal** section.

4 In the V_0 text field, type `sign*Va`.

The right side of the junction (Al_0.25Ga_0.75As) is grounded.

Metal Contact 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 3 only.

The doping concentration stays constant for each material and for any modeled configuration. Accordingly, the variable Doping, defined in the domain variables GaAs and Al_0.25Ga_0.75As, is used for all the added doping feature. Depending on the chosen configuration, the doping type changes on each side of the junction. For this reason, n- and p-type features are created for each side of the junction. To define the desired configurations, doping features are enabled/disabled in their respective study steps.

Donor doping (left)

1 In the **Physics** toolbar, click — **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Donor doping (left)` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **Impurity** section. From the **Impurity type** list, choose **Donor doping (n-type)**.

5 In the N_{D0} text field, type `Doping`.

Donor doping (right)

1 In the **Physics** toolbar, click — **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Donor doping (right)` in the **Label** text field.

3 Select Domain 2 only.

4 Locate the **Impurity** section. From the **Impurity type** list, choose **Donor doping (n-type)**.

5 In the N_{D0} text field, type `Doping`.

Acceptor doping (left)

1 In the **Physics** toolbar, click — **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Acceptor doping (left)` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **Impurity** section. In the N_{A0} text field, type `Doping`.

Acceptor doping (right)

1 In the **Physics** toolbar, click — **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Acceptor doping (right)` in the **Label** text field.

3 Select Domain 2 only.

4 Locate the **Impurity** section. In the N_{A0} text field, type `Doping`.

In order to observe the effect of the different heterojunction models, create an additional feature and change the default continuous quasi-Fermi model for the thermionic emission model.

Continuity/Heterojunction 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Continuity/Heterojunction**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Continuity/Heterojunction**, locate the **Heterojunction** section.

4 From the **Continuity model** list, choose **Thermionic emission**.

Add a material to the model and enter the material properties defined in the domain variables GaAs and Al_0.25Ga_0.75As. This discontinuous material is used to define both sides of the junction.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electron mobility	mun	`mun0`	m²/(V·s)	Semiconductor material
Hole mobility	mup	`mup0`	m²/(V·s)	Semiconductor material
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	`er`	1	Basic
Band gap	Eg0	`Eg`	V	Semiconductor material
Electron affinity	chi0	`chi`	V	Semiconductor material

Property	Variable	Value	Unit	Property group
Effective density of states, conduction band	Nc	Nc0	1/m³	Semiconductor material
Effective density of states, valence band	Nv	Nv0	1/m³	Semiconductor material
Electron lifetime, SRH	taun	taun0	s	Shockley-Read-Hall recombination
Hole lifetime, SRH	taup	taup0	s	Shockley-Read-Hall recombination

Create a fine mesh using the distribution tool.

MESH 1

Edge 1

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

Distribution 1

1. Right-click **Edge 1** and choose **Distribution**.
2. In the **Settings** window for **Distribution**, locate the **Distribution** section.
3. From the **Distribution type** list, choose **Predefined**.
4. In the **Number of elements** text field, type 500.
5. In the **Element ratio** text field, type 10.
6. Select the **Symmetric distribution** check box.
7. Click **Build All**.

Create a study to solve the n-n heterojunction with the continuous quasi-Fermi levels model. In order to reduce the number of figure in the model, clear the generate default plots check box.

N-N : CONTINUOUS QUASI-FERMI LEVELS

1. In the **Model Builder** window, click **Study 1**.
2. In the **Settings** window for **Study**, type `n-n : Continuous Quasi-Fermi Levels` in the **Label** text field.
3. Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Select the doping features and heterojunction model needed for this specific configuration. Note that the Voltage continuation sweep proceeds from reverse to forward bias (the sign variable is starting with -1).

Step 1: Stationary

1 In the **Model Builder** window, under **n-n : Continuous Quasi-Fermi Levels** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (left)**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (right)**.

7 Click **Disable**.

8 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Continuity/Heterojunction 2**.

9 Click **Disable**.

10 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

11 From the **Sweep type** list, choose **All combinations**.

12 Click **Add**.

13 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
sign (Sign of applied voltage)	-1 1	

14 Click **Add**.

15 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Va (Voltage)	range(0.05,0.05,1)	V

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

16 From the **Reuse solution from previous step** list, choose **Auto**.

The equation system for heterojunctions is highly nonlinear and numerically challenging. In this tutorial we show a few different ways to achieve better convergence. First, we can manually scale the solution variables to their expected magnitudes.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 1**.

3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.

4 From the **Method** list, choose **None**.

5 In the **Model Builder** window, expand the **n-n : Continuous Quasi-Fermi Levels> Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** node, then click **Electron solution variable (comp1.Ne)**.

6 In the **Settings** window for **Field**, locate the **Scaling** section.

7 From the **Method** list, choose **Manual**.

8 In the **Scale** text field, type `1.0e22`.

9 In the **Model Builder** window, click **Hole solution variable (comp1.Ph)**.

10 In the **Settings** window for **Field**, locate the **Scaling** section.

11 From the **Method** list, choose **Manual**.

12 In the **Scale** text field, type `1.0e4`.

Change the default relative tolerance to 1E-10. This gives a better resolution to the current density.

13 In the **Model Builder** window, click **Stationary Solver 1**.

14 In the **Settings** window for **Stationary Solver**, locate the **General** section.

15 In the **Relative tolerance** text field, type `1E-10`.

16 Click **Compute**.

Create another study for the n-n heterojunction using the thermionic emission model.

ADD STUDY

1 In the **Study** 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 **General Studies>Stationary**.

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

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

N-N : THERMIONIC EMISSION

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

2 In the **Settings** window for **Study**, type `n-n : Thermionic Emission` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Select the doping features and heterojunction model needed for this specific configuration. Start with the initial condition given by the solution from the previous study - this is another way to achieve better convergence. Note that the Voltage sweep proceeds from reverse to forward bias (the sign variable is starting with -1).

Step 1: Stationary

1 In the **Model Builder** window, under **n-n : Thermionic Emission** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (left)**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (right)**.

7 Click **Disable**.

8 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

9 From the **Method** list, choose **Solution**.

10 From the **Study** list, choose **n-n : Continuous Quasi-Fermi Levels, Stationary**.

11 From the **Parameter value (Va (V),sign)** list, choose **1: Va=0.05 V, sign=-1**.

12 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

13 From the **Sweep type** list, choose **All combinations**.

14 Click **Add**.

15 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
sign (Sign of applied voltage)	-1 1	

16 Click **Add**.

17 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Va (Voltage)	`range(0.05,0.05,1)`	V

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

18 From the **Reuse solution from previous step** list, choose **Auto**.

Change the default relative tolerance to 1E-10. This will give a better resolution on the current density.

Solution 2 (sol2)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Stationary Solver 1**.

3 In the **Settings** window for **Stationary Solver**, locate the **General** section.

4 In the **Relative tolerance** text field, type `1E-10`.

5 Click **Compute**.

Load the reference's results in two tables.

RESULTS

n-n : Cont.

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

2 Right-click **Results>Tables** and choose **Table**.

3 In the **Settings** window for **Table**, type `n-n : Cont.` in the **Label** text field.

4 Locate the **Data** section. Click **Import**.

5 Browse to the model's Application Libraries folder and double-click the file `heterojunction_1d_case1_cont.txt`.

n-n : TE

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `n-n : TE` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `heterojunction_1d_case1_te.txt`.

Plot the J-V curve comparison.

n-n : Jx Comparison

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

2 In the **Settings** window for **1D Plot Group**, type `n-n : Jx Comparison` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

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

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Va (V)`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `abs(Jx) (A/cm^2)`.

9 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Table Graph 1

1 Right-click **n-n : Jx Comparison** and choose **Table Graph**.

2 In the **Settings** window for **Table Graph**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **None**.

4 From the **Color** list, choose **Black**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Asterisk**.

6 From the **Positioning** list, choose **In data points**.

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

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

9 In the table, enter the following settings:

Legends
Reference Cont.

10 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

Table Graph 2

1 Right-click **Table Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Table** list, choose **n-n : TE**.

4 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

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

Legends
Reference TE

Point Graph 1

1 In the **Model Builder** window, right-click **n-n : Jx Comparison** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **n-n : Continuous Quasi-Fermi Levels/Solution 1 (sol1)**.

4 Select Boundary 2 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `abs(semi.JX)`.

6 In the **Unit** field, type `A/cm^2`.

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

Point Graph 2

1 Right-click **Point Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Point Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **n-n : Thermionic Emission/Solution 2 (sol2)**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

n-n : Jx Comparison

1 In the **Model Builder** window, click **n-n : Jx Comparison**.

2 In the **n-n : Jx Comparison** toolbar, click **Plot**.

Create another study for the p-n configuration with the thermionic emission mode. In this study, we show yet another way to achieve better convergence: use the **Semiconductor Equilibrium** study step to obtain a good initial condition.

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>Semiconductor Equilibrium**.

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

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

STUDY 3

Step 1: Semiconductor Equilibrium

1 In the **Settings** window for **Semiconductor Equilibrium**, locate the **Physics and Variables Selection** section.

2 Select the **Modify model configuration for study step** check box.

3 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Donor doping (left)**.

4 Click **Disable**.

5 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (right)**.

6 Click **Disable**.

In order to reduce the number of figure in the model, clear the generate default plots check box.

7 In the **Model Builder** window, click **Study 3**.

8 In the **Settings** window for **Study**, type `p-n : Thermionic Emission` in the **Label** text field.

9 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Add a second stationary step to sweep the voltage from reverse to forward bias. This step will automatically use the solution of the previous step as the initial condition. Right click p-n : thermionic emission then select Study Steps and Stationary.

Stationary

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Donor doping (left)**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (right)**.

7 Click **Disable**.

8 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

9 From the **Sweep type** list, choose **All combinations**.

10 Click **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
sign (Sign of applied voltage)	-1 1	

12 Click **Add**.

13 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Va (Voltage)	range(0.05,0.05,1.7)	V

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

Change the default relative tolerance to 1E-10. This gives a better resolution to the current density.

Solution 3 (sol3)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node, then click **Stationary Solver 2**.

3 In the **Settings** window for **Stationary Solver**, locate the **General** section.

4 In the **Relative tolerance** text field, type 1E-10.

5 Click **Compute**.

Load the references results in a table.

RESULTS

p-n : TE

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type p-n : TE in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file heterojunction_1d_case2_te.txt.

p-n : Jx Comparison

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

2 In the **Settings** window for **1D Plot Group**, type p-n : Jx Comparison in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Va (V)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `abs(Jx) (A/cm^2)`.

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

Table Graph 1

1 Right-click **p-n : Jx Comparison** and choose **Table Graph**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Table** list, choose **p-n : TE**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

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

6 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

7 From the **Positioning** list, choose **In data points**.

8 Locate the **Legends** section. Select the **Show legends** check box.

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

10 In the table, enter the following settings:

Legends
Reference TE

11 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

Point Graph 1

1 In the **Model Builder** window, right-click **p-n : Jx Comparison** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **p-n : Thermionic Emission/Solution 3 (sol3)**.

4 Select Boundary 2 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `abs(semi.JX)`.

6 In the **Unit** field, type `A/cm^2`.

7 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

p-n : Jx Comparison

1 In the **Model Builder** window, click **p-n : Jx Comparison**.

2 In the **p-n : Jx Comparison** toolbar, click **Plot**.

Another way to achieve better convergence is to ramp up nonlinear contributions to the equation system from small values. The Semiconductor physics interface provides a convenient mechanism to ramp up several quantities simultaneously by using a common continuation parameter as a multiplication factor. Here we will ramp up the doping and thermionic current. Enter the continuation parameter, `ramp`, in the interface continuation parameter field.

SEMICONDUCTOR (SEMI)

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

2 In the **Settings** window for **Semiconductor**, click to expand the **Continuation Settings** section.

3 In the C_p text field, type `ramp`.

4 From the **Doping and trap density continuation parameter** list, choose **Use interface continuation parameter**.

Select the interface continuation parameter to ramp the thermionic current. (The doping features are by default ramped with the doping and trap density continuation parameter, which is in turn by default set to be the interface continuation parameter.)

Continuity/Heterojunction 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)** click **Continuity/Heterojunction 2**.

2 In the **Settings** window for **Continuity/Heterojunction**, click to expand the **Continuation Settings** section.

3 From the **Continuation type** list, choose **Use interface continuation parameter**.

Create a study to solve the n-p heterojunction with the thermionic emission model. In order to reduce the number of figure in the model, clear the generate default plots check box.

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 **General Studies>Stationary**.

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

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

N-P : THERMIONIC EMISSION

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

2 In the **Settings** window for **Study**, type `n-p : Thermionic Emission` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Add the ramping step.

Step 1: Stationary

1 In the **Model Builder** window, under **n-p : Thermionic Emission** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Donor doping (right)**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (left)**.

7 Click **Disable**.

8 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

9 Click **Add**.

10 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
ramp (Continuation parameter)	`1e-8 1e-6 1e-4 1e-2 0.1 0.25 0.5 0.75 1`	

Add the second stationary step to sweep the voltage from reverse to forward bias. In this case, the sign variable starts at 1. Right click n-p : thermionic emission then select Study Steps and Stationary.

Stationary 2

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Donor doping (right)**.

5 Click **Disable**.

6 In the **Physics and variables selection** tree, select **Component 1 (comp1)> Semiconductor (semi)>Acceptor doping (left)**.

7 Click **Disable**.

8 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

9 From the **Sweep type** list, choose **All combinations**.

10 Click **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
sign (Sign of applied voltage)	1 -1	

12 Click **Add**.

13 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Va (Voltage)	range(0.05,0.05,1.7)	V

For assistance in entering ranges of different kinds in the **Parameter value list** column, click the **Range** button to launch the **Range** dialog.

14 From the **Reuse solution from previous step** list, choose **Auto**.

Change the default relative tolerance to 1E-10. This gives a better resolution to the current density.

Solution 5 (sol5)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 5 (sol5)** node, then click **Stationary Solver 2**.

3 In the **Settings** window for **Stationary Solver**, locate the **General** section.

4 In the **Relative tolerance** text field, type 1E-10.

5 Click **Compute**.

Load the references results in a table.

RESULTS

n-p : TE

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type n-p : TE in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `heterojunction_1d_case3_te.txt`.

n-p : Jx Comparison

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

2 In the **Settings** window for **1D Plot Group**, type `n-p : Jx Comparison` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Va (V)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `abs(Jx) (A/cm^2)`.

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

Table Graph 1

1 Right-click **n-p : Jx Comparison** and choose **Table Graph**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Table** list, choose **n-p : TE**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

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

6 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

7 From the **Positioning** list, choose **In data points**.

8 Locate the **Legends** section. Select the **Show legends** check box.

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

10 In the table, enter the following settings:

Legends
Reference TE

11 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

Point Graph 1

1 In the **Model Builder** window, right-click **n-p : Jx Comparison** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **n-p : Thermionic Emission/Solution 5 (sol5)**.

4 Select Boundary 2 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `abs(semi.JX)`.

6 In the **Unit** field, type `A/cm^2`.

7 Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

n-p : Jx Comparison

1 In the **Model Builder** window, click **n-p : Jx Comparison**.

2 In the **n-p : Jx Comparison** toolbar, click **Plot**.

Generate the thermionic emission model energy diagram figures for each configuration.

n-n : Energy Diagram

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `n-n : Energy Diagram` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **n-n : Thermionic Emission/Solution 2 (sol2)**.

4 From the **Parameter selection (sign)** list, choose **Last**.

5 From the **Parameter selection (Va)** list, choose **First**.

6 Locate the **Title** section. From the **Title type** list, choose **None**.

7 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Line Graph 1

1 Right-click **n-n : Energy Diagram** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Fermi levels and band edges> Energies>semi.Ec_e - Conduction band energy level - J**.

5 Locate the **y-Axis Data** section. From the **Unit** list, choose **eV**.

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

7 In the **Expression** text field, type `x`.

8 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Blue**.

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

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

11 In the table, enter the following settings:

Legends
Ec

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Fermi levels and band edges>Energies>semi.Efn_e - Electron quasi-Fermi energy level - J**.

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

4 From the **Color** list, choose **Black**.

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

Legends
Efn

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Fermi levels and band edges>Energies>semi.Efp_e - Hole quasi-Fermi energy level - J**.

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

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

Legends
Efp

Line Graph 4

1 Right-click **Line Graph 3** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor>Fermi levels and band edges>Energies>semi.Ev_e - Valence band energy level - J**.

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

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

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

Legends
Ev

n-n : Energy Diagram

1 In the **Model Builder** window, click **n-n : Energy Diagram**.

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

3 Select the **y-axis label** check box.

4 In the associated text field, type `Energy (eV)`.

5 Select the **x-axis label** check box.

6 In the **n-n : Energy Diagram** toolbar, click **Plot**.

p-n : Energy Diagram

1 Right-click **n-n : Energy Diagram** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `p-n : Energy Diagram` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **p-n : Thermionic Emission/ Solution 3 (sol3)**.

4 From the **Parameter selection (Va)** list, choose **From list**.

5 In the **Parameter values (Va (V))** list, select **1.05**.

6 In the **p-n : Energy Diagram** toolbar, click **Plot**.

n-p : Energy Diagram

1 Right-click **p-n : Energy Diagram** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `n-p : Energy Diagram` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **n-p : Thermionic Emission/ Solution 5 (sol5)**.

4 In the **n-p : Energy Diagram** toolbar, click **Plot**.