Bands and electronic devices

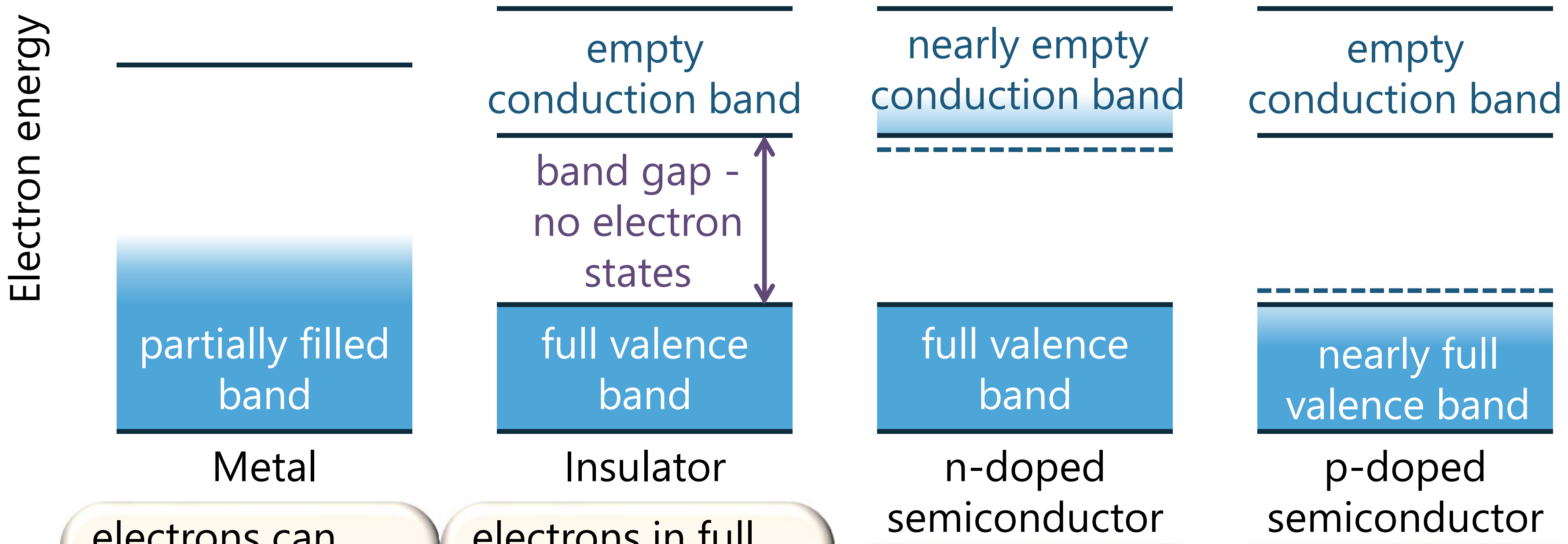
Electrons and holes in bands

Modern physics for engineers

David Miller

Metals, semiconductors and insulators - revision

Metals, insulators and semiconductors - revision



Metal: electrons can move to new states hence conducts electricity

Insulator: electrons in full bands cannot move to new states does not conduct

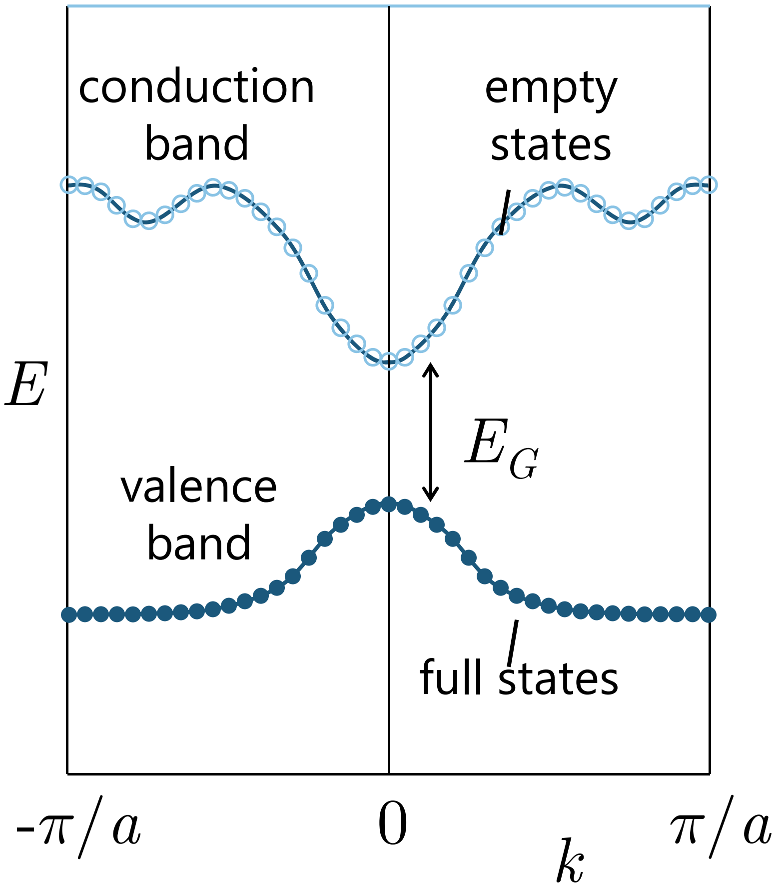
n-doped semiconductor: added free electrons in conduction band conduct

p-doped semiconductor: missing free electrons in valence band allow conduction

Semiconductors and insulators - revision

Semiconductors and insulators
- have an (almost) completely full band
  - the valence band

separated by a “bandgap” energy E_G
- from an (almost) completely empty band
  - the conduction band



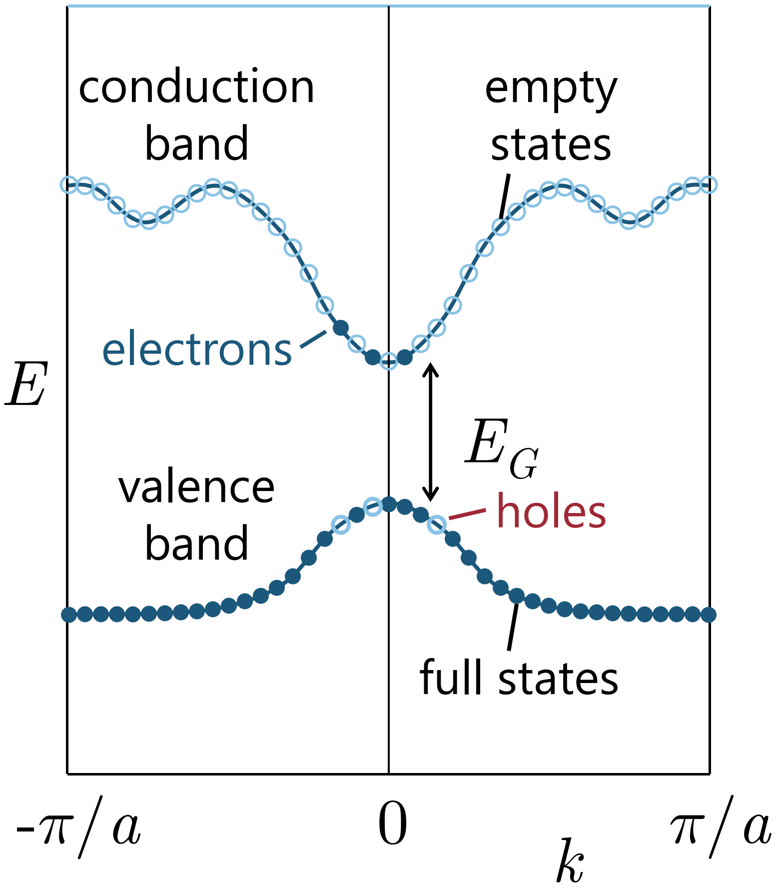
Semiconductors

Now we look at behaviors of electrons (and holes) in bands

- for example, for "transport"
  - the movement of charge for conducting electrical current

and some of the consequences of thermal distributions of them

- for devices



Transport in semiconductors

Transport of electrons

For an electron in some parabolic minimum (or maximum)

we can rewrite $E = \dfrac{\hbar^2 k^2}{2m_{eff}}$

in terms of "crystal" momentum $p_C = \hbar k$ as

$$E = \frac{p_C^2}{2m_{eff}}$$

Then $\dfrac{dE}{dp_C} = \dfrac{p_C}{m_{eff}}$

Transport of electrons

With $\frac{dE}{dp_C} = \frac{p_C}{m_{eff}}$

then thinking of a velocity v_g such that $p_C = m_{eff} v_g$

we have for this velocity at which we expect the particle is moving

$$v_g = \frac{dE}{dp_C}$$

This particular velocity v_g

is called the "group velocity"

Transport of electrons

Suppose we apply an "external" force F to the particle

such as from an electric field

Then the work done in applying the force through a distance dx is

$$dE = Fdx$$

The distance dx equals

the group velocity v_g times

the time, dt, for which the force is applied

so we have

$$dE = Fdx = Fv_g dt$$

Transport of electrons

Hence $$F = \frac{1}{v_g}\frac{dE}{dt} = \frac{1}{v_g}\frac{dE}{dp_C}\frac{dp_C}{dt}$$

or, using $v_g = dE / dp_C$ $$F = \frac{dp_C}{dt} \equiv \frac{d\left(\hbar k\right)}{dt}$$

So applying a force to an electron leads to

"force is equal to rate of change of (crystal) momentum"

This crystal momentum behaves like the momentum of an effective particle of mass m_{eff}

In this picture, applying a force

moves the electron steadily through the Brillouin zone

Ballistic transport of electrons

This kind of transport

where the electron is continuously accelerated by the applied field

is called "ballistic transport"

It does exist in materials like semiconductors

and is part of device analysis

but it only applies for

very short distances

or very short time-scales

Drift transport of electrons

More typically, the electron is accelerated ("ballistically")

for some average or effective "scattering" time t_s

then the electron is scattered by some collision

with other electrons

or crystal vibrations ("phonons")

or crystal impurities or defects

Drift transport of electrons

In the “drift” model

- the scattering events are random
  - but so strong that, on the average
    - the electron velocity is randomized by them

So the average electron velocity after the collision is zero

- because it could just as well be going in any direction

Drift transport of electrons

Specifically, for an electric field of magnitude $\mathcal{E}$

the magnitude of the force on an electron is $F = e\mathcal{E}$

If we accelerate (from zero velocity)

using such a force for a time t_s

the peak momentum just before scattering will be

$$p_C = \frac{dp_C}{dt} t_s = F t_s = e\mathcal{E} t_s = m_{eff} v_{peak}$$

The average velocity is half this peak value

$$v_{av} = \frac{e t_s}{2 m_{eff}} \mathcal{E}$$

Drift transport of electrons

So, in drift transport, the average velocity of the electron

is proportional to the applied electric field $\mathcal{E}$

and the average velocity is called the "drift velocity"

Such transport is often written as

$$v_{av} = \mu_e \mathcal{E}$$

where

$$\mu_e = \frac{e t_s}{2 m_{eff}}$$

is called the "mobility"

This gives rise to behavior like Ohm's law

with current proportional to the voltage

Hole transport in semiconductors

Holes

- At a maximum at the top of the valence band
  - the electron effective mass is negative
    - Electrons would go backwards if pushed
- Though counter-intuitive, this is correct
  - The group velocity can be “backwards”
    - e.g., in the “wrong” direction when pushed by an electric field

Holes

- For a set of electrons in states near such a negative effective mass maximum
  - but with a state (or wave packet of states) not occupied
    - that “empty” state or wave packet will move along
      - in the same “backwards” direction as the electrons do

Holes

This "absence of an electron" wavepacket

- is moving in the wrong direction for electron electrical current
  - but in the correct direction for the electrical current of a positively charged particle
    - in this electric field

Holes

- So we can pretend this “absence-of-an-electron”
  - in a “negative electron effective mass” maximum
- behaves like a positive charge with a positive mass
  - going in the “correct” direction

Holes

This "cancellation of two minus signs"

- exchanging an absence of negative charge with a negative mass
  - for an effective positive charge with a positive mass (of the same magnitude)
    - lets us define the idea of a "hole" with positive charge and mass

Hole transport otherwise obeys the same behaviors as electron transport

Hole energies

Holes

- We can think of the hole kinetic energy as being positive
  - if we look at the band diagram upside down
    - just as we can similarly think of positive hole energies in the hole Fermi-Dirac distribution
      - when looking at the band diagram upside down

Holes

Generally, for holes

we "stand on our heads" in looking at energy diagrams

just as we would for thinking about

the energy of bubbles in a liquid

which is a higher energy for a bubble "deeper" in the liquid

Bands and electronic devices

Semiconductor doping and diodes

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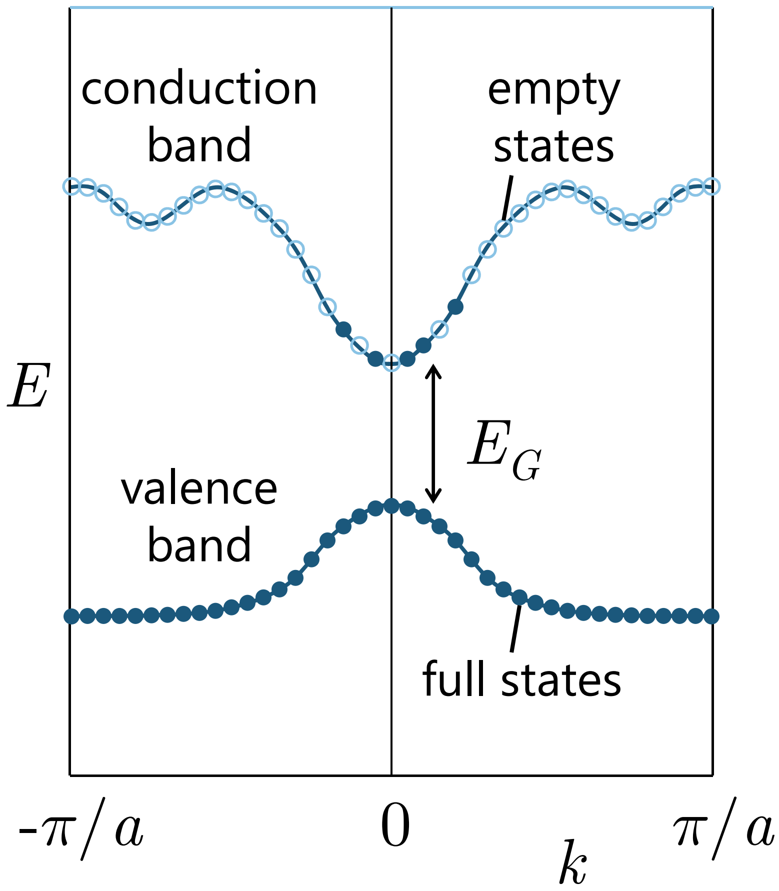
Doping in semiconductors

Doping semiconductors

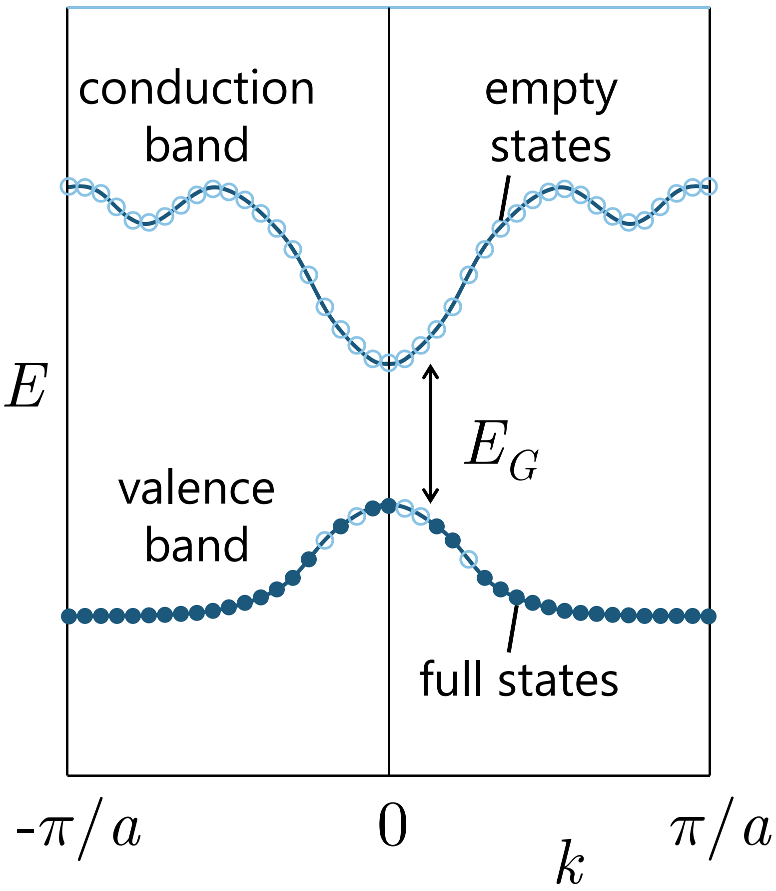
- Substituting a few atoms with more electrons
  - e.g., a Group V element like phosphorus in a Group IV semiconductor like silicon
    - known as n-type doping
  - makes the material conduct more
    - using these additional electrons



Doping semiconductors

Substituting a few atoms with fewer electrons

- e.g., a Group III element like boron in a Group IV semiconductor like silicon
  - known as p-type doping
- makes the material conduct more
  - using these additional "holes"



Semiconductor diodes

Semiconductor diode

Conceptually, to make a diode

we join

a piece of p-doped semiconductor

with ionized acceptors

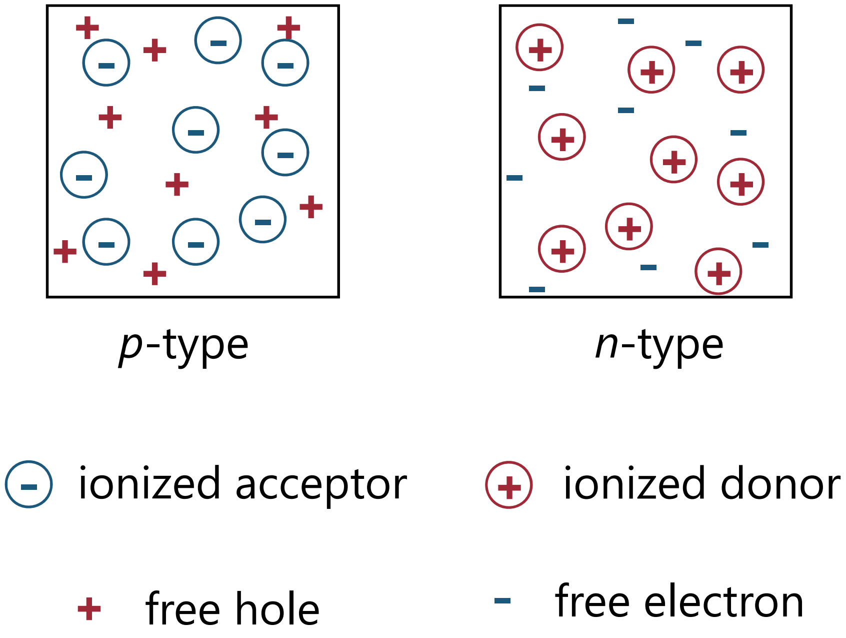
and free holes

to

a piece of n-doped semiconductor

with ionized donors

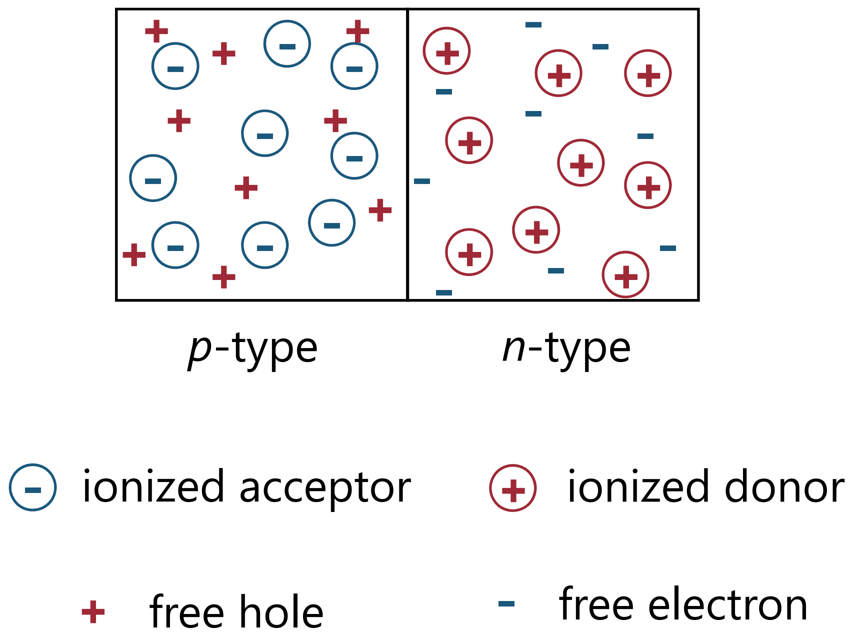
and free electrons



Semiconductor diode

Conceptually, to make a diode

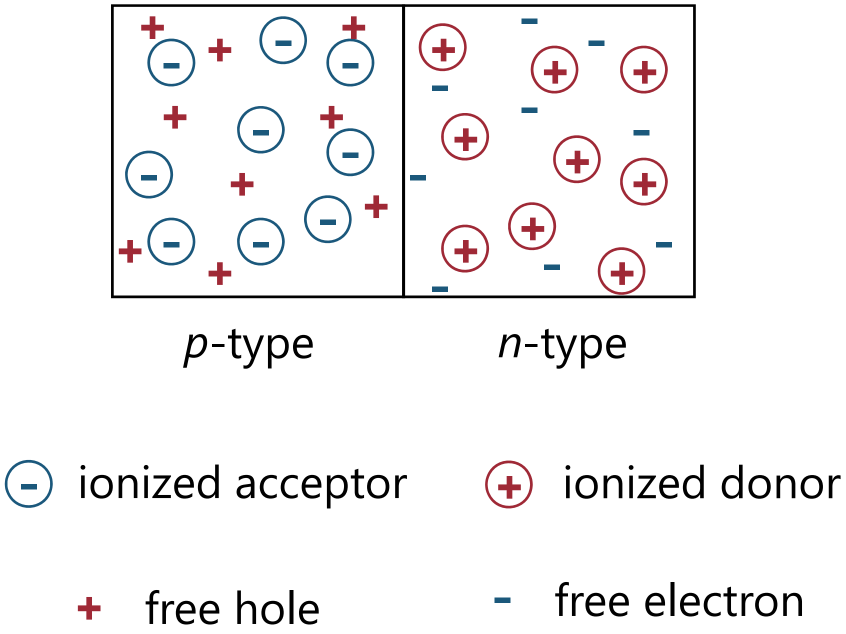
- we join
  - a piece of p-doped semiconductor
    - with ionized acceptors
      - and free holes
- to
  - a piece of n-doped semiconductor
    - with ionized donors
      - and free electrons



Semiconductor diode

Once they are joined

- free electrons move
  - from the side with more
    - to the side with less
      - by "diffusion"
- and similarly for free holes



Semiconductor diode

Diffusion is the process where

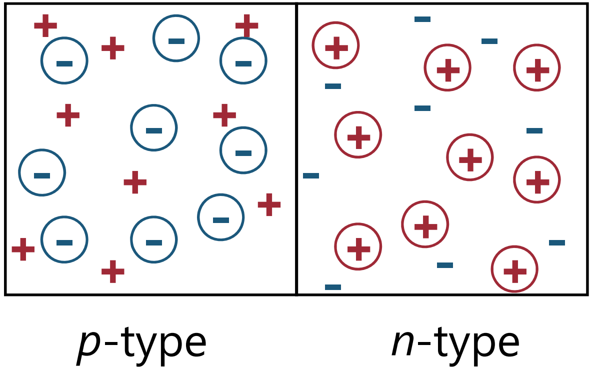
as a result of a "random walk"

there is net flow

from regions of high concentration

to regions of low concentration

like smoke diffusing through a room



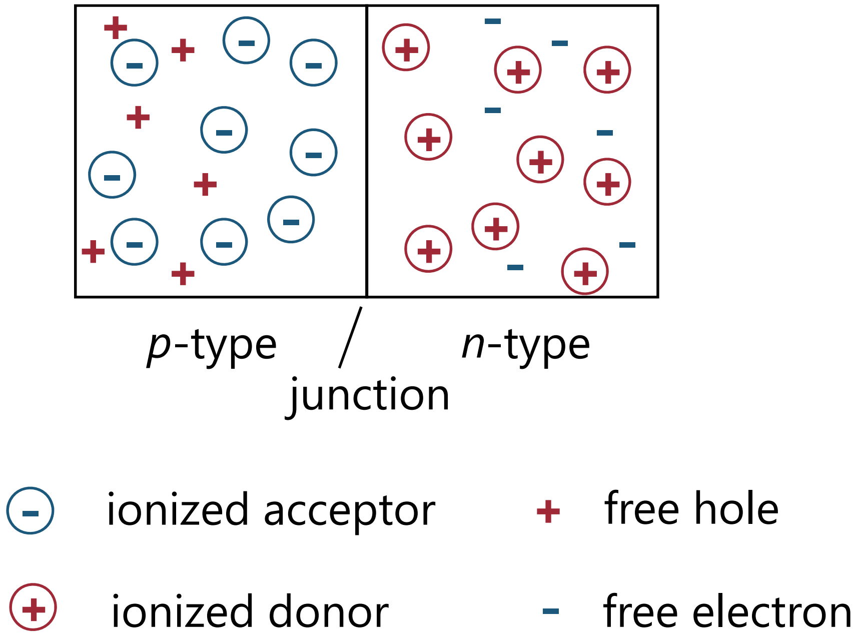
⊖ ionized acceptor ⊕ ionized donor

+ free hole - free electron

Semiconductor diode

Free electrons and free holes

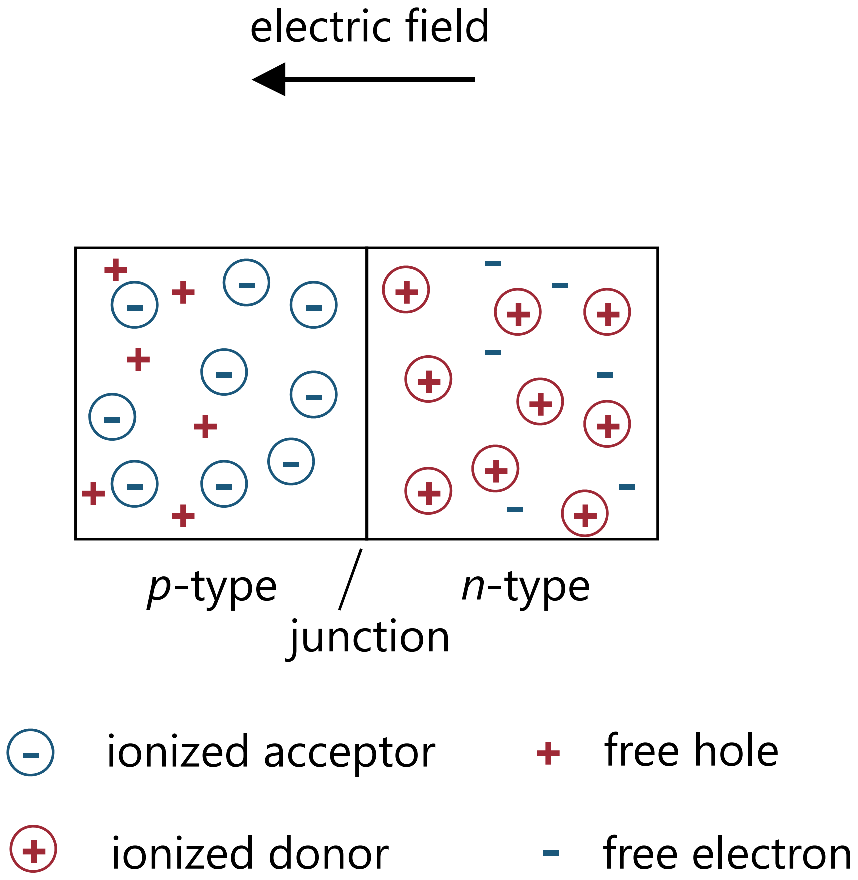
- arriving in the same region as a result of diffusion
- effectively "annihilate" one another by recombination



Semiconductor diode

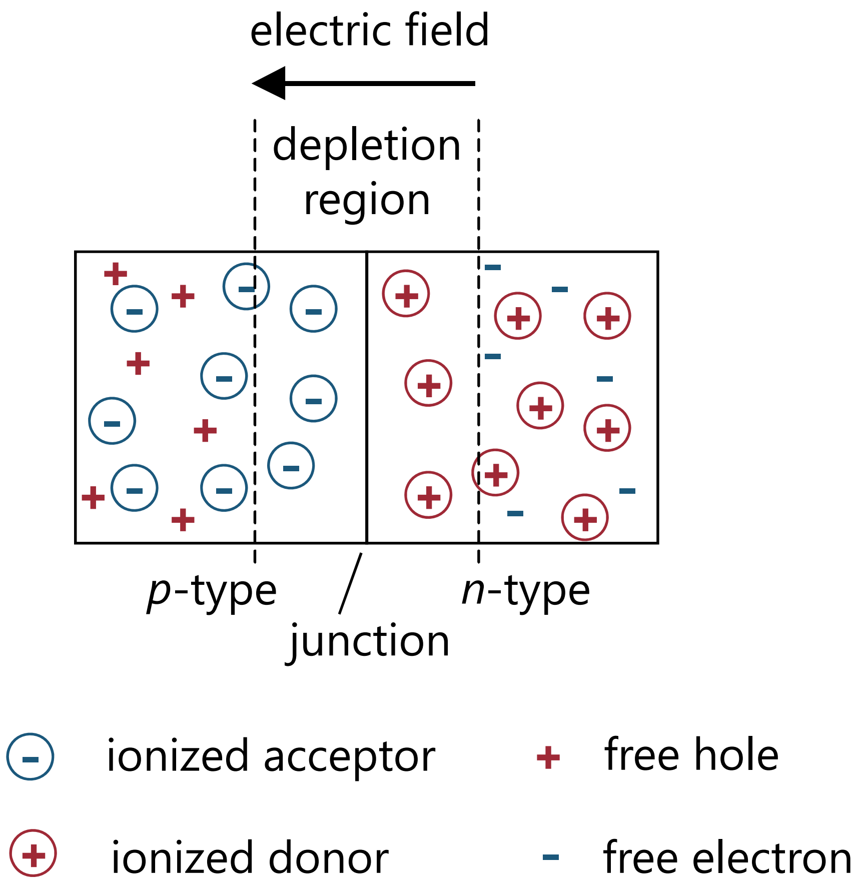
As the electrons and holes move and "annihilate"

- they leave behind net "bare" fixed charges
  - the ionized donors and acceptors
    - which means an electric field is generated
      - in the direction that opposes the diffusion



Semiconductor diode

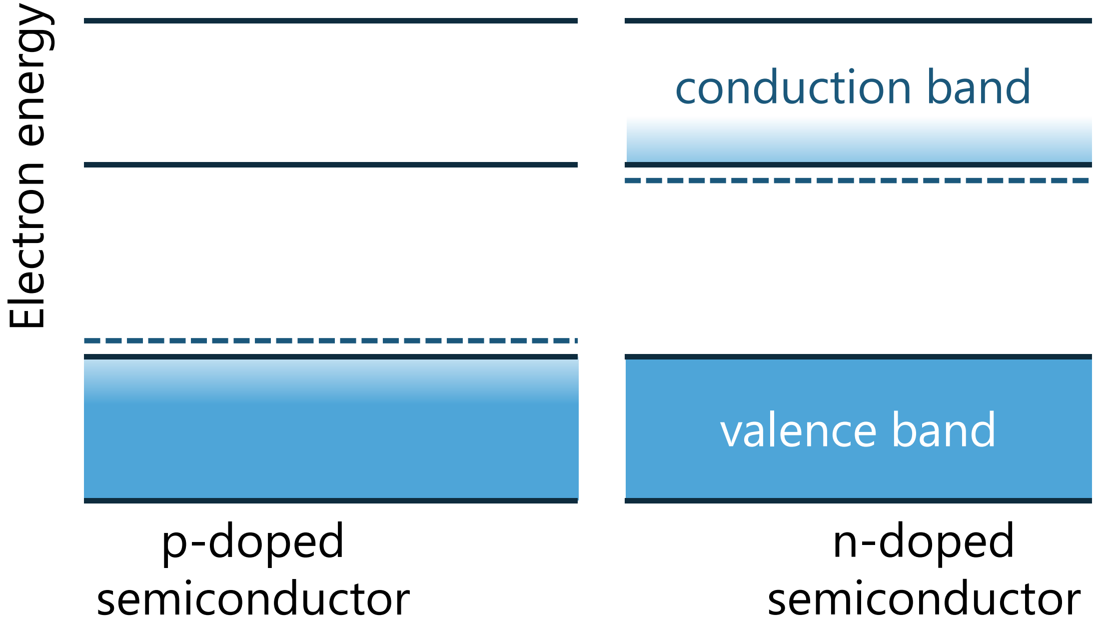
The result is to create a
"depletion region"
on either side of the junction
with essentially no free
charges in it
and an electric field



Semiconductor diode

In terms of bands

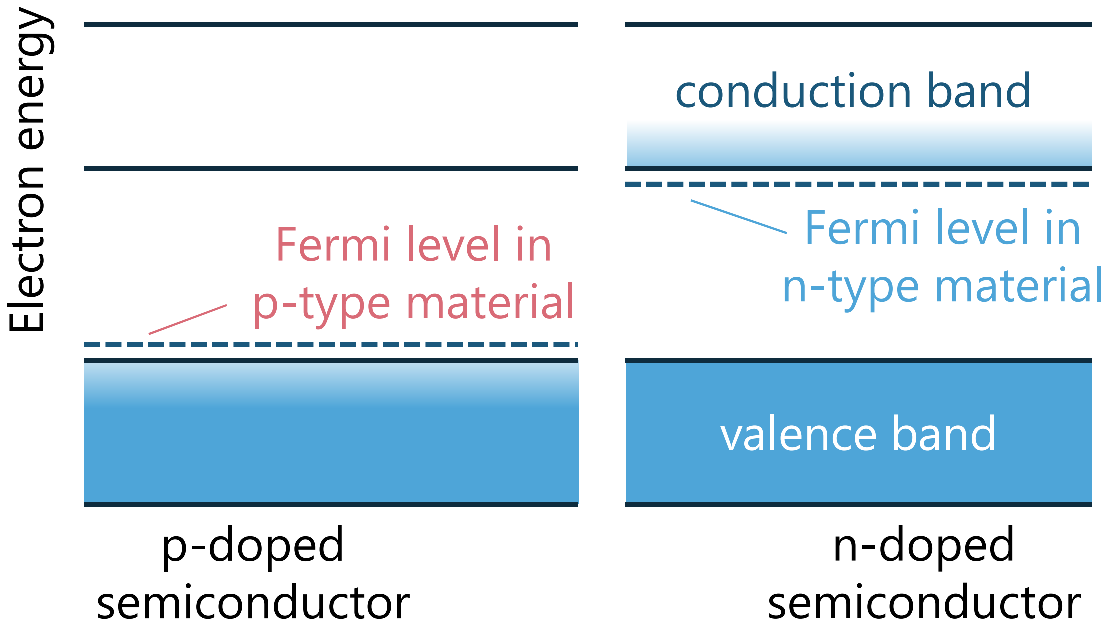
- we might view the bands as being "lined up" before this diffusion



Semiconductor diode

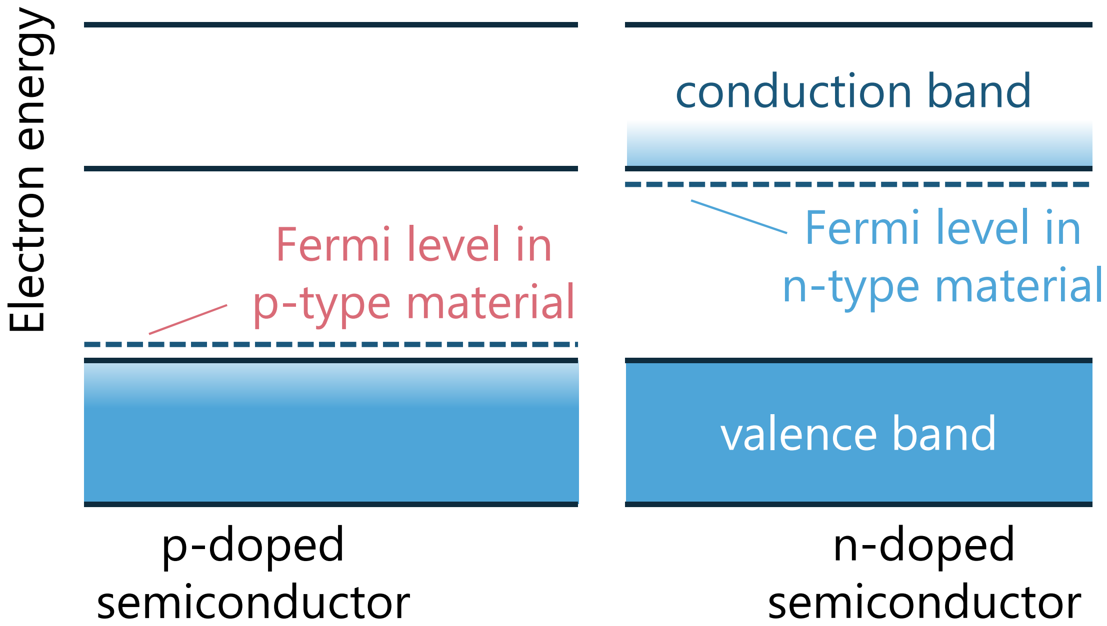
Before diffusion, the Fermi level must be

- near the conduction band edge in n-type material
  - to have many electrons in the conduction band
- near the valence band edge in p-type material
  - to have many holes in the valence band



Semiconductor diode

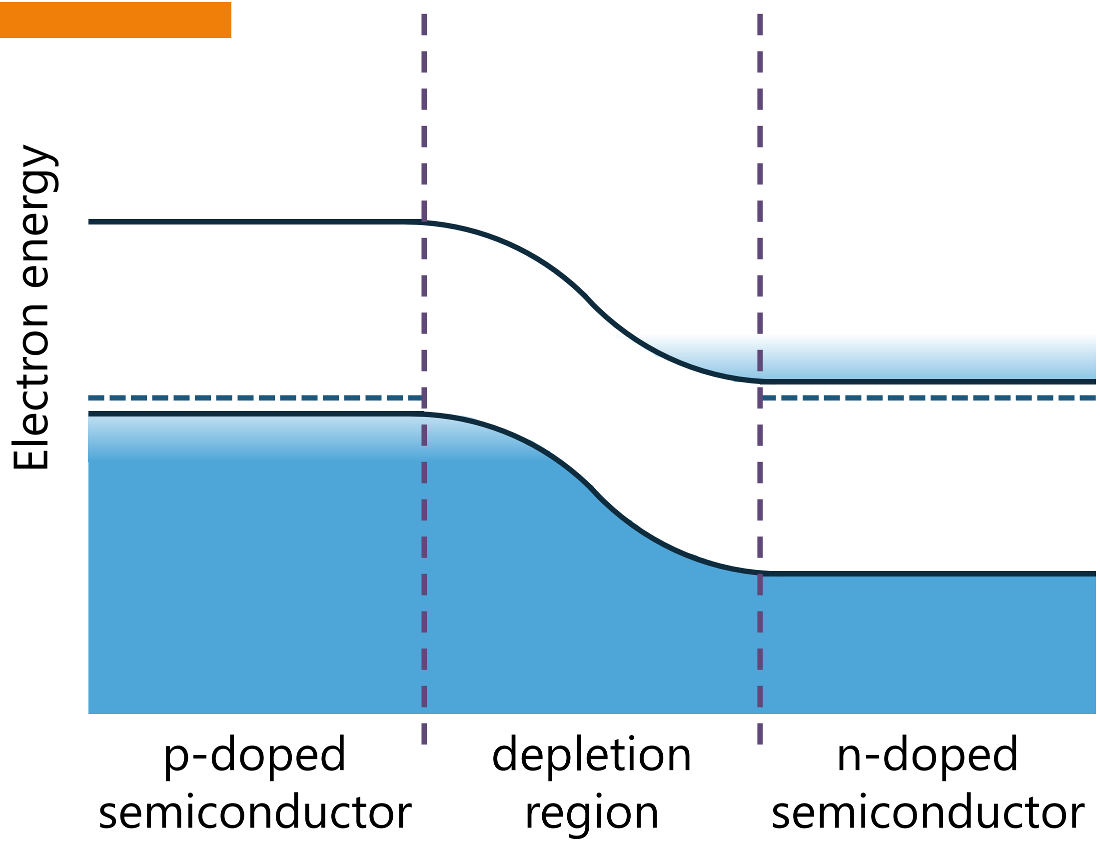
- Note that we move the Fermi level
  - closer to the valence band
    - by adding p-type dopants
  - closer to the conduction band
    - by adding n-type dopants



Semiconductor diode

After the diffusion
- the electrostatic potential has
  - "bent" the bands

Formally
- once the diffusion is finished
  - the "Fermi levels" or "chemical potentials"
    - are equalized



Bands and electronic devices

Voltages and Fermi levels

Modern physics for engineers

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Voltages and Fermi levels

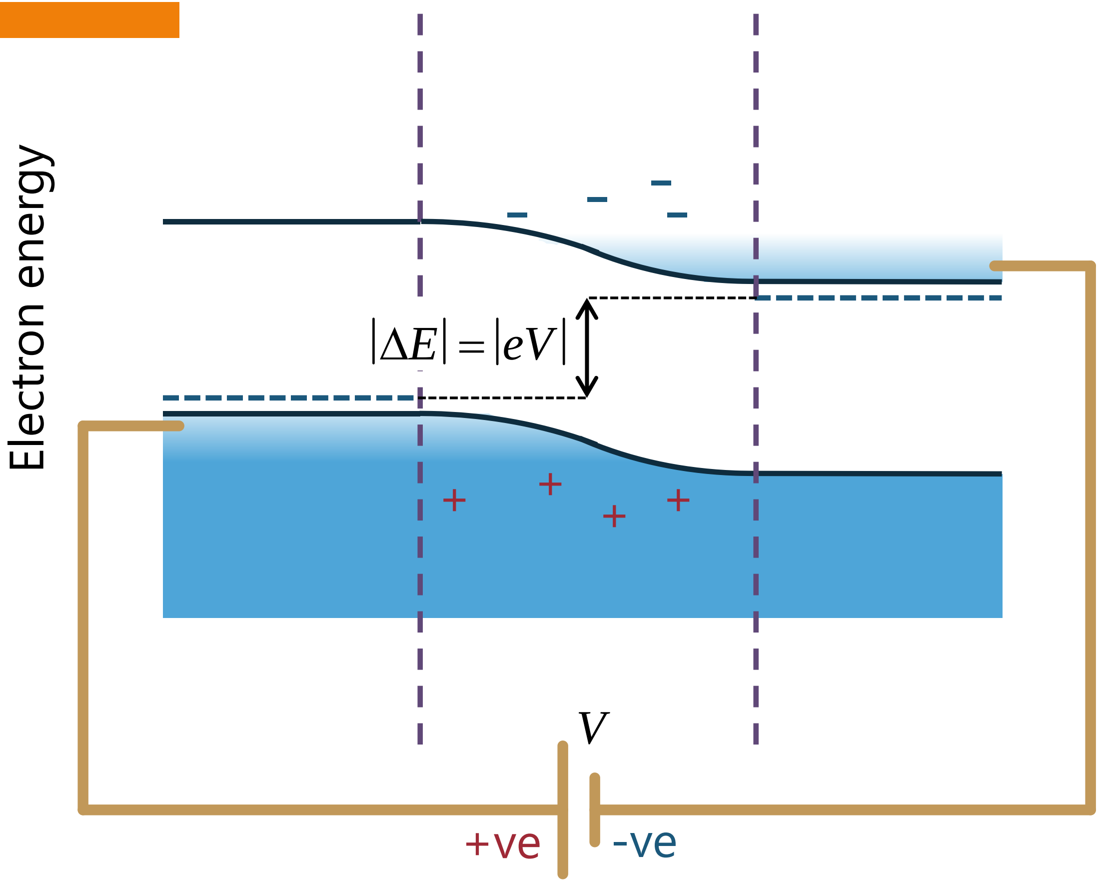
Why is it that

when we apply a voltage V between the two sides of a diode

we separate the Fermi levels

by an amount

$$|\Delta E| = |eV| \text{ ?}$$



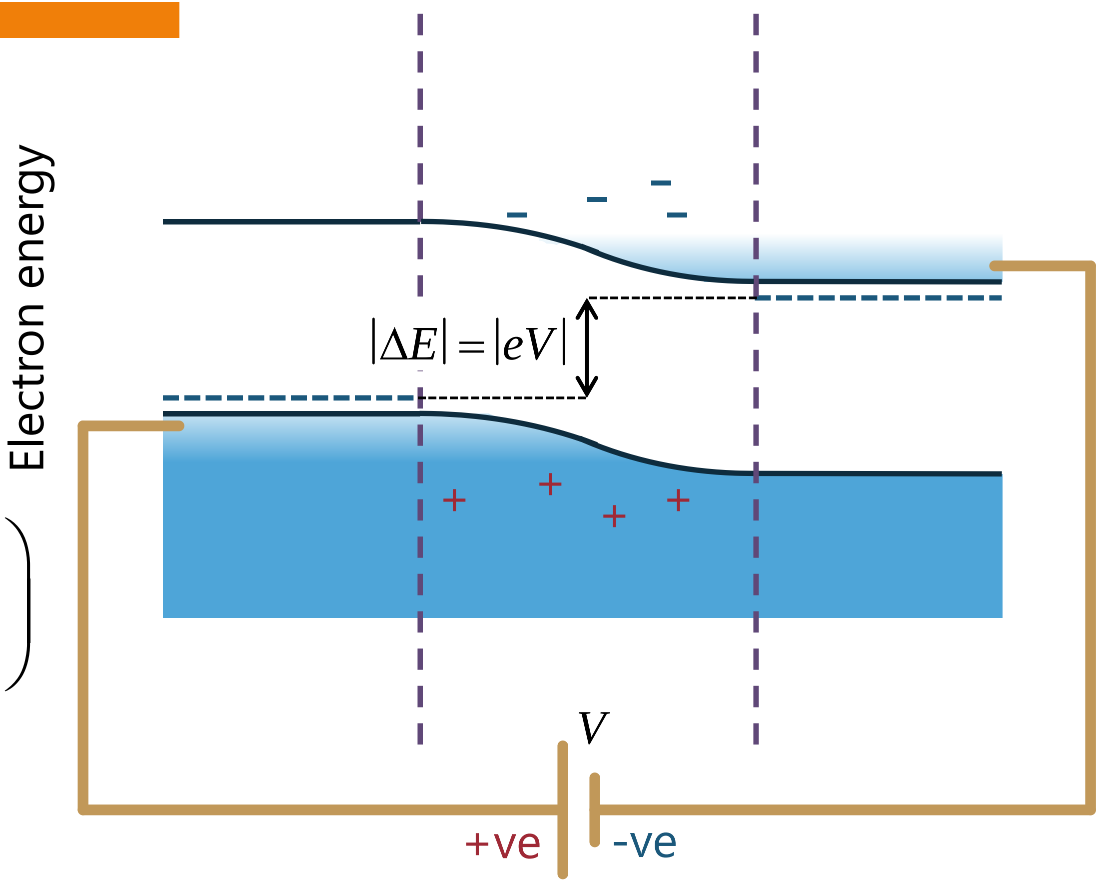
Voltages and Fermi levels

To understand this

we need an alternate but equivalent definition of chemical potential

$$\mu_C = \left(\frac{\partial U}{\partial N}\right)\bigg|_S \quad \left(\equiv -\tau \left(\frac{\partial \sigma}{\partial N}\right)\bigg|_U \right)$$

where U is energy

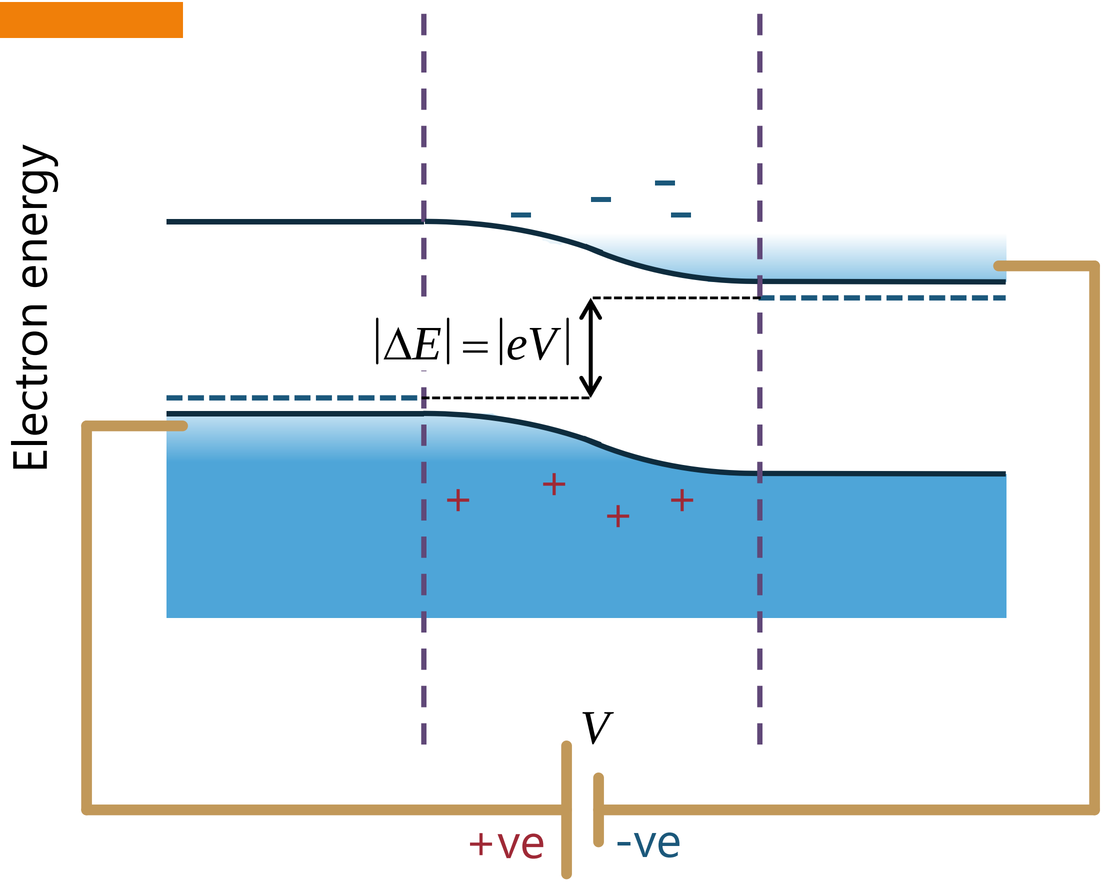


Voltages and Fermi levels

First, we can understand why this alternative form

$$\mu_C = \left(\frac{\partial U}{\partial N} \right) \Bigg|_S$$

gives the result we need



Voltages and Fermi levels

Note that $\left(\frac{\partial U}{\partial N}\right)\Big|_S$ is

the energy per particle at constant entropy

Adding a potential energy $|\Delta E| = |eV|$ to every electron

by changing the voltage V

changes the energy per particle by $|\Delta E| = |eV|$

without changing the entropy at all

and hence changes the chemical potential

$\mu_C = \left(\frac{\partial U}{\partial N}\right)\Big|_S$ by the same amount

Q.E.D

Voltages and Fermi levels

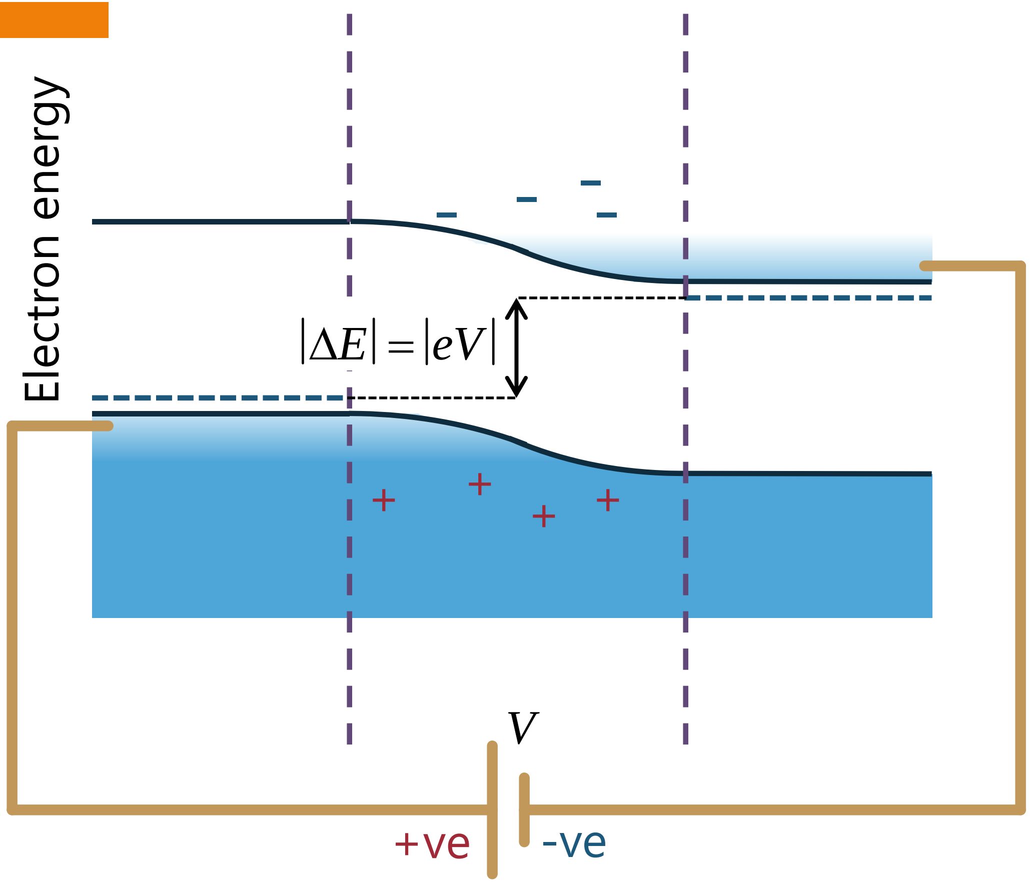
Hence adding $|\Delta E| = |eV|$

to each electron on the "right"

compared to the electrons on the "left"

raises the Fermi level (chemical potential) on the "right" by $|\Delta E| = |eV|$

compared to that on the "left"



Proof of equivalence of chemical potential definitions

Consider the differential of entropy $d\sigma$ for a system with energy U and particle number N

Then, considering a situation of constant entropy, we would have

$$d\sigma = \left(\frac{\partial\sigma}{\partial U}\right)\bigg|_N dU + \left(\frac{\partial\sigma}{\partial N}\right)\bigg|_U dN = 0$$

So, at such a constant entropy, we have

$$\left(\frac{\partial\sigma}{\partial U}\right)\bigg|_N dU = -\left(\frac{\partial\sigma}{\partial N}\right)\bigg|_U dN$$

Proof of equivalence of chemical potential definitions

With $\left(\frac{\partial\sigma}{\partial U}\right)\bigg|_N dU = -\left(\frac{\partial\sigma}{\partial N}\right)\bigg|_U dN$ at constant entropy

we can therefore write $\left(\frac{\partial\sigma}{\partial U}\right)\bigg|_N \left(\frac{\partial U}{\partial N}\right)\bigg|_S = -\left(\frac{\partial\sigma}{\partial N}\right)\bigg|_U$

But $\left(\frac{\partial\sigma}{\partial U}\right)\bigg|_N \equiv \frac{1}{\tau}$

So $\left(\frac{\partial U}{\partial N}\right)\bigg|_S = -\tau\left(\frac{\partial\sigma}{\partial N}\right)\bigg|_U = \mu_C$

which is the chemical potential – Q. E. D.

Bands and electronic devices

Biasing semiconductor devices

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Biasing semiconductor diodes

Semiconductor diode

"Forward biasing"

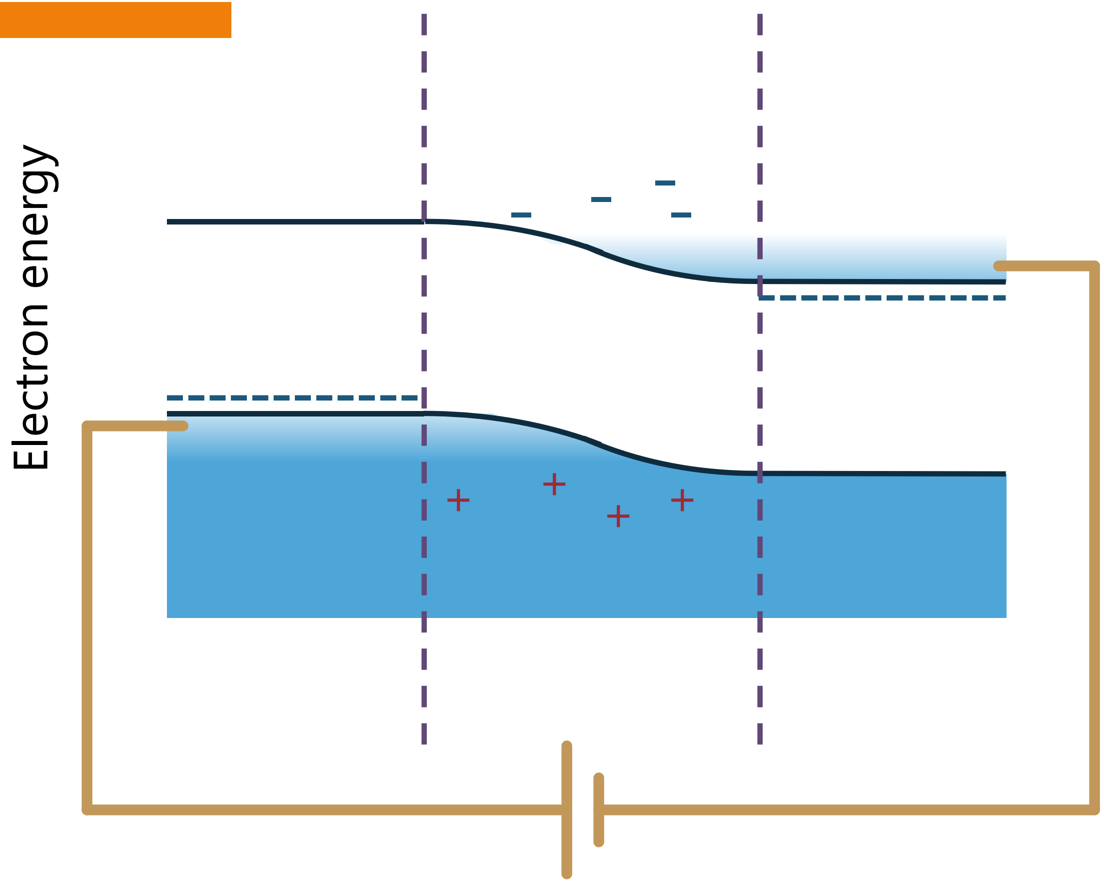
"unbalances" the diffusion again

allowing electrons

with enough thermal energy

to diffuse from right to left

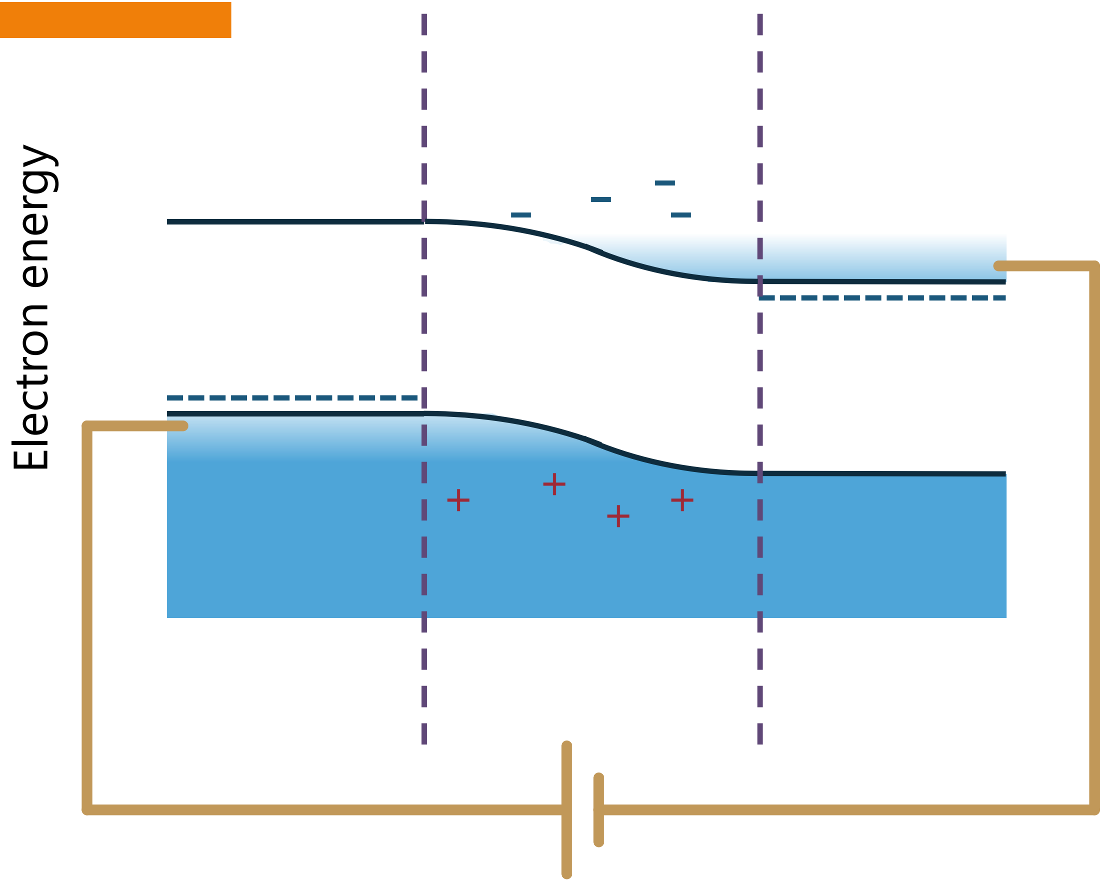
over the potential



Semiconductor diode

and allowing holes
with enough
thermal energy
to diffuse from
left to right
“over” the
potential

This diffusion current is the normal diode forward current



Reverse-biased diode

In a reverse-biased diode

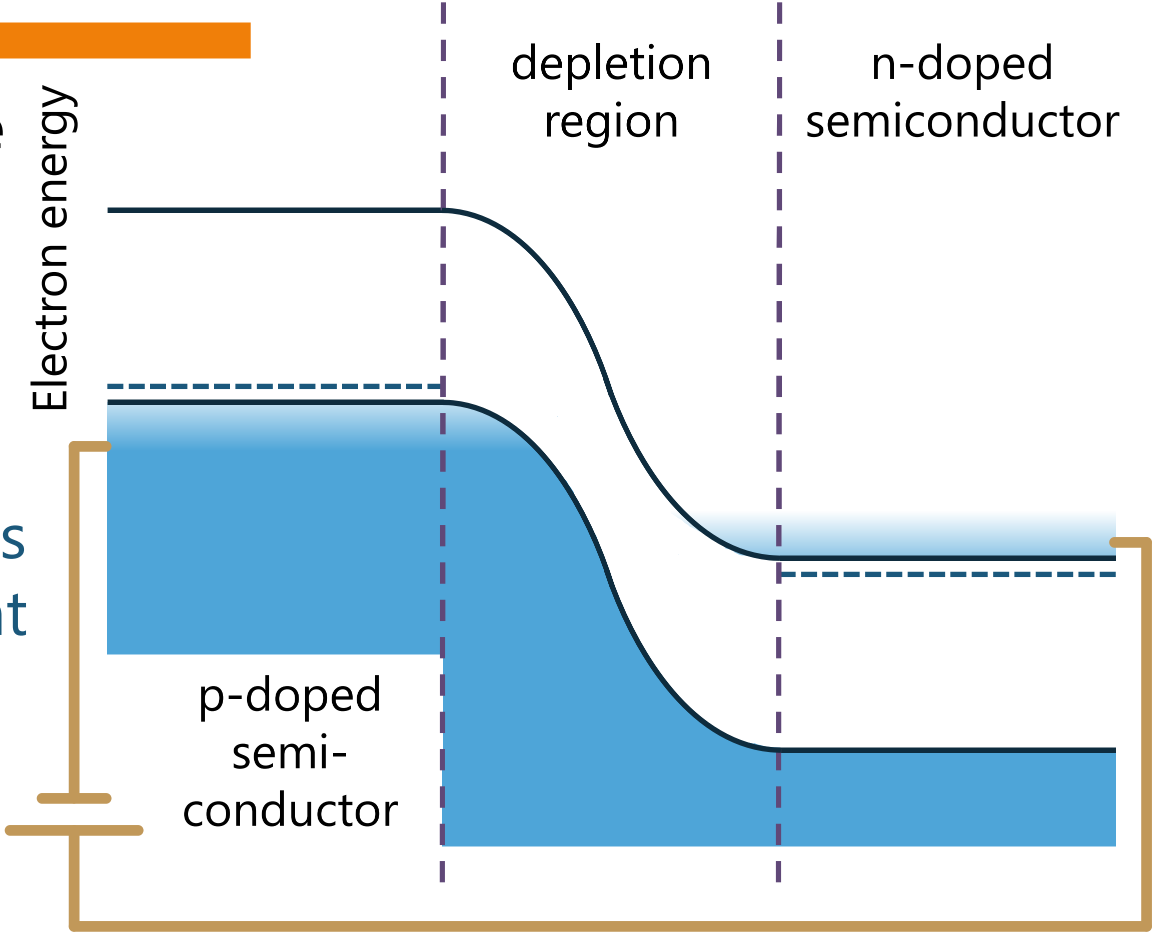
the barriers

for conduction band electrons to diffuse to the left, and

for valence band holes to diffuse to the right

are even higher

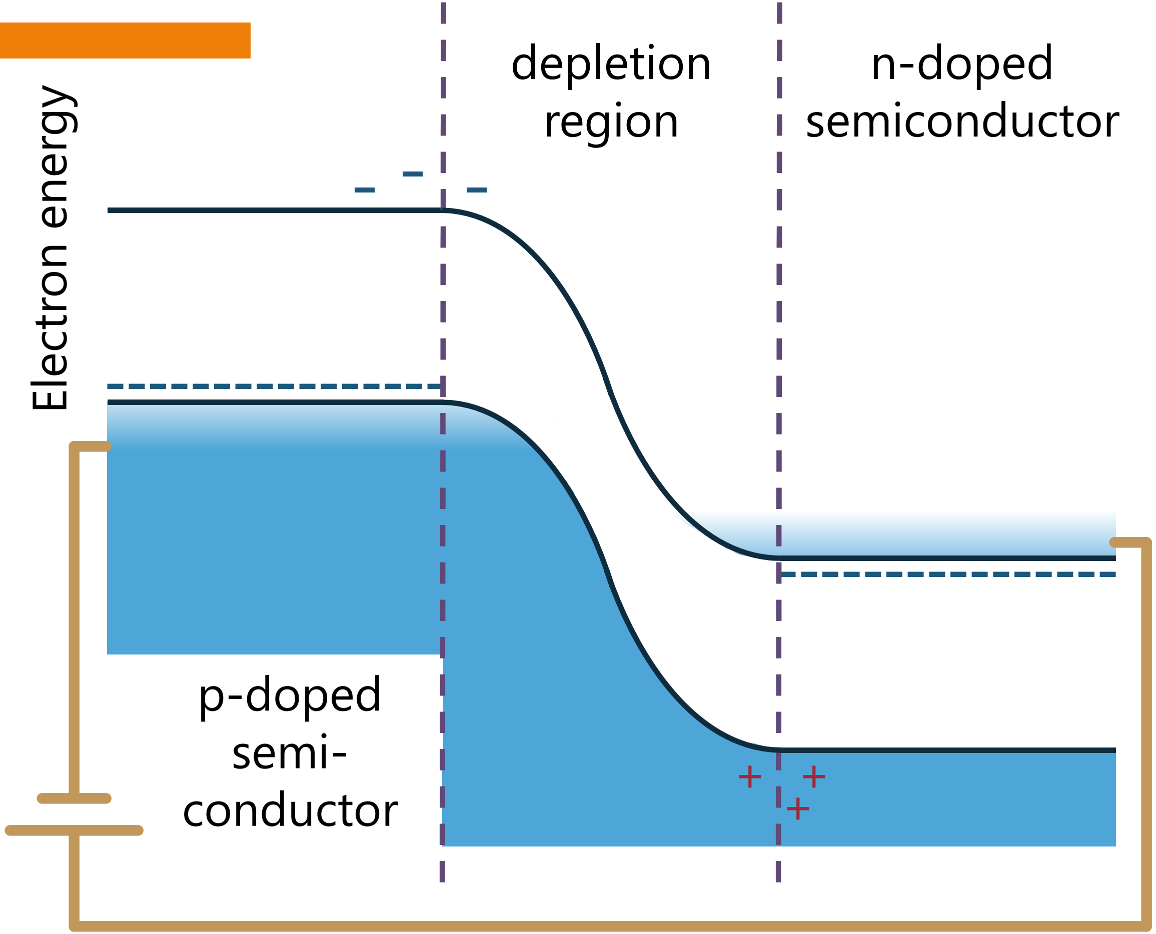
turning off forward diffusion current



Reverse-biased diode

At a finite temperature

- there are also very small "minority carrier" densities of
  - conduction electrons in the p-semiconductor
  - and valence holes in the n-semiconductor



Reverse-biased diode

These minority carriers

can diffuse into the depletion region

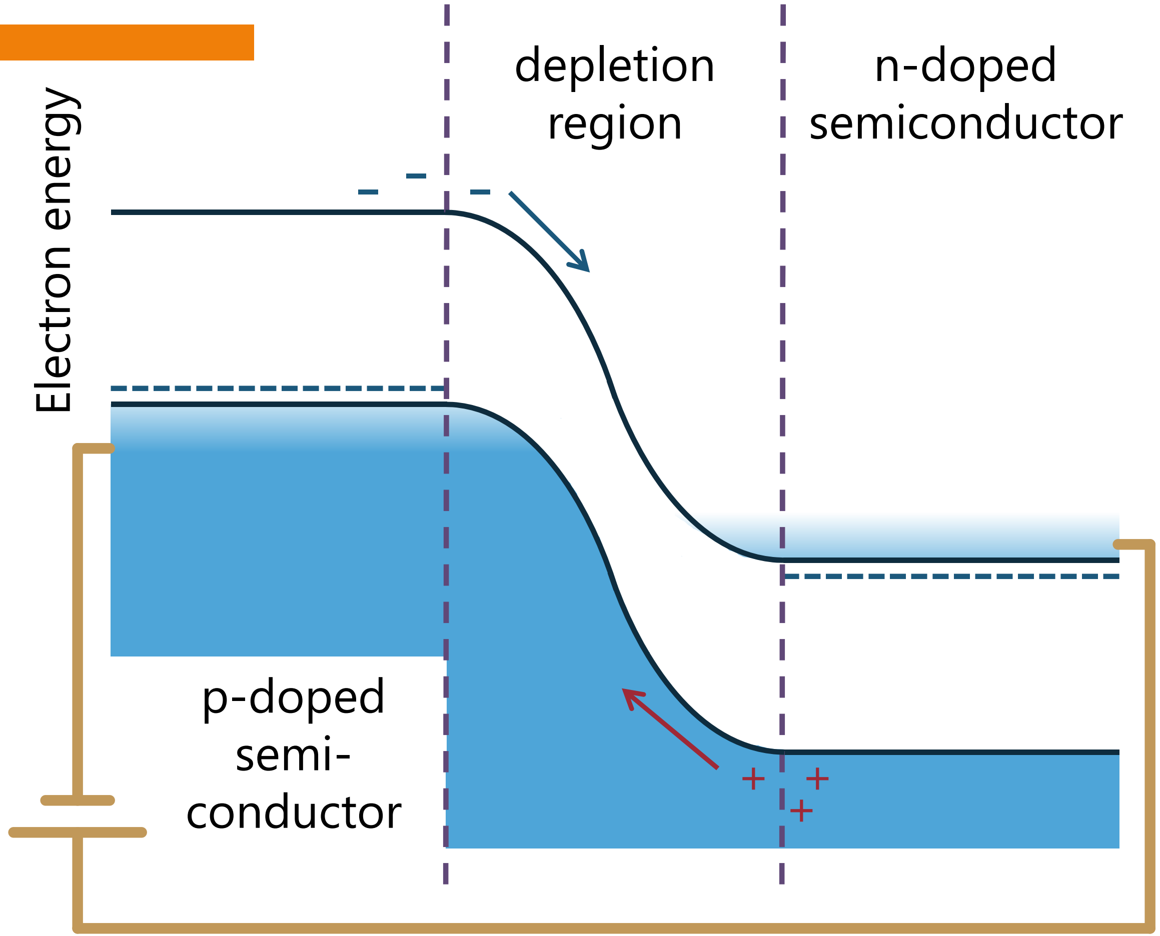
and drift down-hill

Under reverse bias

this gives reverse leakage current

of magnitude I_S

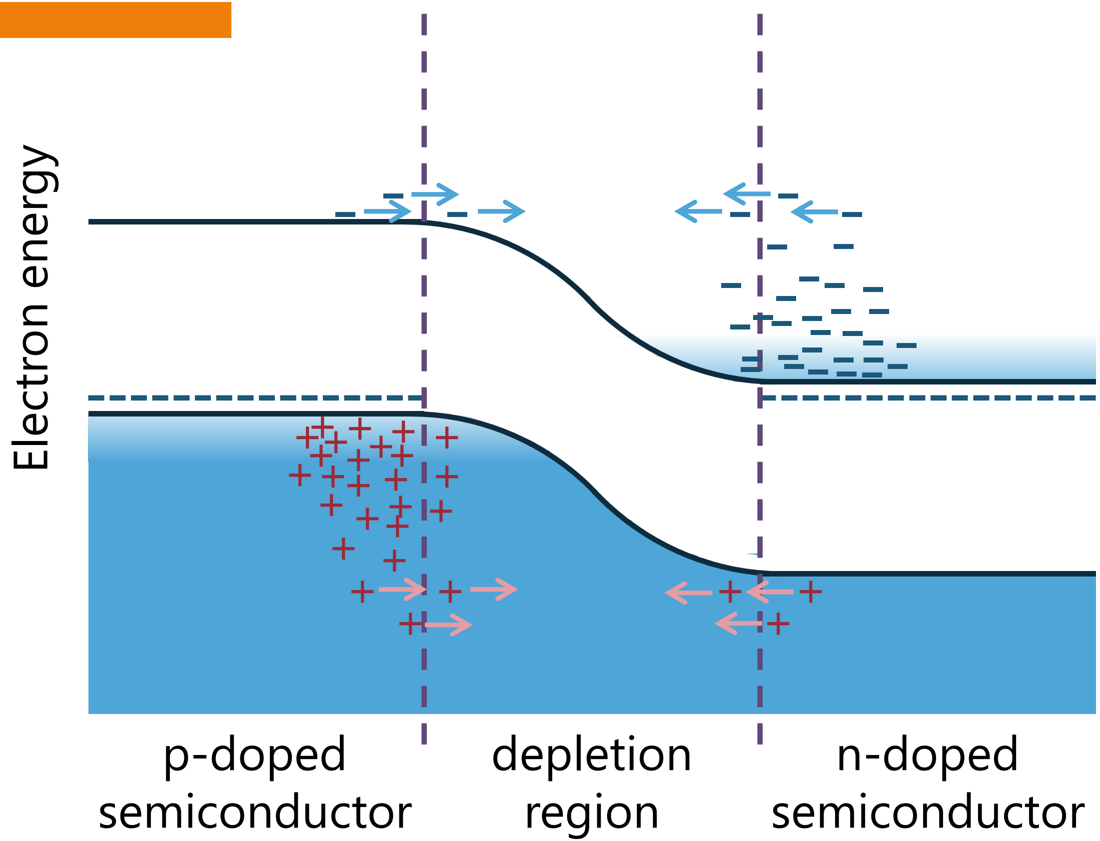
present even in an ideal diode



Semiconductor diode current-voltage characteristic

Current at zero bias voltage

At zero bias voltage
- the number of minority carriers
  - diffusing in “reverse”
- equals the number of “majority carriers”
  - diffusing “forwards”
    - electrons on the n side
    - holes in the p side



Net forward current

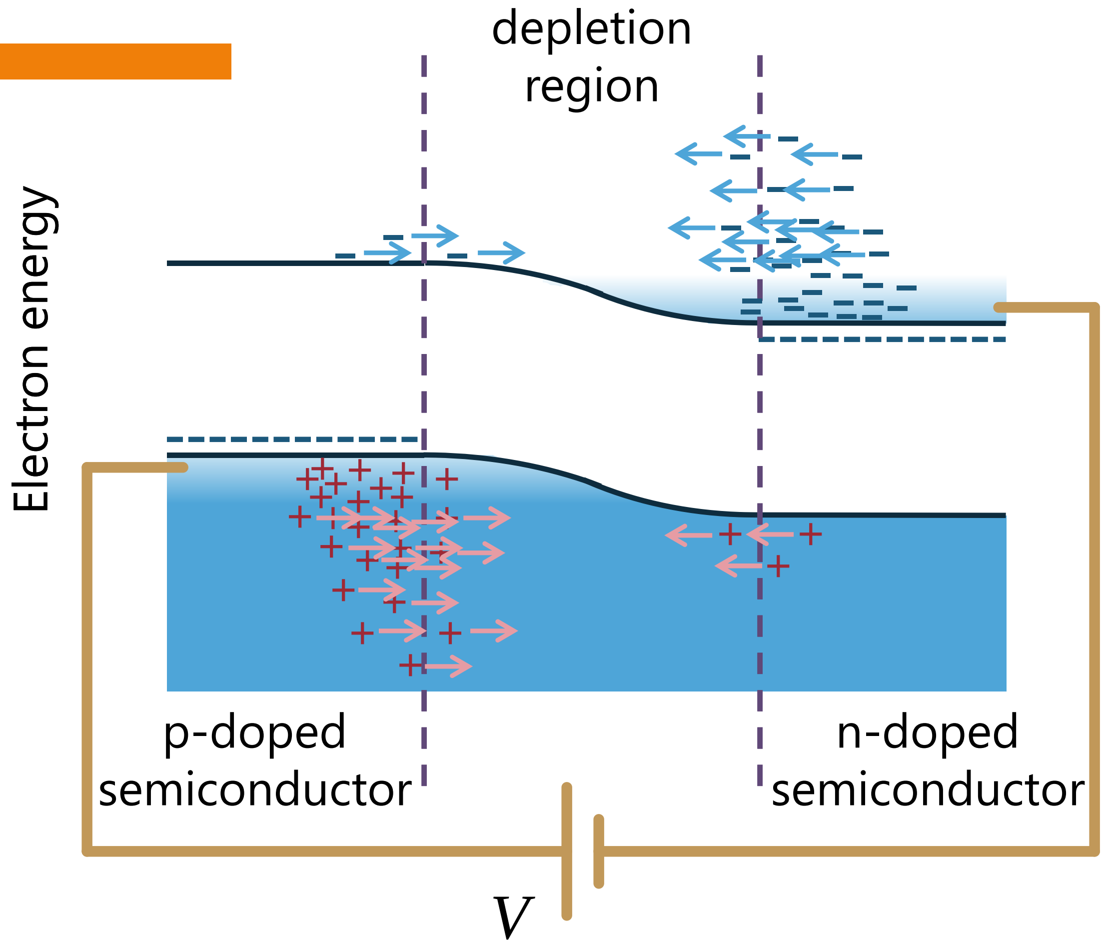
Under forward bias by V volts

the occupation probability of the majority carrier states

presuming the Maxwell-Boltzmann approximation

has increased by

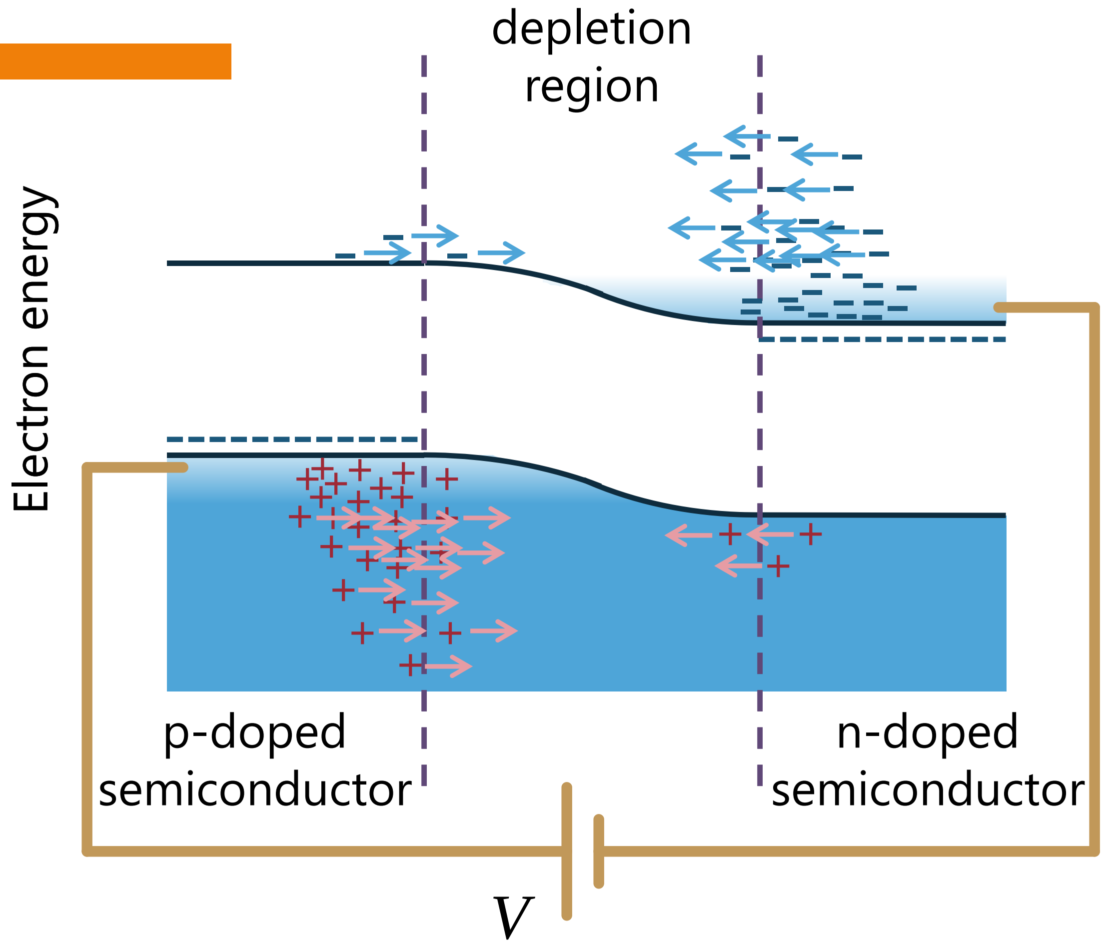
$$\exp\left(eV / k_B T\right)$$



Net forward current

So the net forward current I in a diode is
the forward diffusion
minus
the backward "leakage" diffusion

$$I = I_S\left[\exp\left(\frac{eV}{k_B T}\right) - 1\right]$$



Diode current-voltage (I-V)

Here is current as a function of voltage for an "ideal" diode

At room temperature

$$k_B T / e \simeq 25mV$$

I_S depends on doping levels and material properties

$$I = I_S \left[\exp\left(\frac{eV}{k_B T} \right) - 1 \right]$$