Particles, atoms, and crystals
6

Band structures

Modern physics for engineers

David Miller

Calculating a band structure

For a periodic structure of "rectangular" potential wells

using the periodic boundary conditions

we can calculate the energy eigenvalues

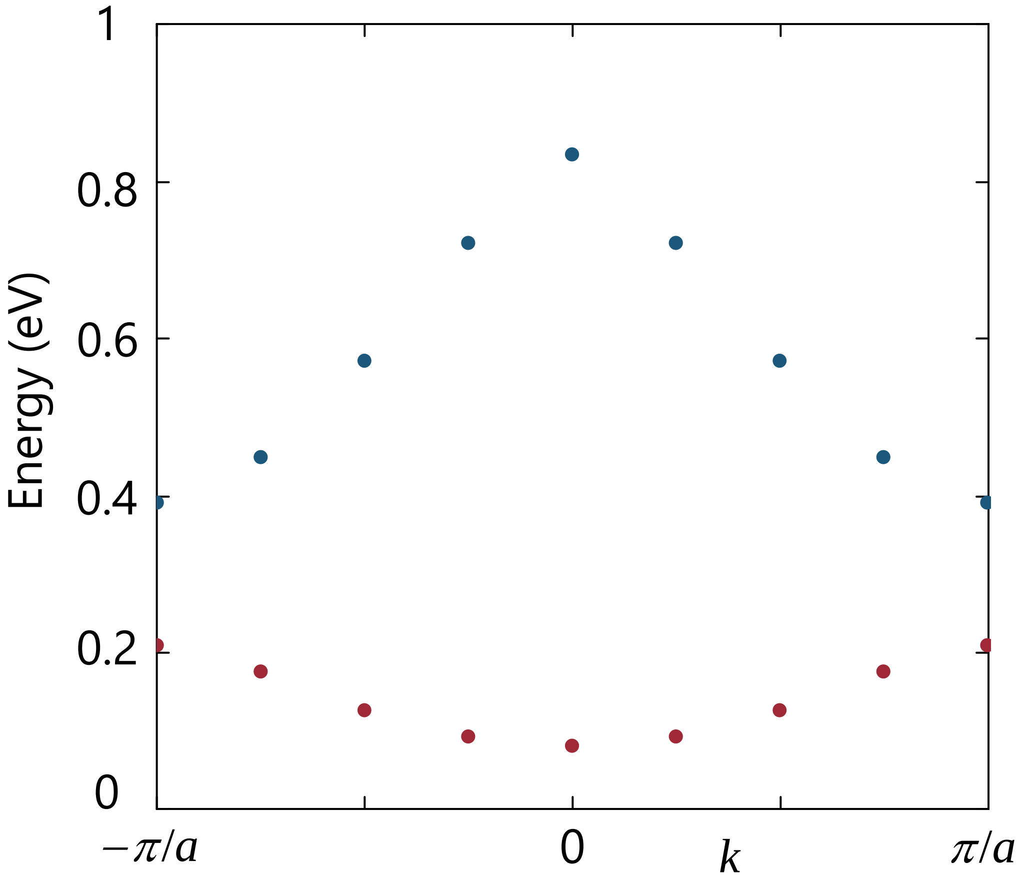
for each allowed value of k

The resulting sets of energies

will allow us to plot

a "band structure"

Calculating a band structure



N = 8 solutions

N = 8 solutions

well width

1.2 nm

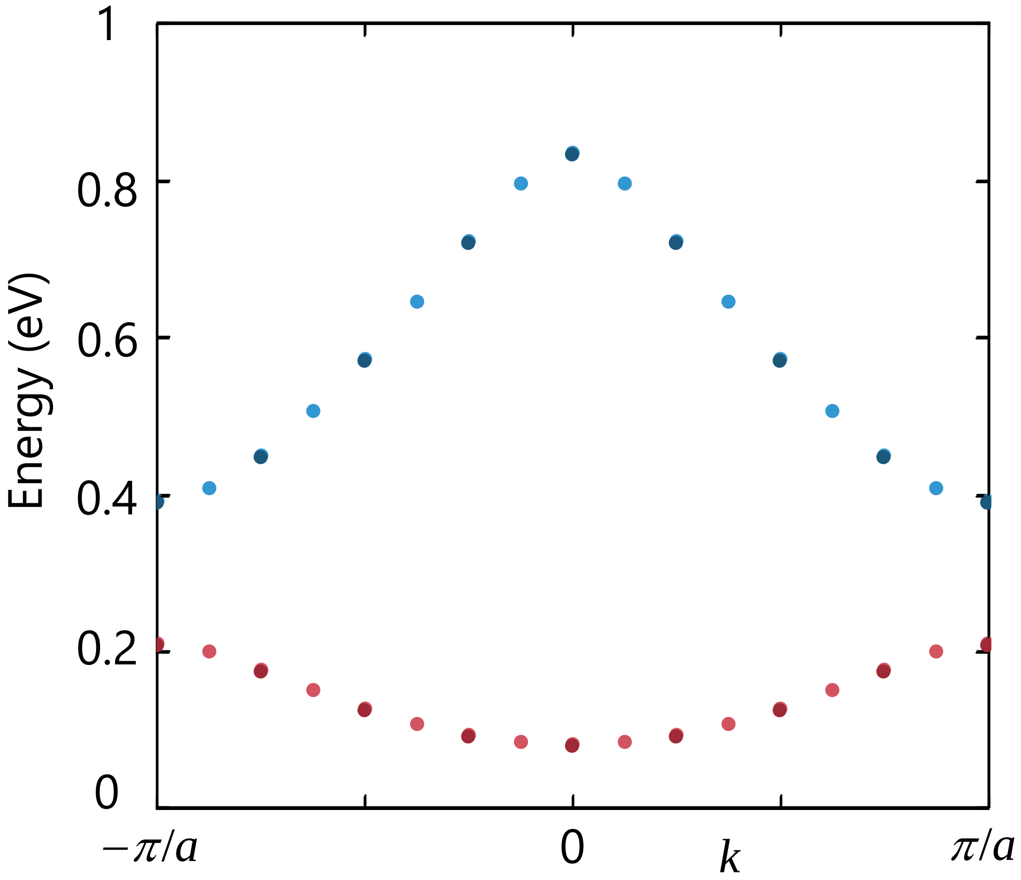
barrier width

0.15 nm

barrier height

1 eV

Calculating a band structure



N = 8 solutions

N = 16 additional solutions

N = 8 solutions

N = 16 additional solutions

well width

1.2 nm

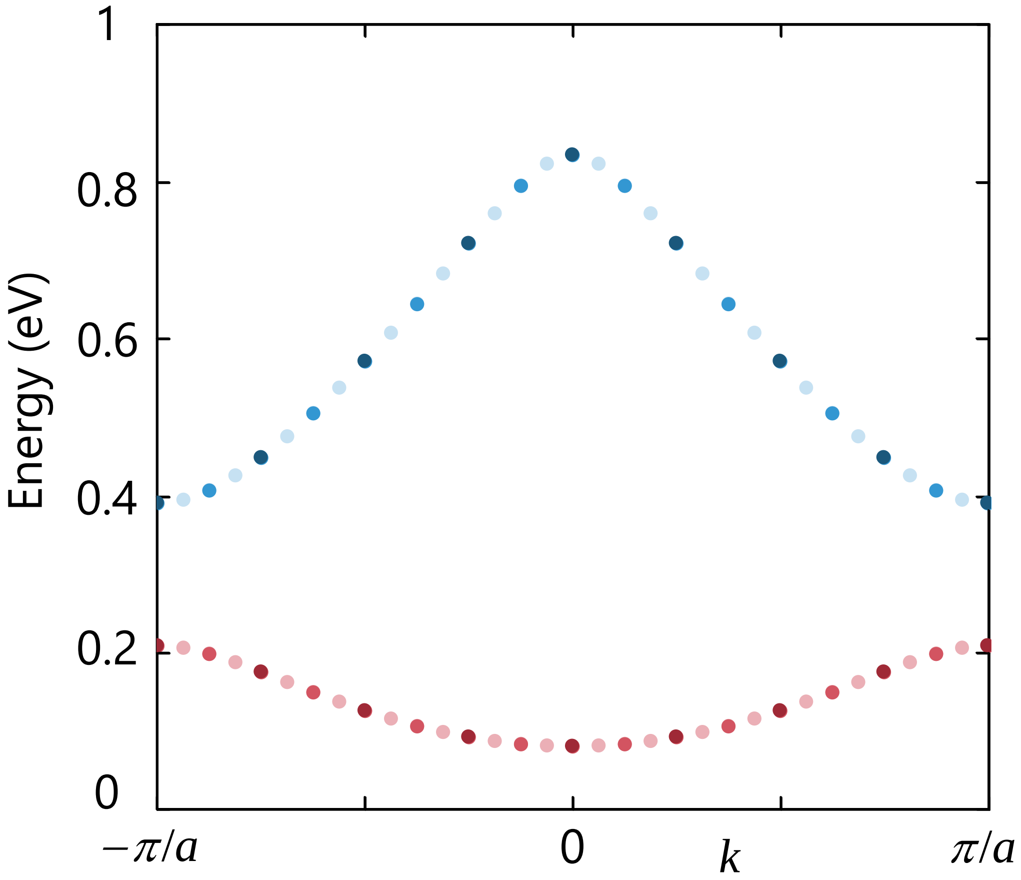
barrier width

0.15 nm

barrier height

1 eV

Calculating a band structure



N = 8 solutions

N = 16 additional solutions

N = 32 additional solutions

N = 8 solutions

N = 16 additional solutions

N = 32 additional solutions

well width

1.2 nm

barrier width

0.15 nm

barrier height

1 eV

Calculating a band structure

well width

1.2 nm

barrier width

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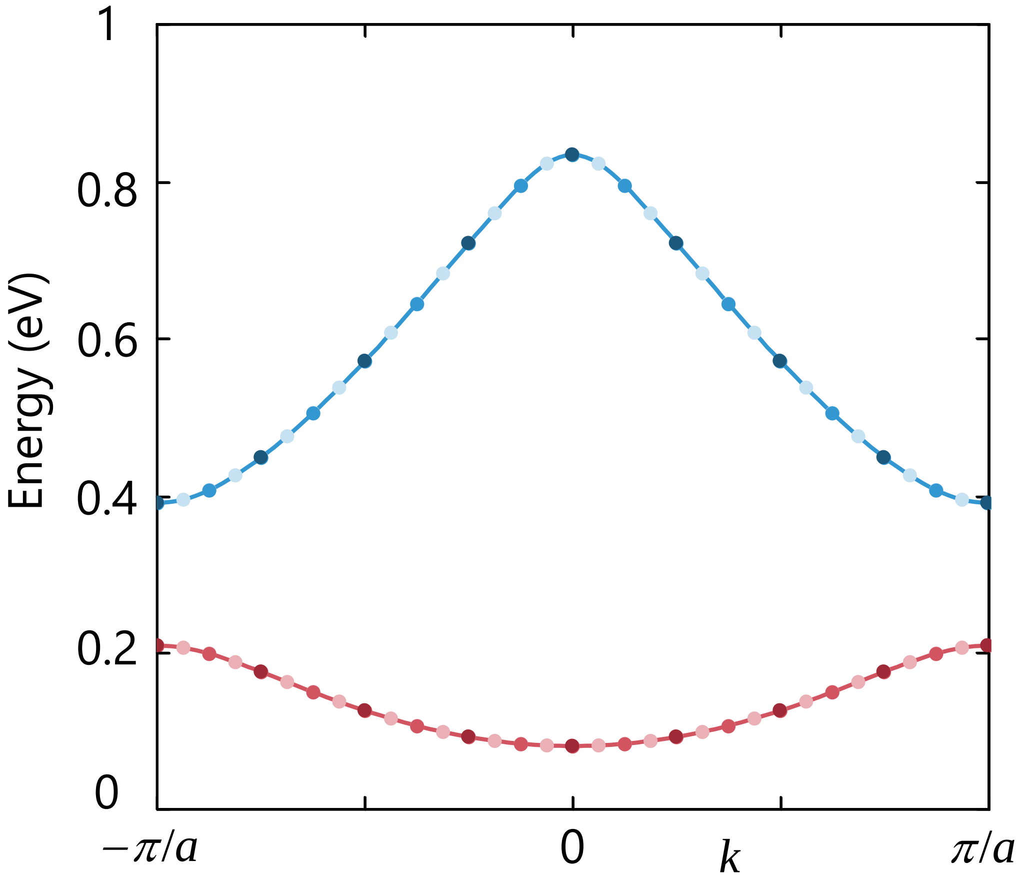
barrier height

1 eV



N = 8 solutions

N = 16 additional solutions

N = 32 additional solutions

N large

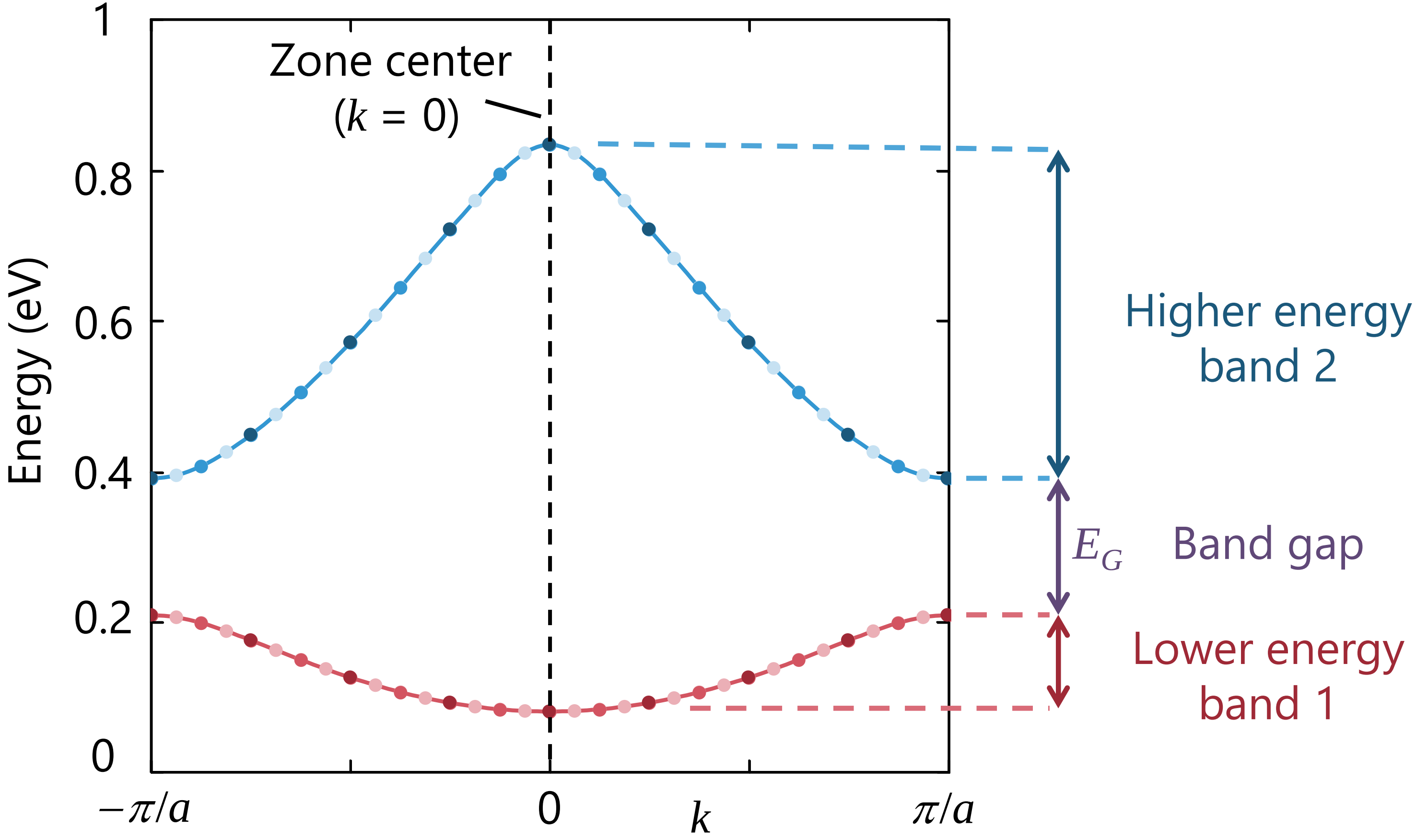
N = 8 solutions

N = 16 additional solutions

N = 32 additional solutions

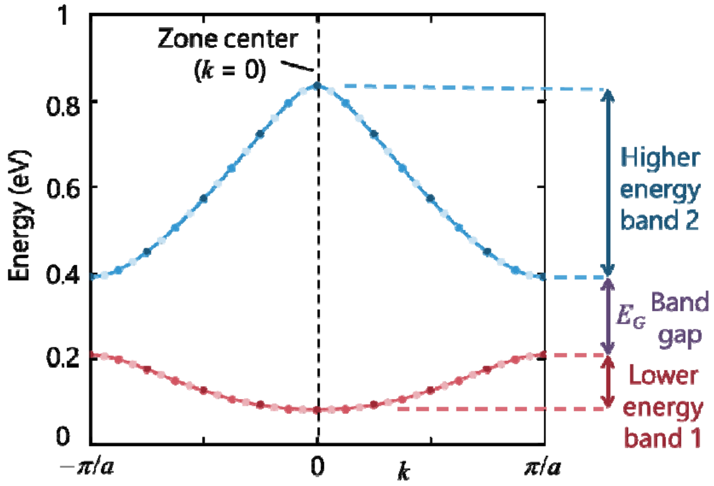
N large

Calculating a band structure



Properties of the band structure

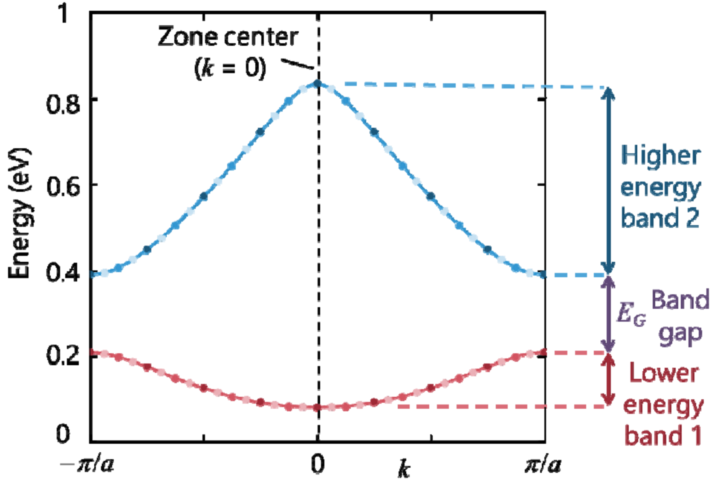
- First
  - note the k values for each choice of N
    - are equally spaced, by $2\pi / Na$
- As we have “pushed” the “atoms” together to make this “crystal”
  - we can keep the same counting of states
    - Some given atomic level in each of N atoms
      - has turned into N energy levels
        - in a band in the combined system



Properties of the band structure

Second

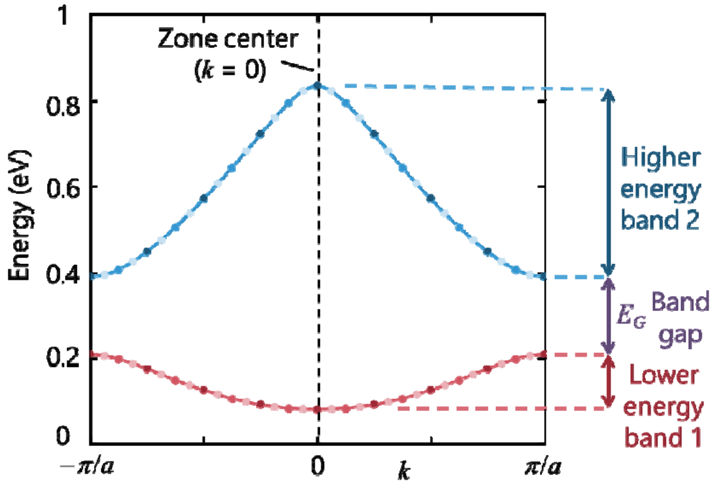
- note that, for each value of k
  - within the energy range from 0 to 1 eV for which we performed calculations
    - there are two possible energy eigenvalues, as given by
      - the “red” dots for the lower band and
      - the “blue” dots for the upper band



Properties of the band structure

Third

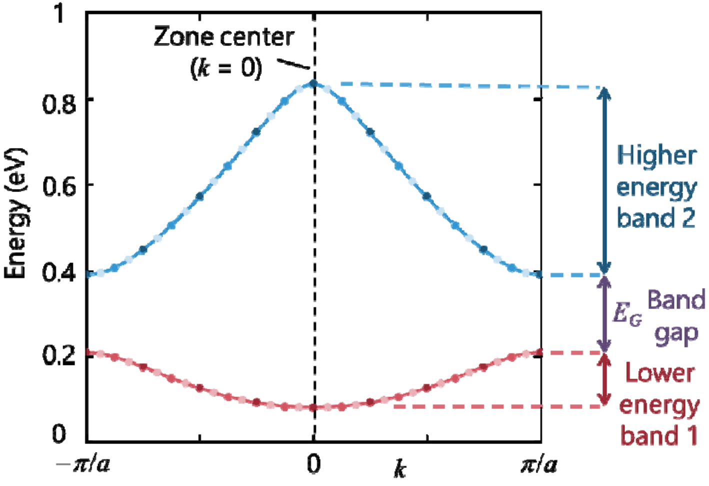
- as we increase N, first to 16, and then to 32
  - we fill in the spaces between the existing "dots"
    - retaining all the previous solutions
- Note that the energy width of the bands
  - does not increase
    - as we increase N arbitrarily
- We end up with smooth continuous bands of definite width
  - and all the energy solutions lie on these curves



Properties of the band structure

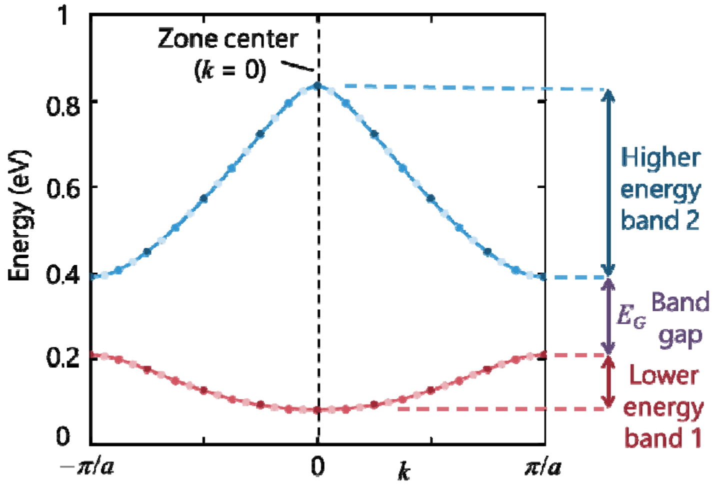
Fourth

- we see a range of energies between the two bands, for which
  - there are no energy eigenstates
    - Such energy ranges are “band gaps”
      - with a band gap energy E_G
- The existence or otherwise of band gaps in a band structure
  - is very important in influencing both
    - the electrical and optical properties of a material



Brillouin zone

- We calculated for the allowed set of N different k values
  - We could keep on calculating
    - for further values of k spaced by the same amount
- We would just repeat ourselves, however
  - finding the same solutions again
    - We would just repeat the same band structure
      - copying the curves and moving them sideways by $2\pi / a$
        - creating an “extended” zone scheme



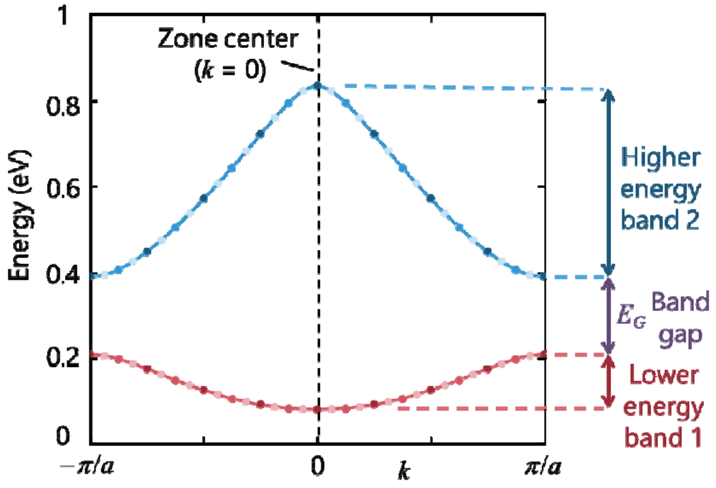
Brillouin zone

Any one such $2\pi / a$ range of k values can be called

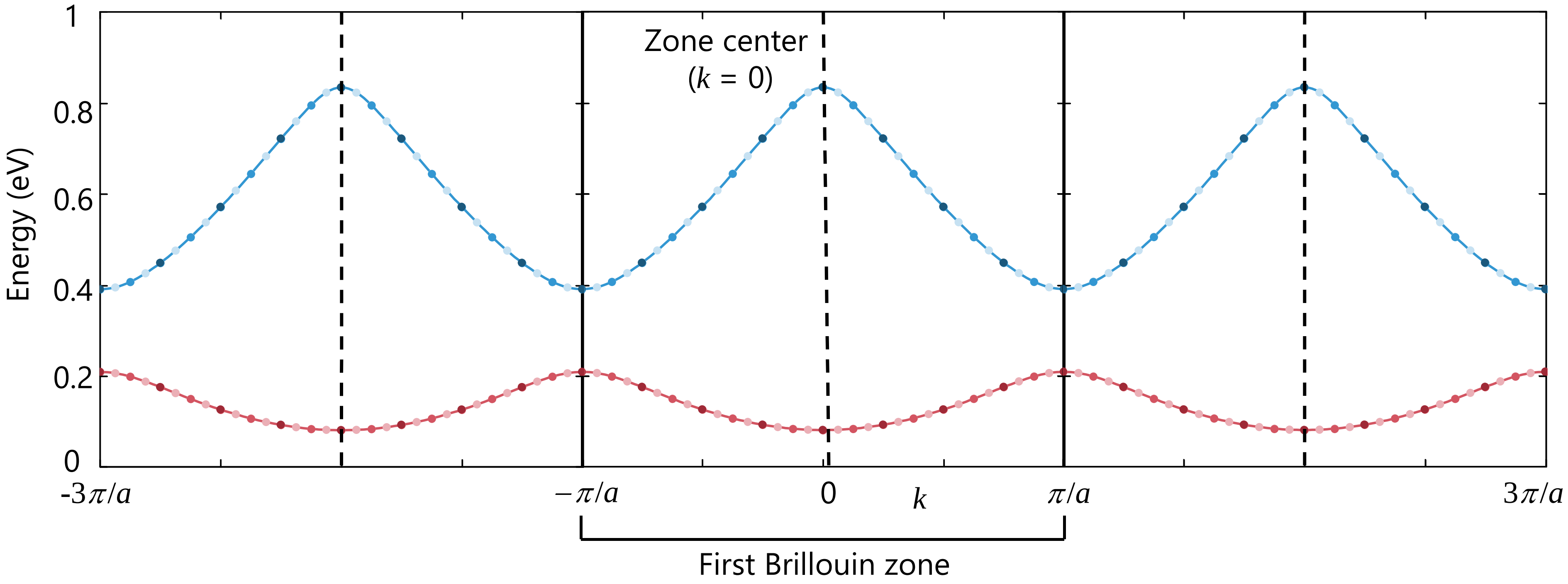
- a “Brillouin zone”
  - The version centered round $k = 0$
    - is called the first Brillouin zone
  - and the point $k = 0$
    - is referred to as “zone center”

We only ever need to calculate the results

- for the first Brillouin zone
  - because it contains all the distinct solutions



Brillouin zones – "extended" scheme



Particles, atoms, and crystals
6

Crystal momentum and effective mass

Modern physics for engineers

David Miller

Crystal momentum

Crystal momentum

For a particle in a uniform potential

- we know the eigen solutions are plane waves

In one dimension, for a particle of mass m_b

- with a given energy E
  - solving Schrödinger's equation for a "forward-going" wave
    - gives a wavefunction $\propto \exp(ikz)$

with eigen energy $E = \dfrac{\hbar^2 k^2}{2m_b}$

Crystal momentum

We also know from de Broglie's hypothesis that

- the magnitude of the momentum is then $p = \hbar k$

For solutions in Bloch form

- the "envelope" part of the solution is
  - a propagating wave of the form $\exp(ikz)$

We can define a similar concept here

- the "crystal momentum" p_C
  - which we write with a similar formula

$$p_C = \hbar k$$

- using the k in the propagating "envelope" function

Crystal momentum

This crystal momentum shows many effective properties

- that behave like actual momentum for an electron in a crystal
  - though this is not actually the electron momentum
    - and we can call it a “pseudo-momentum”

Crystal momentum

An electron accelerated by a force in the crystal

- acquires such an effective momentum

In optical absorption, it can appear that

- "momentum" overall is conserved when we use this pseudo-momentum

Crystal momentum

In all these cases

- we deduce the effective conservation of this pseudo-momentum from deeper analysis
  - The effective “conservation” of this pseudo-momentum comes out of that analysis
    - It is not a principle we put into the analysis

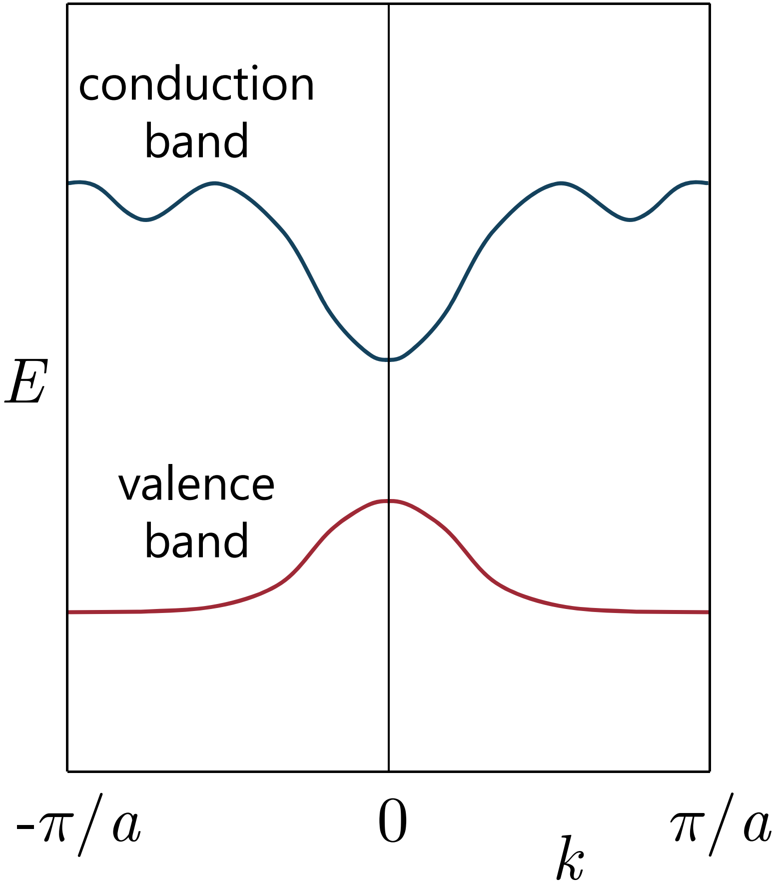
Crystal momentum

- Nonetheless, it is a useful idea for electrons in crystals
  - and is often loosely just called the “momentum”
    - One useful example is associated with the idea of effective mass

Effective mass

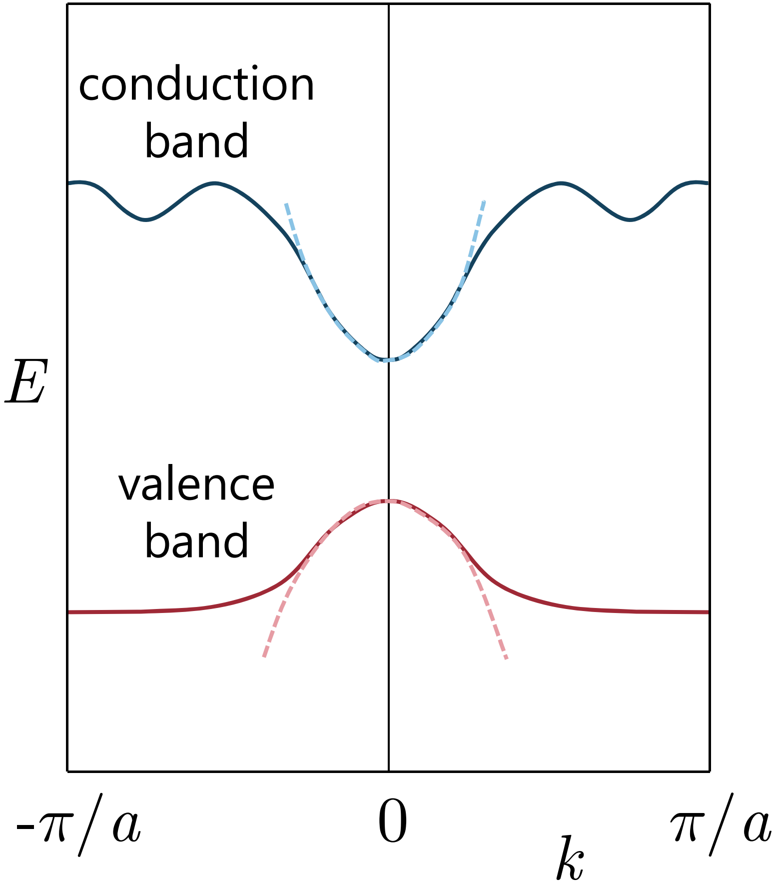
Effective mass approximation

- Consider a hypothetical band structure
  - with a higher band called
    - the “conduction band”
  - and a lower band called
    - the “valence band”



Effective mass approximation

- Near a minimum or maximum
  - in either band
    - we could fit the energy as a function of k with a parabola
- For such a parabola centered round $k = 0$
  - relative to the energy E_o at the minimum or maximum
    - we would have $E - E_o \propto k^2$



Effective mass approximation

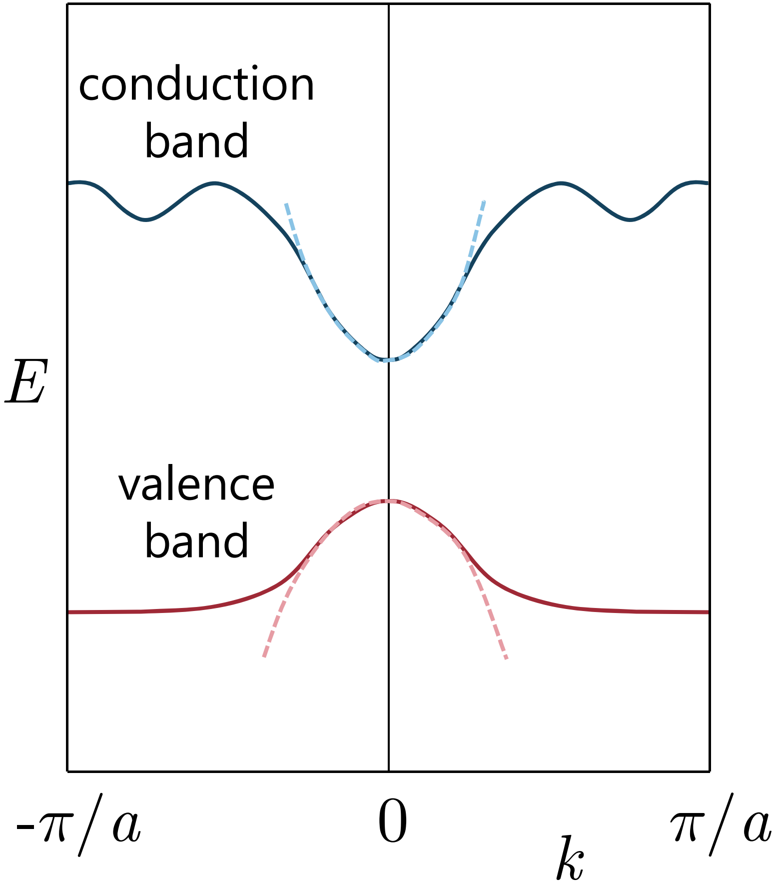
We could choose to write such a relation $E - E_o \propto k^2$

in the form $E - E_o = \dfrac{\hbar^2 k^2}{2m_{eff}}$

where m_{eff} is what we call an "effective mass"

It is a "fitting parameter"

which we choose to get the right curvature on the parabola



Effective mass approximation

In the relation $E - E_o = \dfrac{\hbar^2 k^2}{2m_{eff}}$

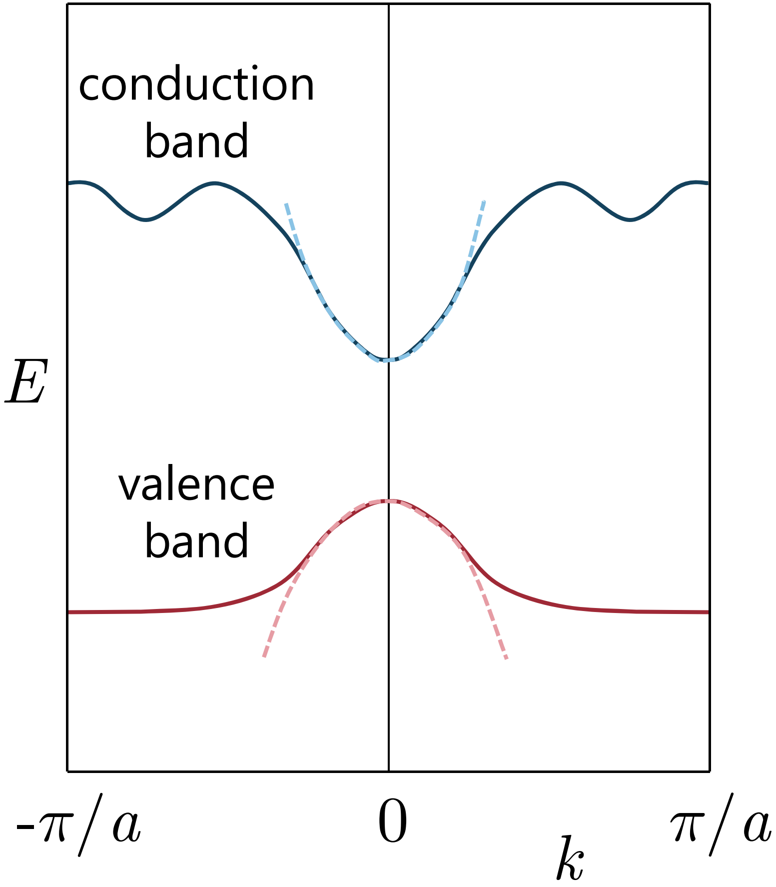
note that

a large effective mass

gives a shallow parabola

a small effective mass

gives a steep parabola



Effective mass approximation

If we then treat p_C as an effective momentum

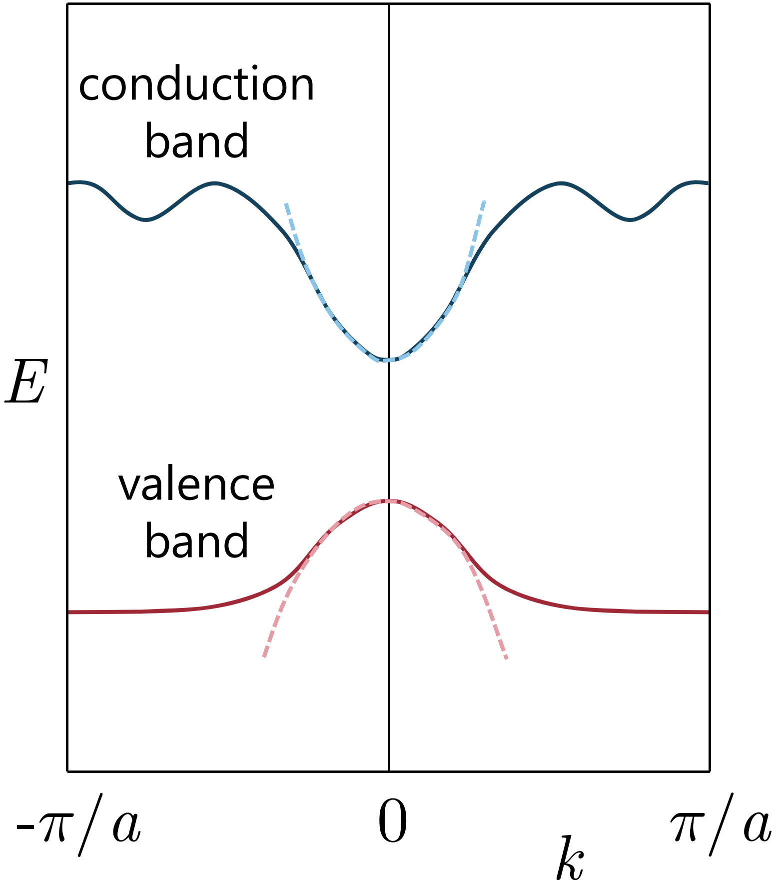
then we can write

$$E - E_o = \frac{\hbar^2 k^2}{2m_{eff}} = \frac{p_C^2}{2m_{eff}}$$

which is consistent with p_C

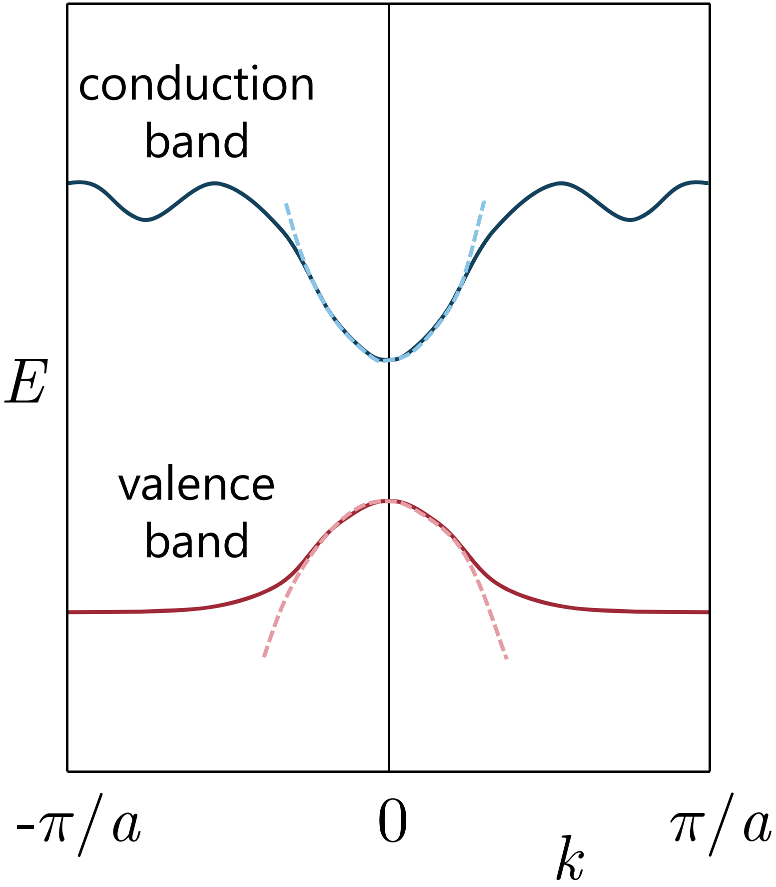
behaving like momentum

for a particle of an effective mass m_{eff}



Effective mass approximation

- This idea of effective mass is very useful
  - especially for electronic and optoelectronic devices
- Note effective mass
  - is only an effective concept
    - We have not changed the electron mass
      - but band structures can make it appear we have



Effective mass approximation

A band structure

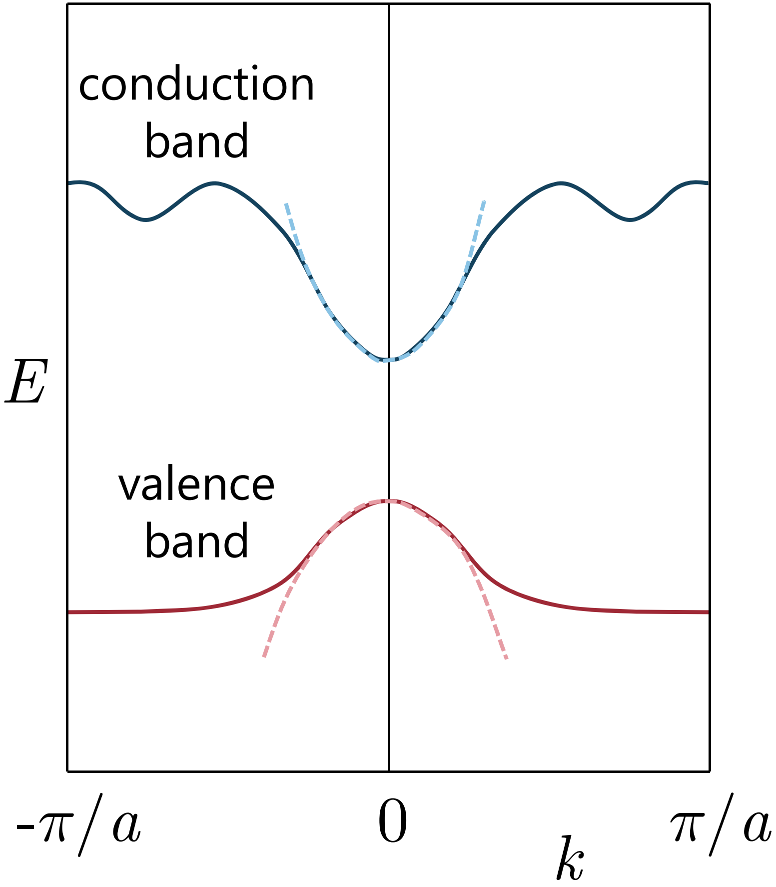
in which the lowest minimum in the conduction band

lies at the same k as

the highest maximum in the valence band

is said to show a

direct bandgap



Effective mass approximation

A band structure

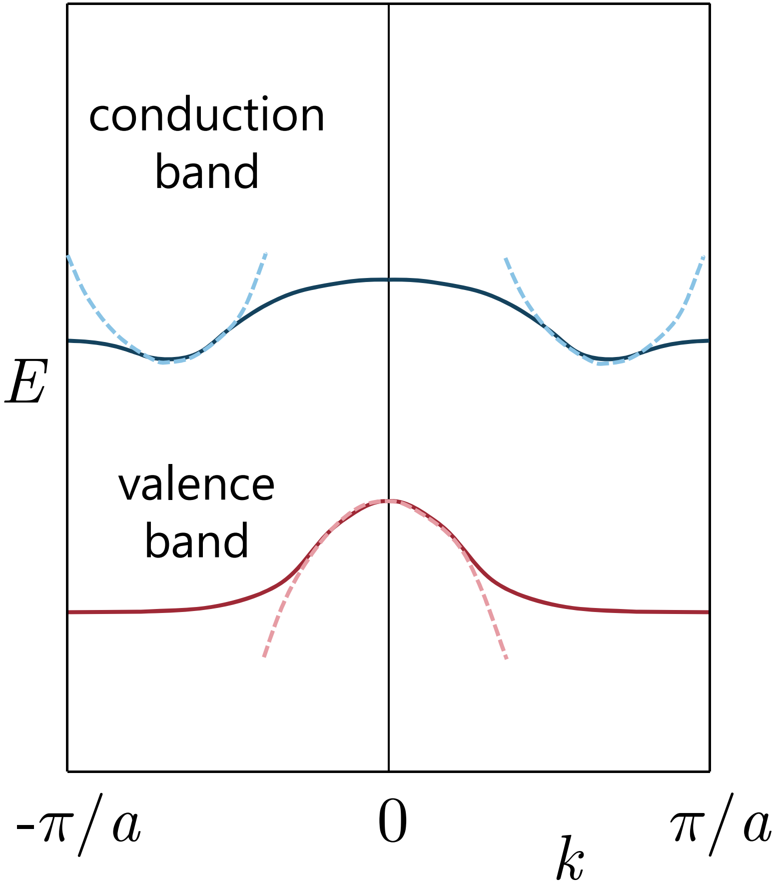
in which the lowest minimum in the conduction band

is *not* at the same k as as

the highest maximum in the valence band

is said to show an

indirect band gap



Particles, atoms, and crystals
6

Band structures in three dimensions

Modern physics for engineers

David Miller

Bloch theorem in two and three dimensions

For two-dimensional or three-dimensional crystals

we presume that we can extend the ideas by writing

$$\psi(\mathbf{r}) = u(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$$

where the unit cell function $u(\mathbf{r})$

is the same in every unit cell of the crystal

in all two or three directions

and the components of the wavevector $\mathbf{k}$

each obey relations similar to $k = \dfrac{2n\pi}{Na}, \;\; n = 0, \pm 1, \pm 2, \ldots \pm \dfrac{N}{2}$

but with (possibly different) “repeat lengths” a for each direction

Band structures in 2D and 3D

- We can construct band structures for two- and three-dimensional (2D and 3D) crystals
  - in similar ways to those for one dimension (1D)
- Such crystals can be more complicated than those for 1D
  - with potentially more complicated forms of unit cells

Band structures in 2D and 3D

To plot a band structure for a 3D crystal

- we would need a four-dimensional diagram
  - three dimensions for the components of a vector **k**
    - and a fourth dimension to indicate the corresponding energies

Brillouin zone in 3D

Before plotting band structures

- we need to understand
  - what form the Brillouin zone takes
    - in higher dimensional crystals

The Brillouin zone itself for a three dimensional crystal

- will be a three-dimensional shape
  - as a function of the components of $\mathbf{k}$
  - and that shape depends on the form of the crystal lattice

Brillouin zone in 3D

The Brillouin zone for the diamond or zinc-blende lattice

can take this shape

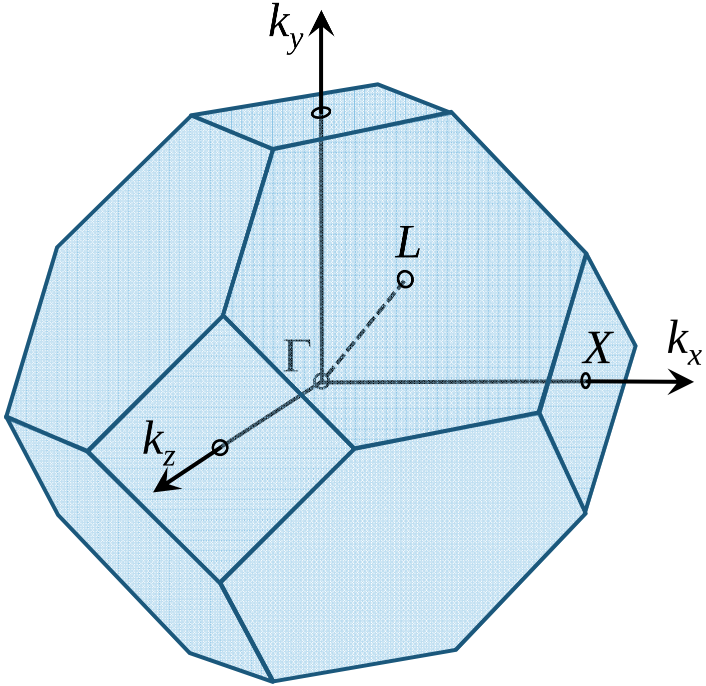
when we plot as a function of $\mathbf{k}$

Two important directions are

X – along one of the x, y, or z coordinate directions

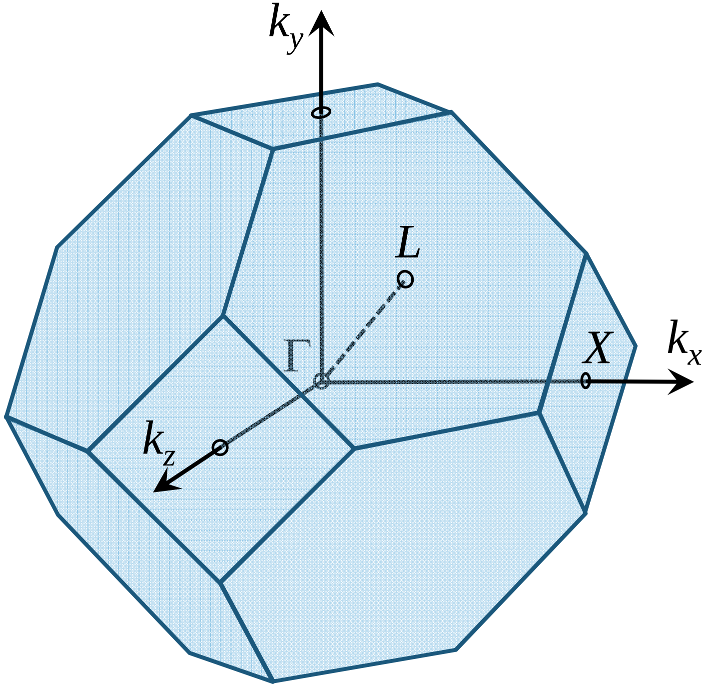
L – along one of the cube space diagonals

The center is the Γ (gamma) point



Band structures for 3D crystals

- At least as a first useful representation of band structure
  - typically the band structure is calculated only along a few directions
    - such as along the lines from the Γ point (at the center of the Brillouin zone)
      - to the X point and the L point



Particles, atoms, and crystals
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Plotting actual band structures

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Plotting band structures

- We typically only plot
  - the last few “full” bands and the first few “empty” bands
    - and/or any partially full bands
- These are the ones of most technological interest
  - Bands associated with deeper, “core” atomic levels
    - typically do not participate in operation of devices

Plotting band structures

One useful simplification is that

- band structures are essentially always symmetric about $k = 0$, which simplifies plotting
  - This is called Kramers degeneracy

Si band structure

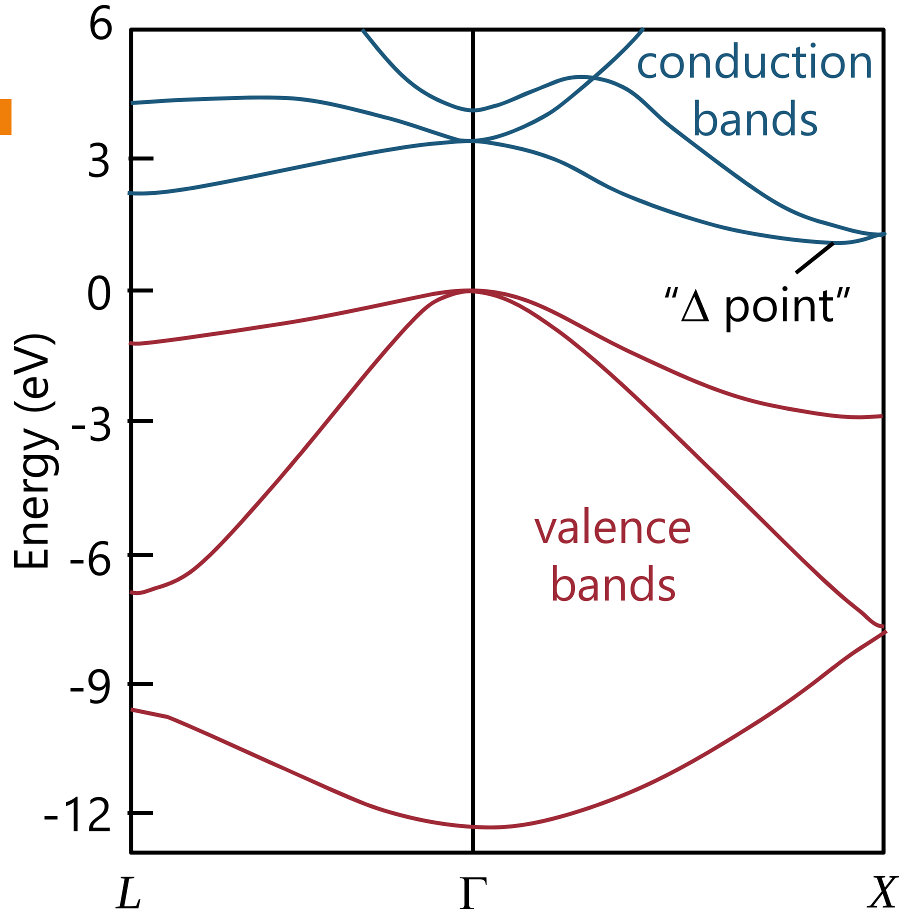
Because band structures are symmetric around $k = 0$

by "Kramers degeneracy"

we need only show one half of the band structure

so we can use the other half of the figure

for the band structure in another direction

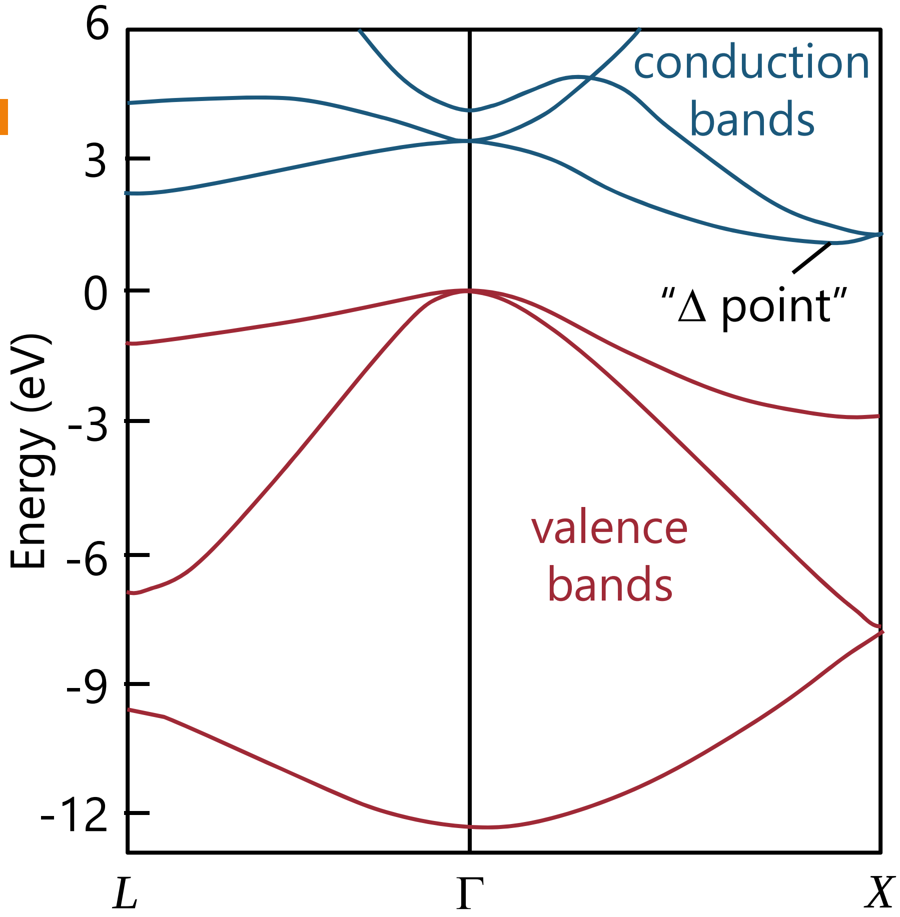


after K. S. Sieh and P. V. Smith, Phys. Status Solidi (b) **129**, 259 (1985)

Si band structure

In contrast to our one-dimensional coupled well cases

- we have multiple bands here
  - some of which do overlap in energy
    - and bands sometimes coincide with one another at specific points

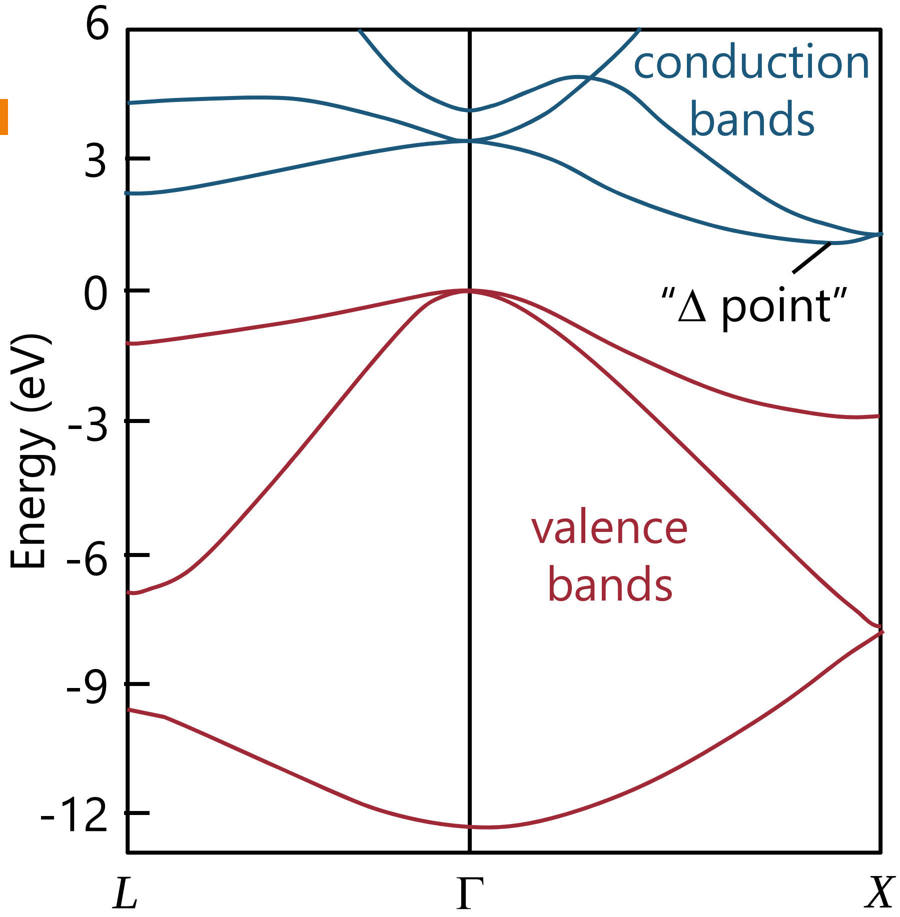


after K. S. Sieh and P. V. Smith, Phys. Status Solidi (b) **129**, 259 (1985)

Si band structure

Sometimes, such as the lowest conduction band in silicon

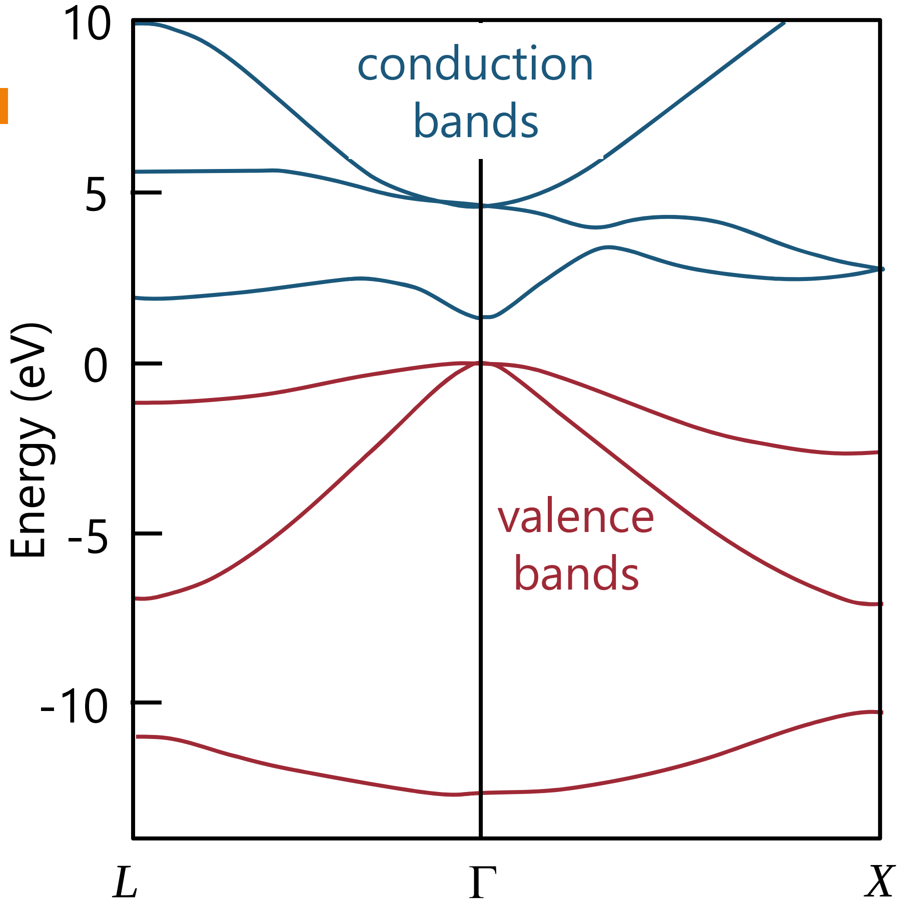
- the lowest energy in the band is neither at the center nor an edge of the Brillouin zone
  - For silicon, the position of this minimum energy is referred to as
    - the Δ (delta) point



after K. S. Sieh and P. V. Smith, Phys. Status Solidi (b) **129**, 259 (1985)

GaAs band structure

- The upper valence bands of GaAs
  - are similar to silicon
    - but the conduction band minimum is at the Γ point
- So GaAs is a direct gap semiconductor
  - unlike Si
    - which is indirect



after M. Rohlfing, P. Krüger and J. Pollmann, Phys. Rev. B **48**, 17791 (1993)

Real band structures

For all such band structures

- for N atoms in the crystal
  - each band has N states in it
    - (multiplied by 2 if electrons of different spins also have the same energy)
  - and all bands have the same set of equally spaced $\mathbf{k}$ values associated with them

Band structures

For Group IV materials like carbon, silicon and germanium

- in the outer, highest energy orbitals
  - we are dealing with the combination of 2 "s" orbitals and 6 "p" orbitals
    - where we include both spin states
      - which gives 8 orbitals that together hold 4 electrons

Band structures

Putting atoms of one such type together to form a crystal

- leads to the formation of two sets of bands
- Loosely, one of these sets of bands is based on
  - "bonding" versions of the combined orbitals
    - and the other is based on "antibonding" versions of those same orbitals
- The bonding versions can have lower energy than the antibonding versions

Band structures

If those “bonding” and “antibonding” sets of bands do not overlap in energy

for these Group IV materials

the bonding versions will be essentially fully occupied

to give what are called the “valence” bands

and the antibonding versions will be essentially unoccupied

to give what are called the “conduction” bands

Band structures

Such non-overlapping band behavior
  - with a band gap energy between them
    - is characteristic of a semiconductor or an insulator

In practical terms
  - the GaAs material
    - and its various other III-V cousins
      - behave like effective Group IV materials
        - with similar forms of band structures

Particles, atoms, and crystals
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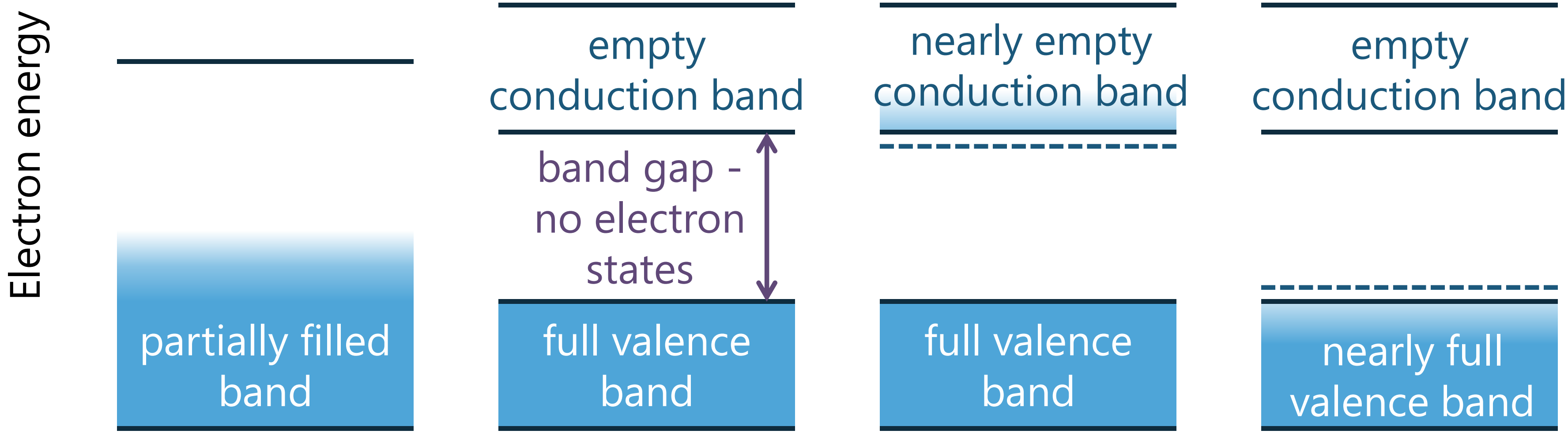
Metals, semiconductors and insulators

Modern physics for engineers

David Miller

Metals, insulators and semiconductors



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

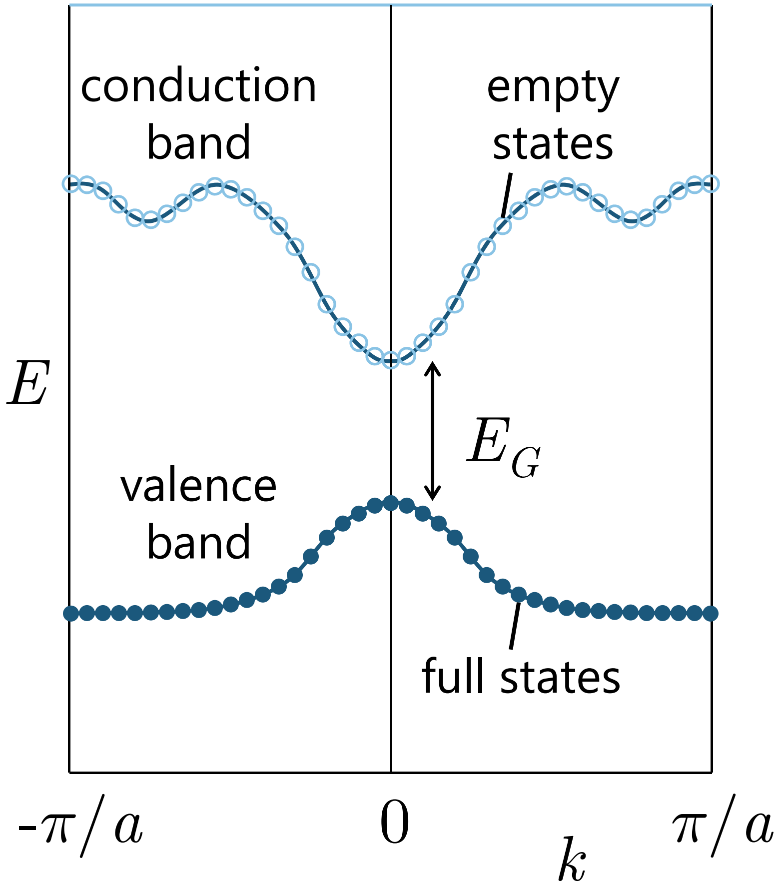
p-doped semiconductor

missing free electrons in valence band
allow conduction

Semiconductors and insulators

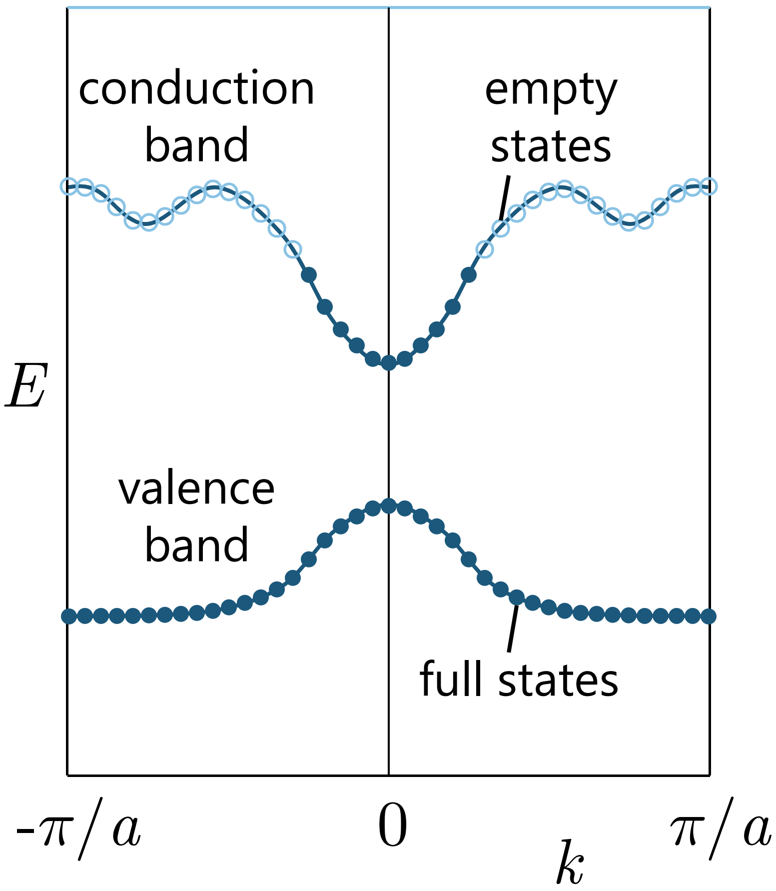
Semiconductors and insulators
- have an (almost) completely full band
  - the valence band

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



Metals

- Because of the number of electrons in the metal atoms
  - the highest band is partially full of electrons e.g., half-full
  - even at zero temperature
- Metals may or may not have band gaps
- Applying a field “skews” the electron distribution
  - allowing metals to conduct electricity well



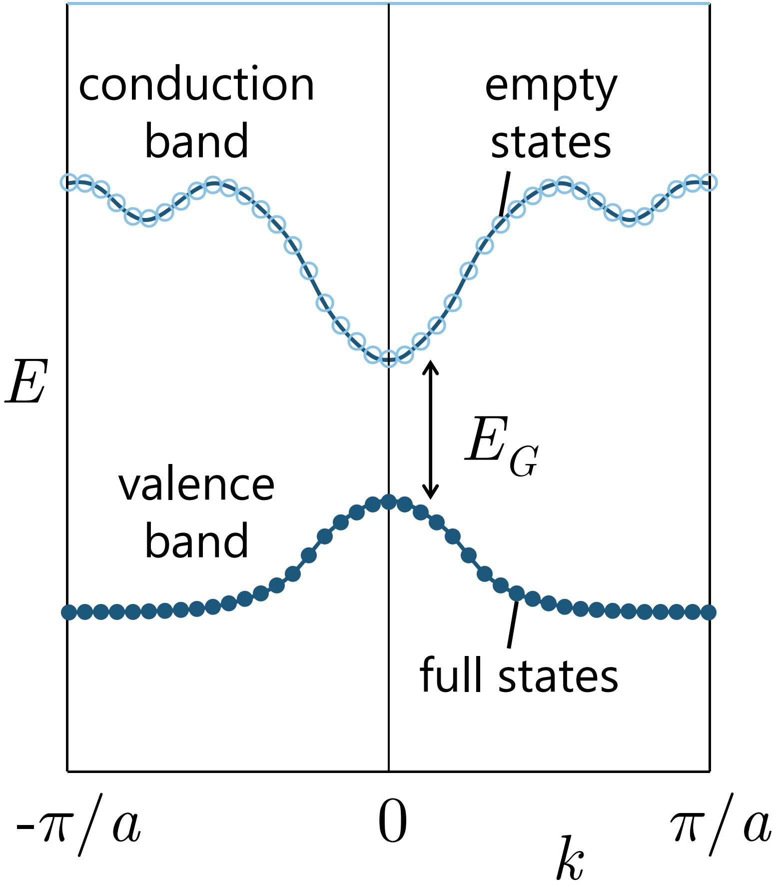
Semiconductors and insulators

Note that

- an empty band does not conduct electricity
  - There are no mobile electrons

Also

- a full band does not conduct electricity
  - The electrons cannot change states within the band
    - because all the states are full



Semiconductors and insulators

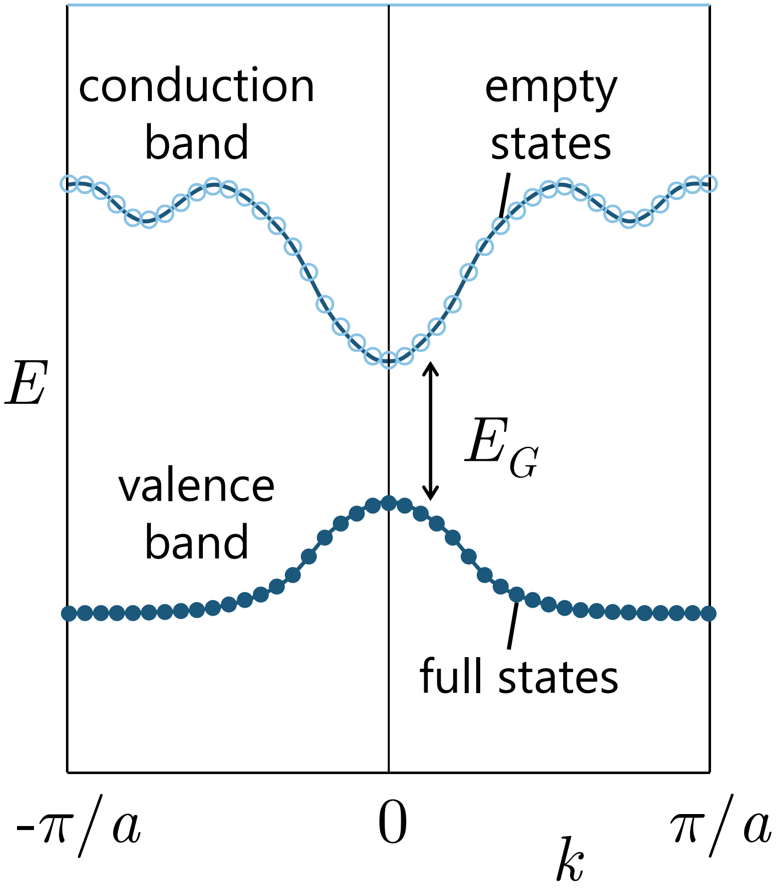
The difference between semiconductors and insulators is primarily that

insulators have such a large bandgap energy

that there is negligible thermal excitation of electrons

from the valence band

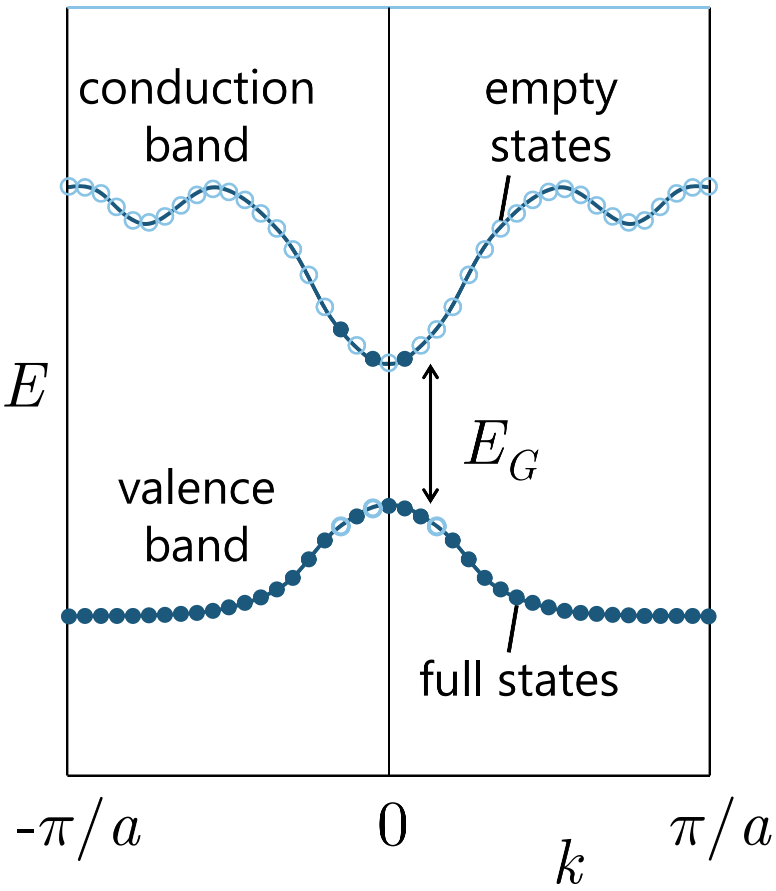
to the conduction band



Semiconductors

At finite temperatures in a semiconductor

- a small number of electrons are excited
  - from the valence band
    - to the conduction band



Semiconductors

These electrons in the conduction band

and

absences of electrons or “holes” in the valence band

can conduct electricity within their bands

So semiconductor materials conduct electricity weakly

hence the name