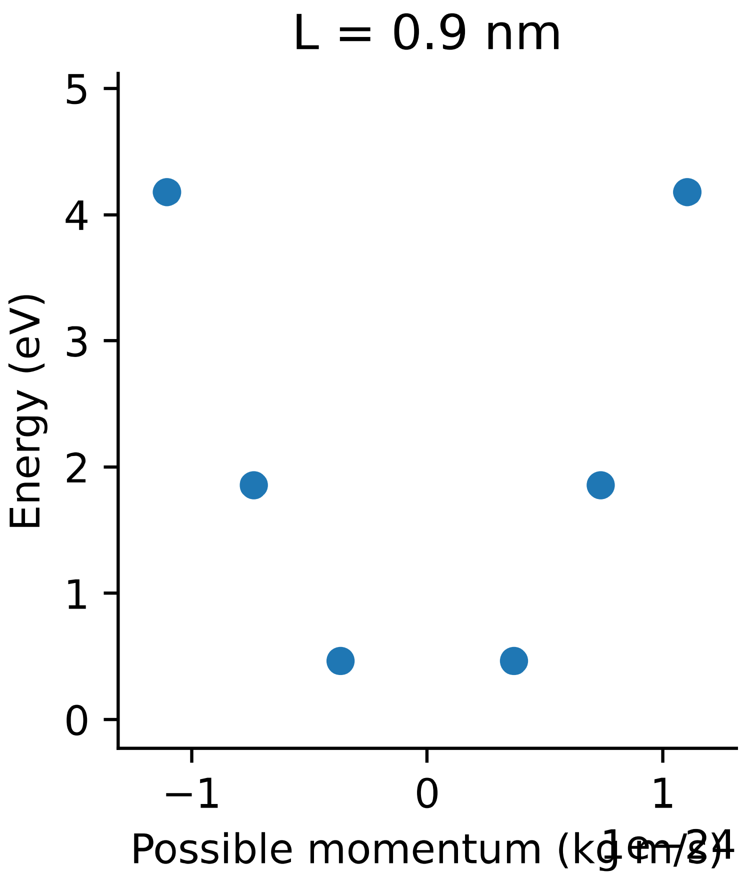
Lecture 12: Band structure

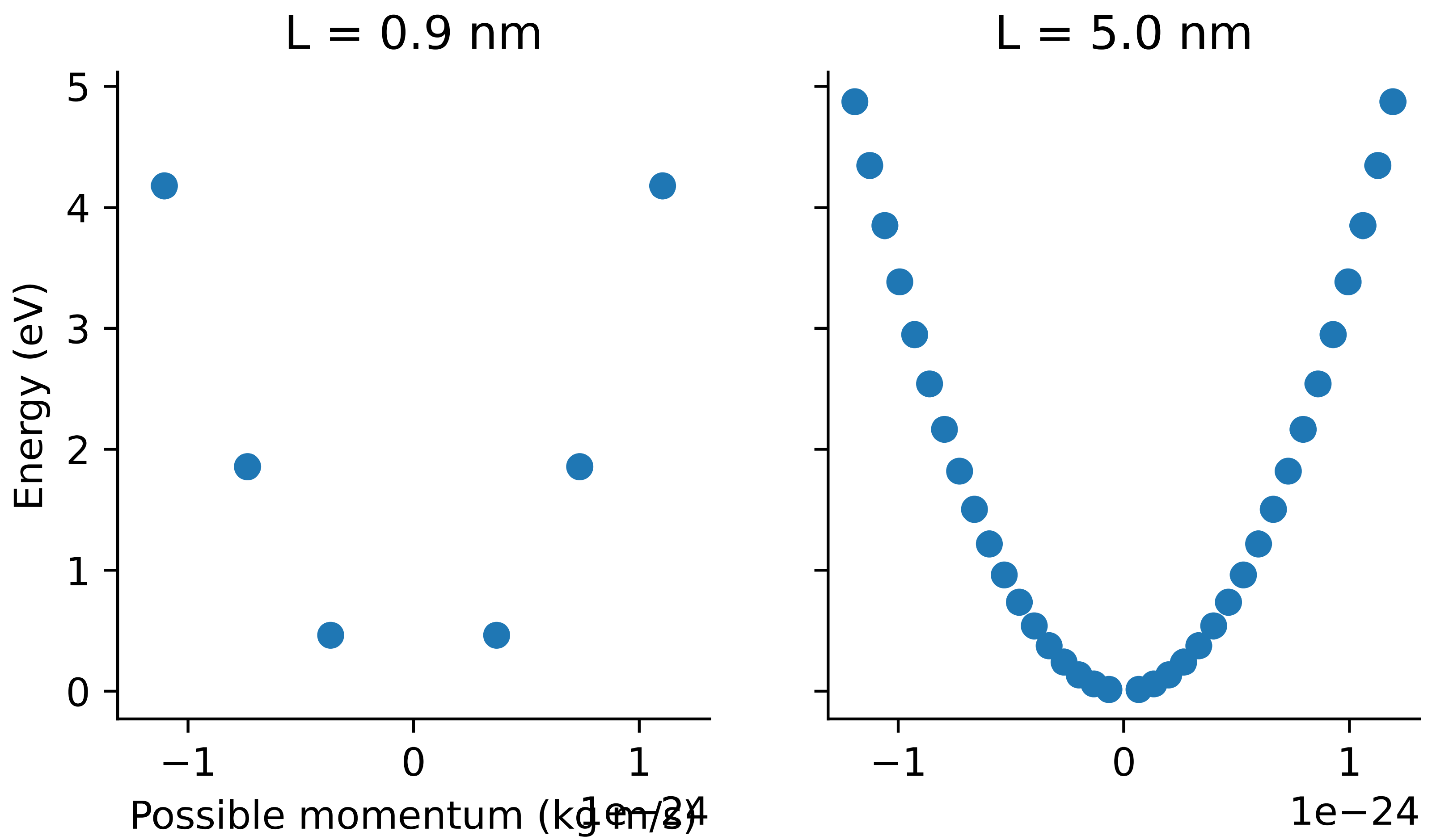
Ground state of Ne (10 electrons)

Name an atom, any atom (in the first 3 rows)

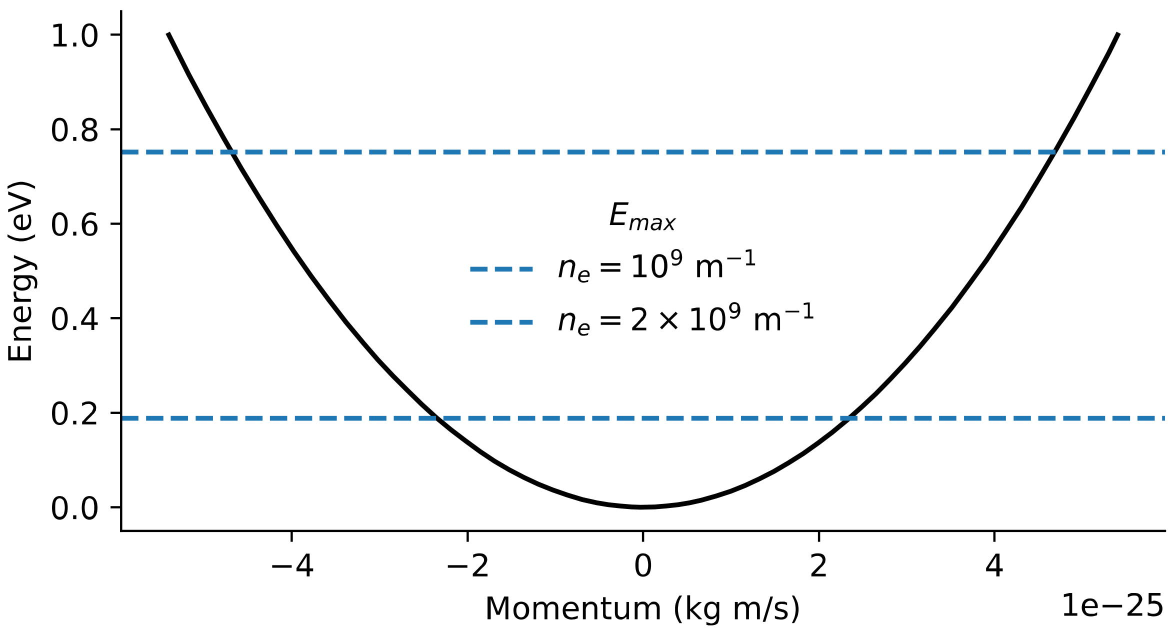
Infinite square well: momentum versus energy



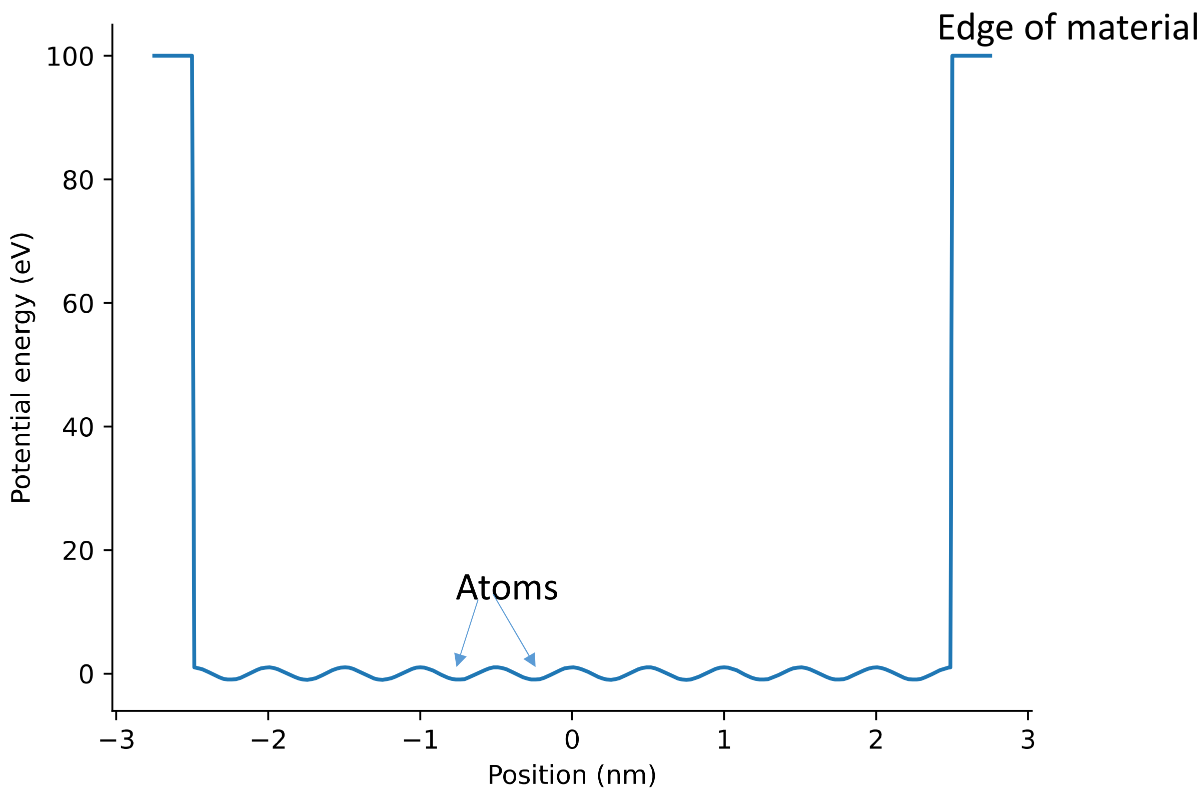
Infinite square well: fermi level



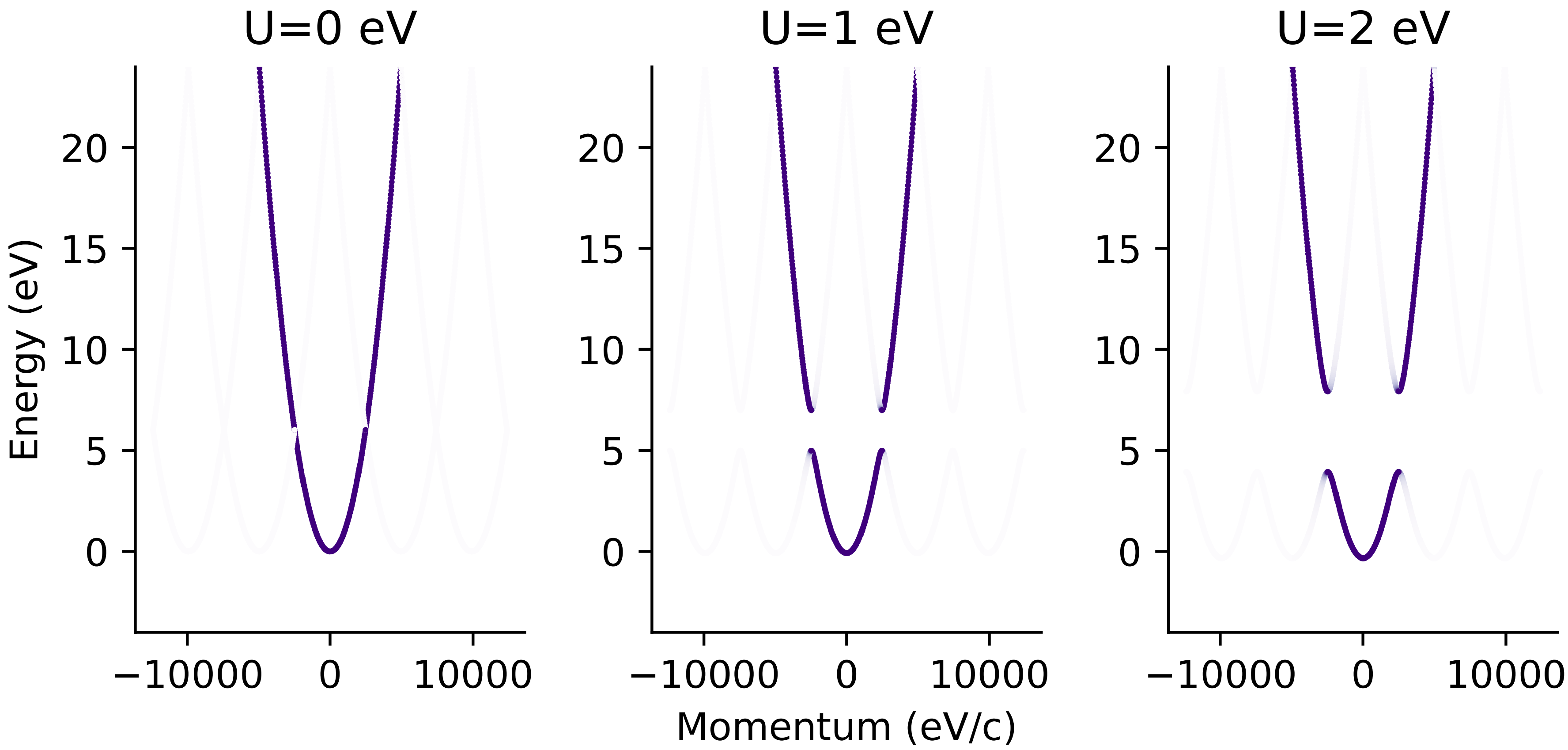
Fermi Level: the infinite limit



Slightly more accurate model

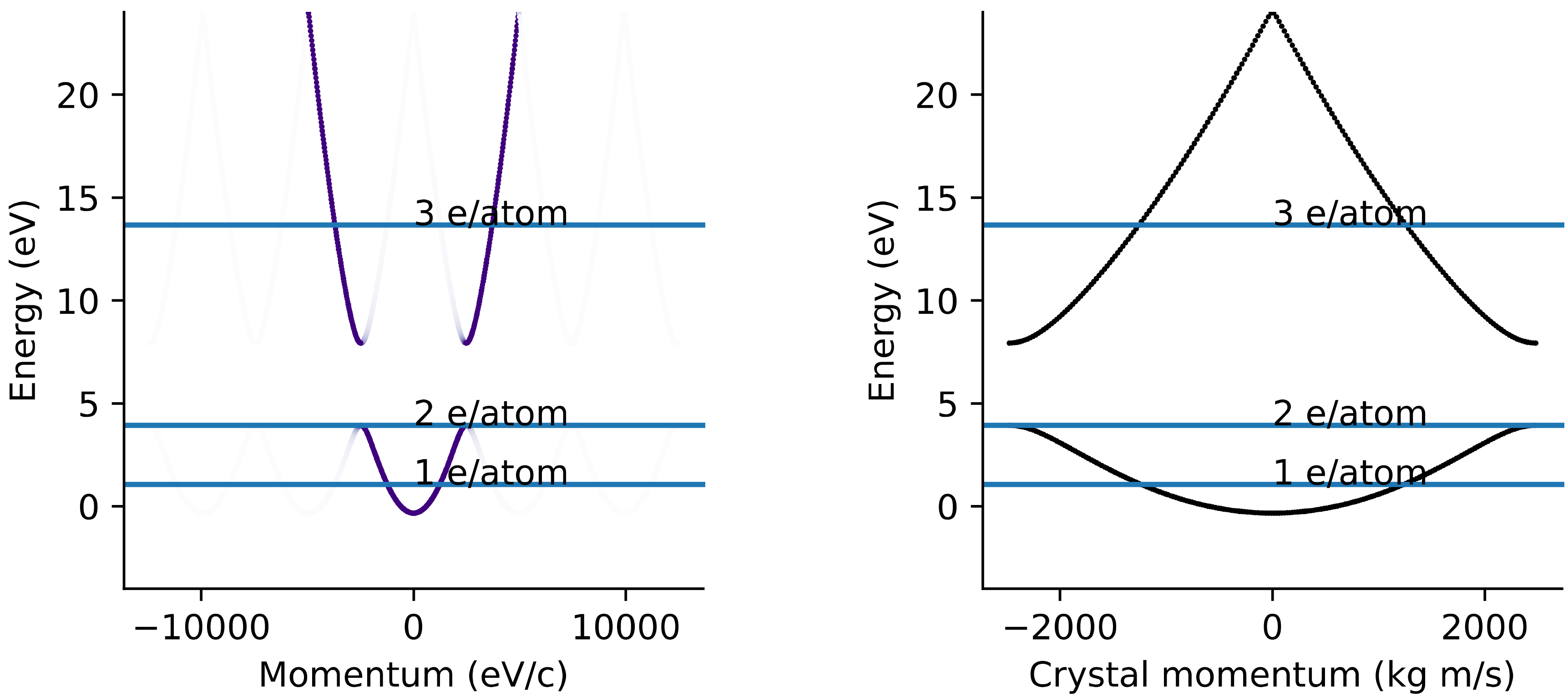


Gaps

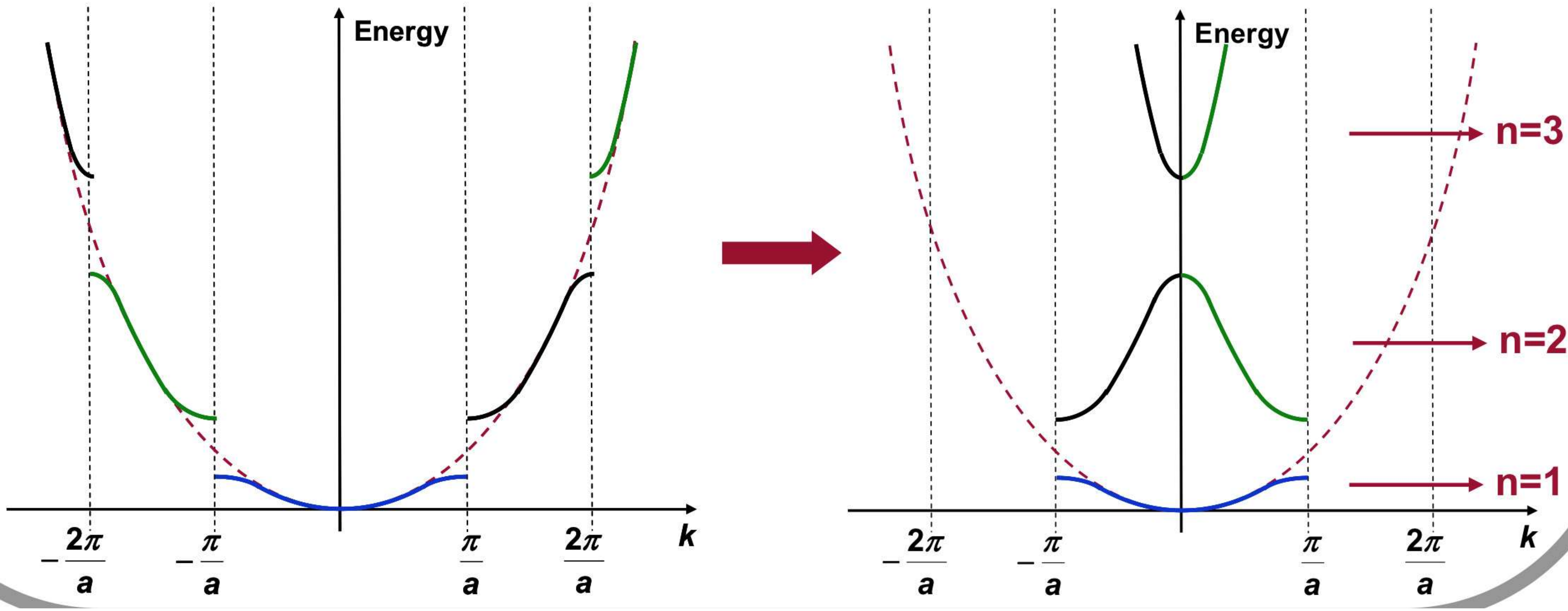


U=0 eV
U=1 eV
U=2 eV
Energy (eV)
20
15
10
5
0
−10000
0
10000
Momentum (eV/c)

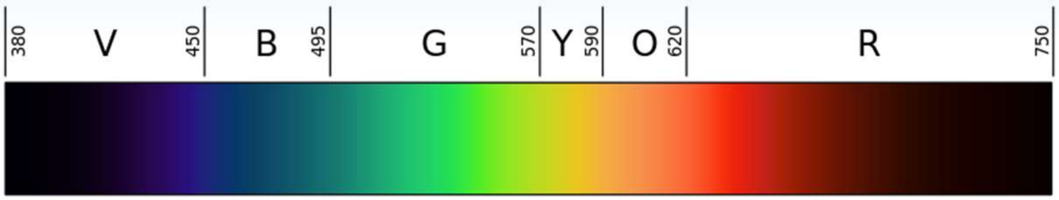
Typical band plots



Band Folding



Energy gaps



This is a piece of silicon. Which is true?

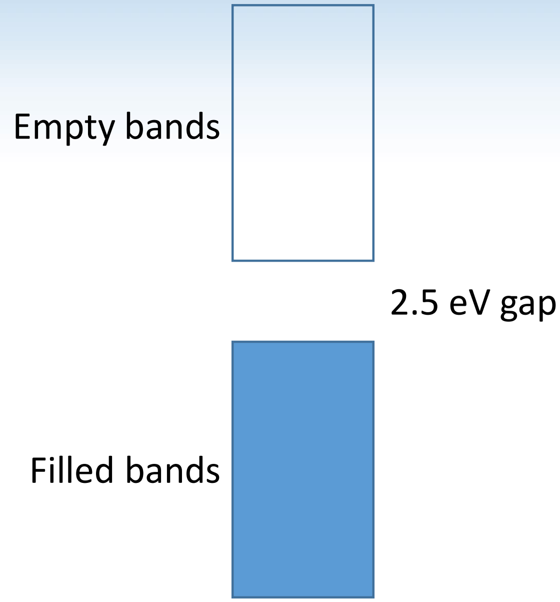
$$a)\ E_g = \frac{hc}{380\ nm}$$
$$b)\ E_g = \frac{hc}{750\ nm}$$
$$c)\ E_g > \frac{hc}{380\ nm}$$
$$d)\ E_g < \frac{hc}{750\ nm}$$

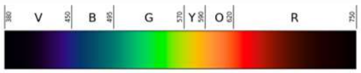
Energy levels

A material has energy levels as diagrammed.

What is true about the material?

a) It will conduct electricity very well.
b) Red light will pass through it.
c) Blue light will pass through it.





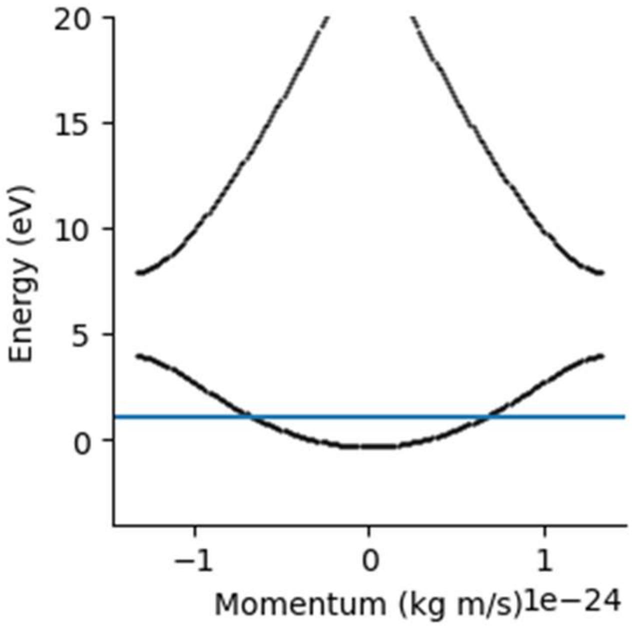
Color	Wavelength	Frequency	Photon energy
Violet	380–450 nm	680–790 THz	2.95–3.10 eV
Blue	450–485 nm	620–680 THz	2.64–2.75 eV
Cyan	485–500 nm	600–620 THz	2.48–2.52 eV
Green	500–565 nm	530–600 THz	2.25–2.34 eV
Yellow	565–590 nm	510–530 THz	2.10–2.17 eV
Orange	590–625 nm	480–510 THz	2.00–2.10 eV
Red	625–740 nm	405–480 THz	1.65–2.00 eV

Energy gaps

Which is true for a piece of glass?

$$a)\, E_g = \frac{hc}{380\ nm}$$
$$b)\, E_g = \frac{hc}{750\ nm}$$
$$c)\, E_g > \frac{hc}{380\ nm}$$
$$d)\, E_g < \frac{hc}{750\ nm}$$

Pokal, from Ikea

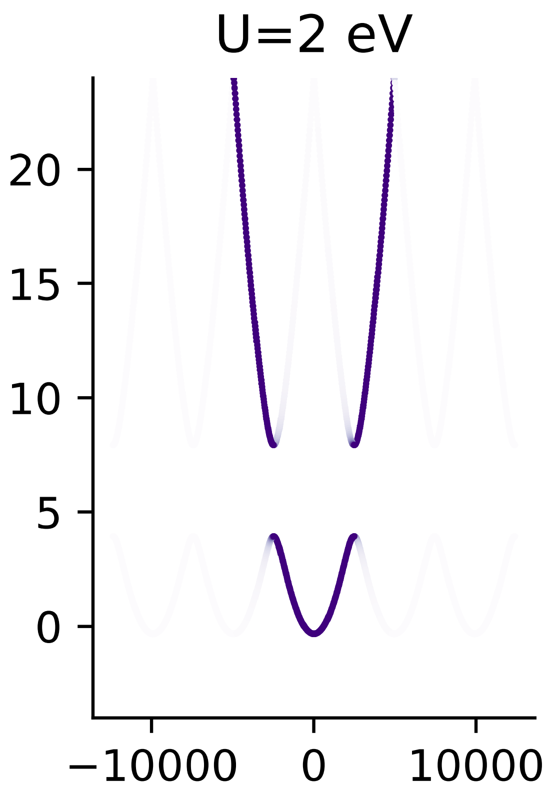


A material has a number of electrons such that in the ground state, all states below the line are occupied with electrons, and all above are unoccupied.

Is this material metallic (does it conduct electricity easily when an electric field is applied)?

a) Yes
b) No

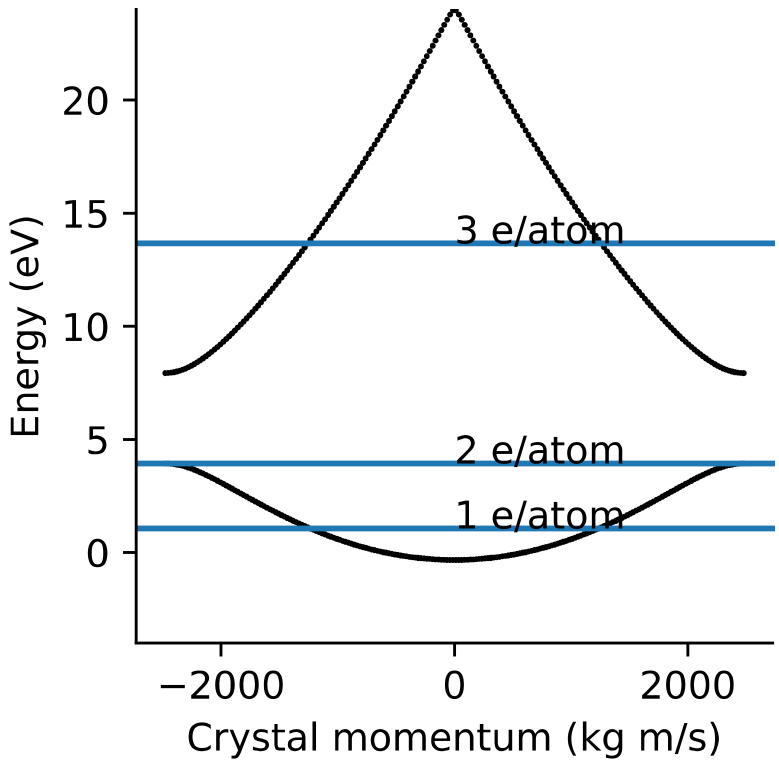
Conductor vs insulator



Roughly what Fermi level energy would result in an insulator?

a) 0 eV
b) 4 eV
c) 7 eV
d) 15 eV

Insulators and metals



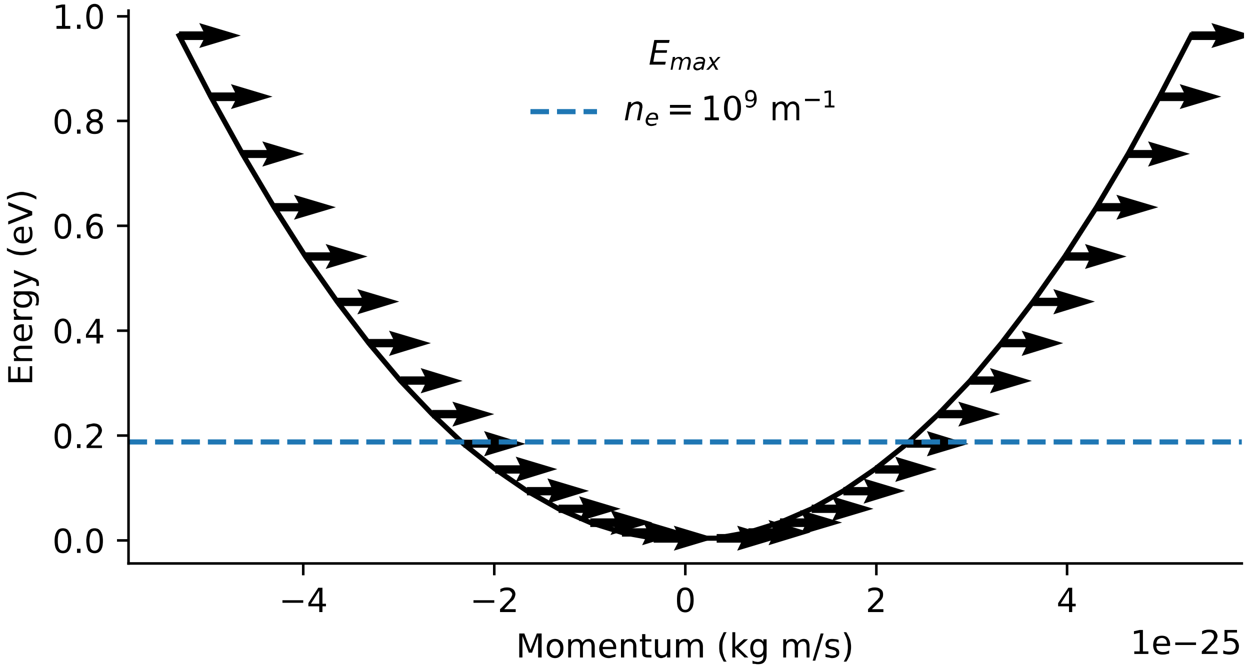
What electron density corresponds to an insulator?

a) 1 e/atom
b) 2 e/atom
c) 3 e/atom

Semiclassical example

Consider a completely free electron; approximate it as a classical particle. At t=0, it starts at rest in an electric field $\mathcal{E}$. How fast will it be moving at time t?

Conduction of electrons: semiclassical model

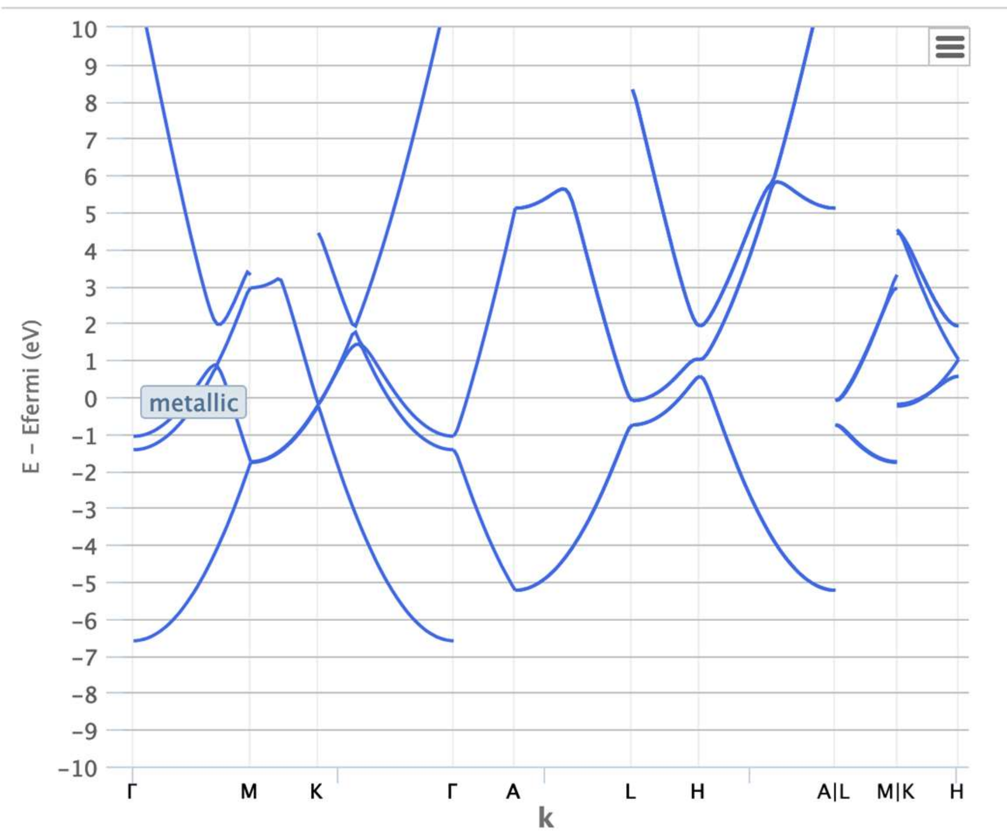


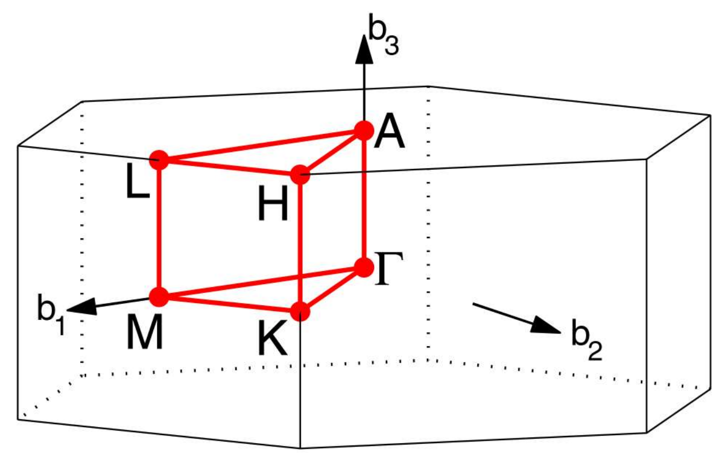
Question from last night: Why is magnesium metallic?

The bands cross in Mg, unlike our simple model!

So there is no gap.

If the bands didn't cross, it would be an insulator.





HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Band structure from materialsproject.org – estimated band structures for almost all known crystalline materials

Summary

Electron levels + filling determine the properties of materials

Gap: energy it takes to get from the ground state to the first excited state
Metals: Zero gap
Insulators: Non-zero gap

Semi-classical model of electrons: $q\mathcal{E} = \frac{dp}{dt}$; gaps block changes in momentum