Fundamentals of Solid State Physics

Electronic Properties - Metals and Insulators

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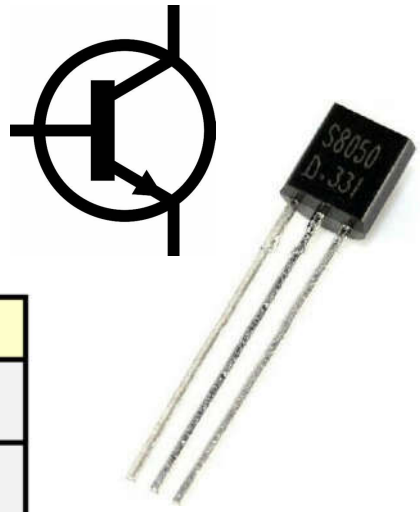
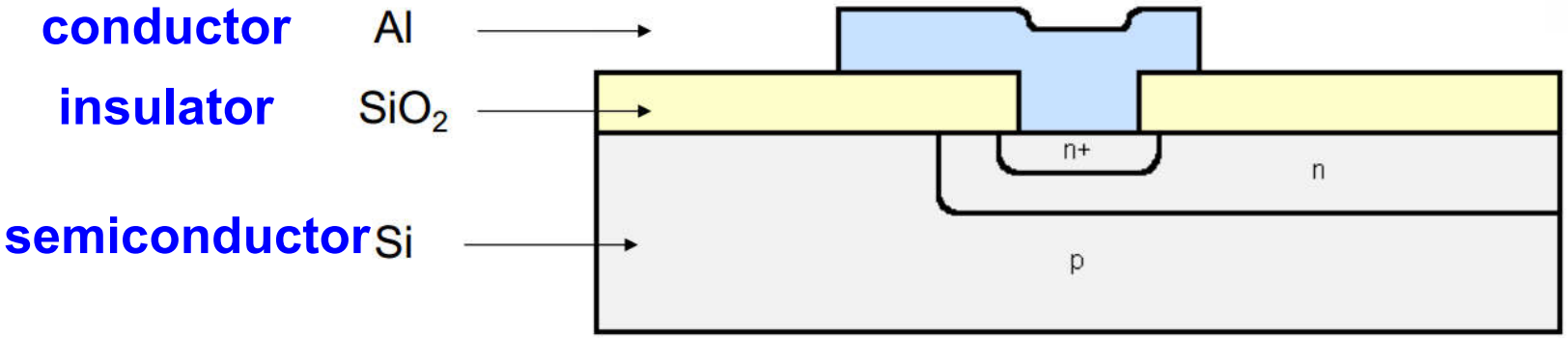
Electronic Properties of Materials

CMOS transistor
- Complementary Metal-Oxide-Semiconductor



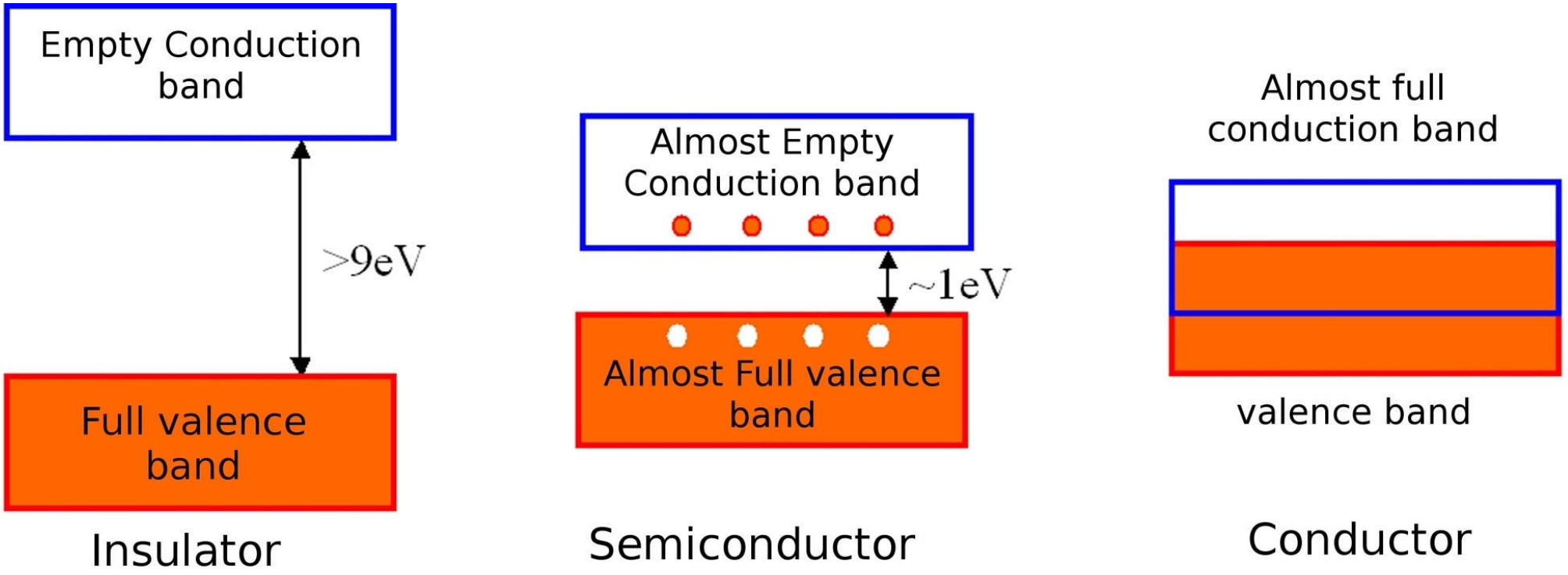


Metal

SiO_2

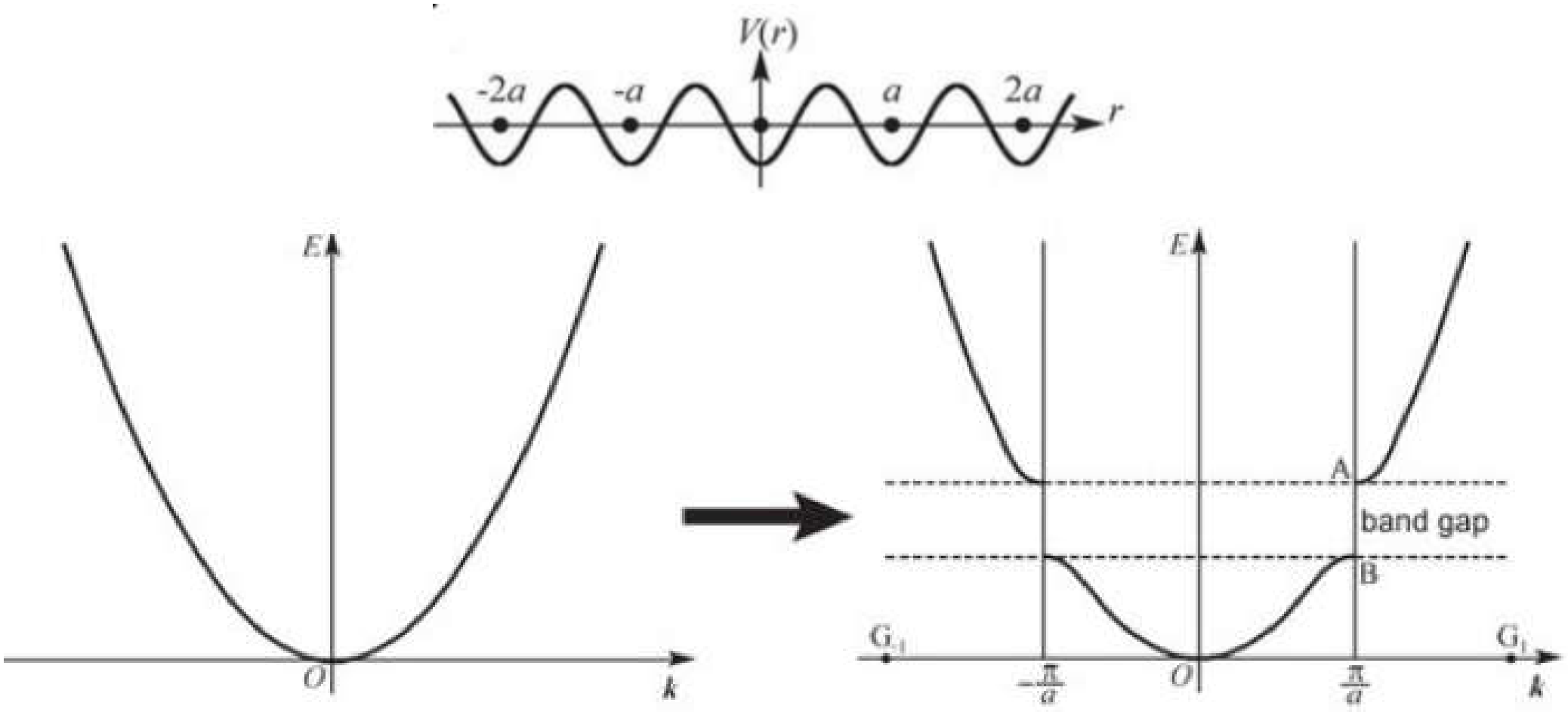
Silicon

Summary


Empty Conduction band
>9eV
Full valence band
Insulator
Almost Empty Conduction band
~1eV
Almost Full valence band
Semiconductor
Almost full conduction band
valence band
Conductor

Formation of Band Gaps

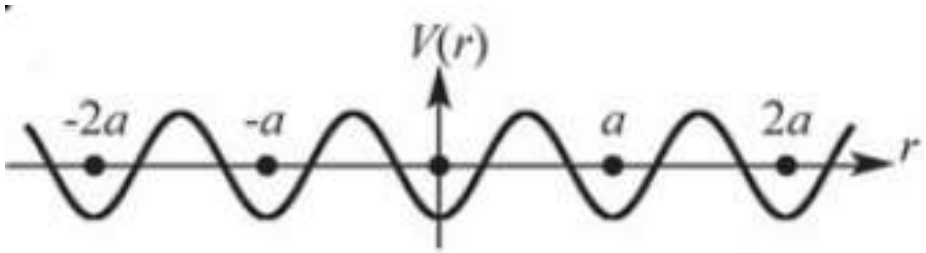
Free electrons are perturbed by a periodic potential

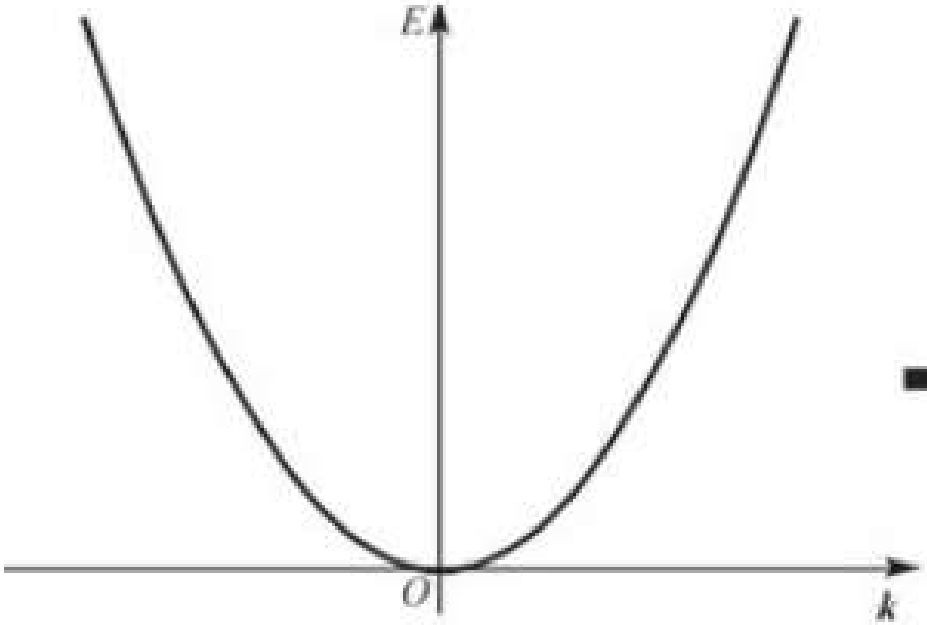


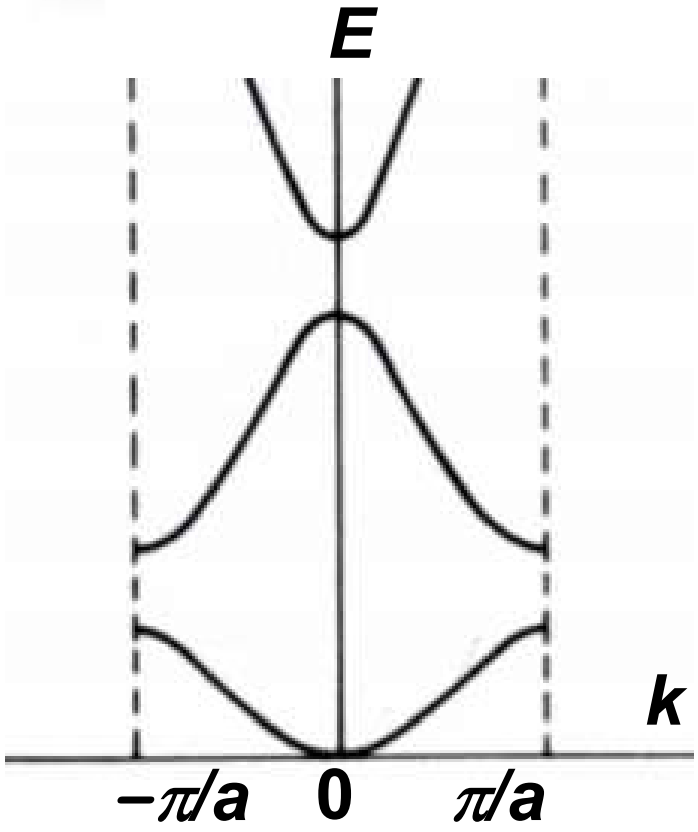
Q: Is it a metal or insulator?

Formation of Band Gaps

Free electrons are perturbed by a periodic potential







Q: Is it a metal or insulator?

State vs. Electron

energy state / level / orbital
能态 / 能级 / 轨道

determined by space, lattice, environments, ...

electron / phonon / ...
电子 / 声子 / ...

Energy States

How many energy states in each band?

$$N = 2 \cdot \frac{\text{size of FBZ}}{\text{density of } k \text{ points}}$$

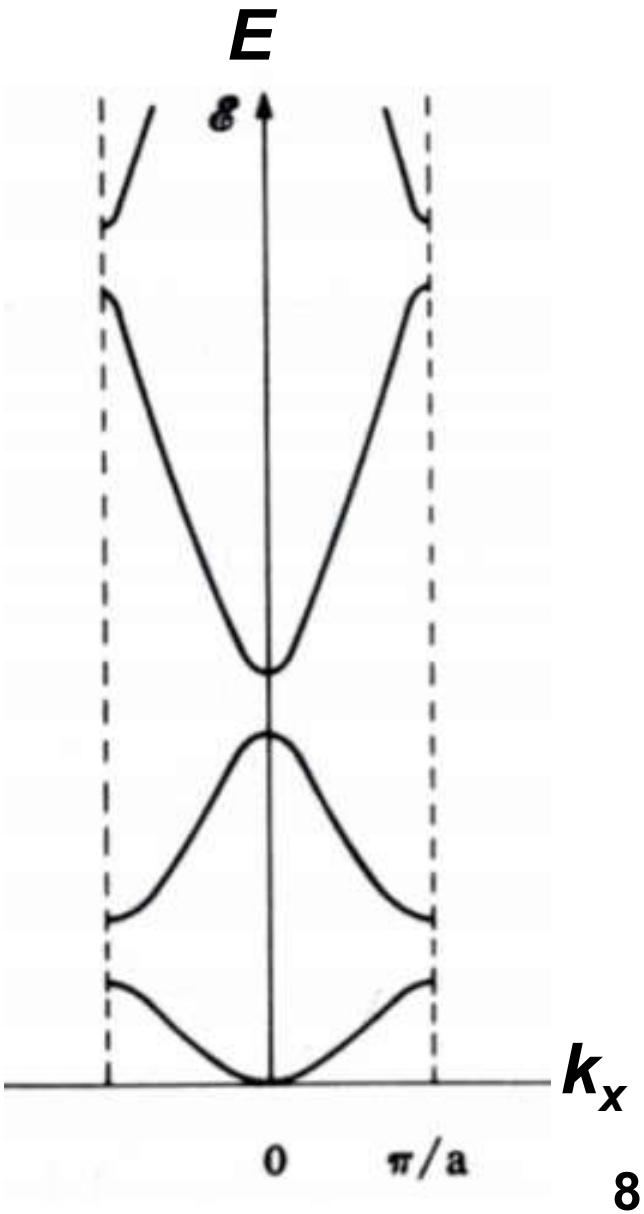
$$= 2 \cdot \frac{2\pi / a}{2\pi / L_x}$$

$$= 2\frac{L_x}{a}$$

$$= 2n$$

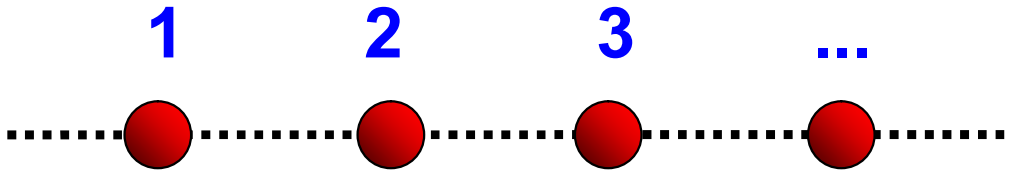
FBZ - First Brillouin Zone
***N* - total number of states**
***n* = *L/a* - number of primitive cells**

Q: How about 2D and 3D cases?



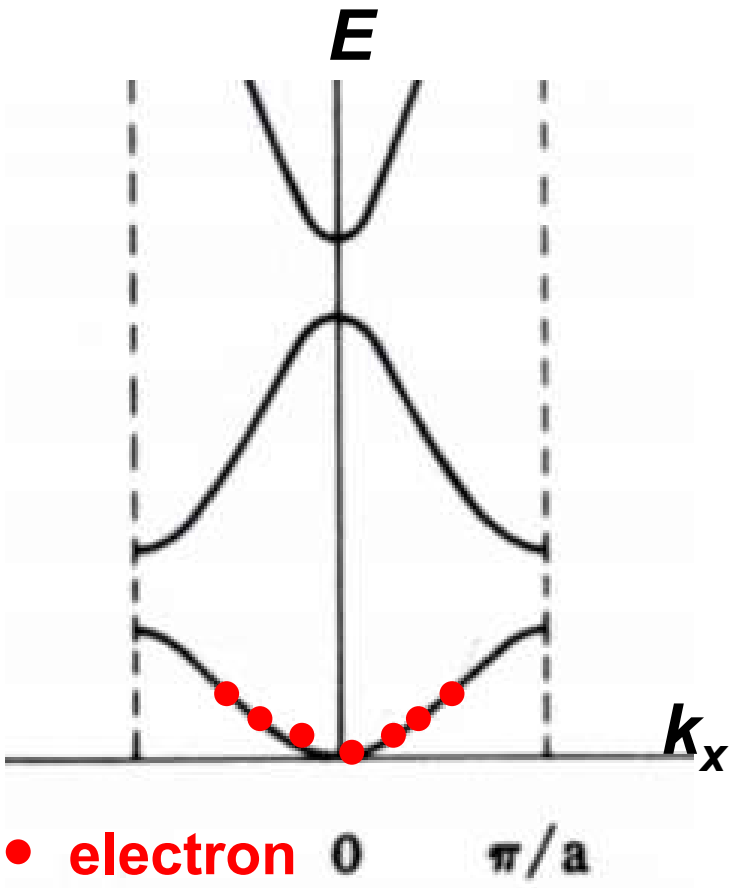
1D Chain of *Monovalent* Atoms

Each atom has *one* valence electron (Na, K, ...)



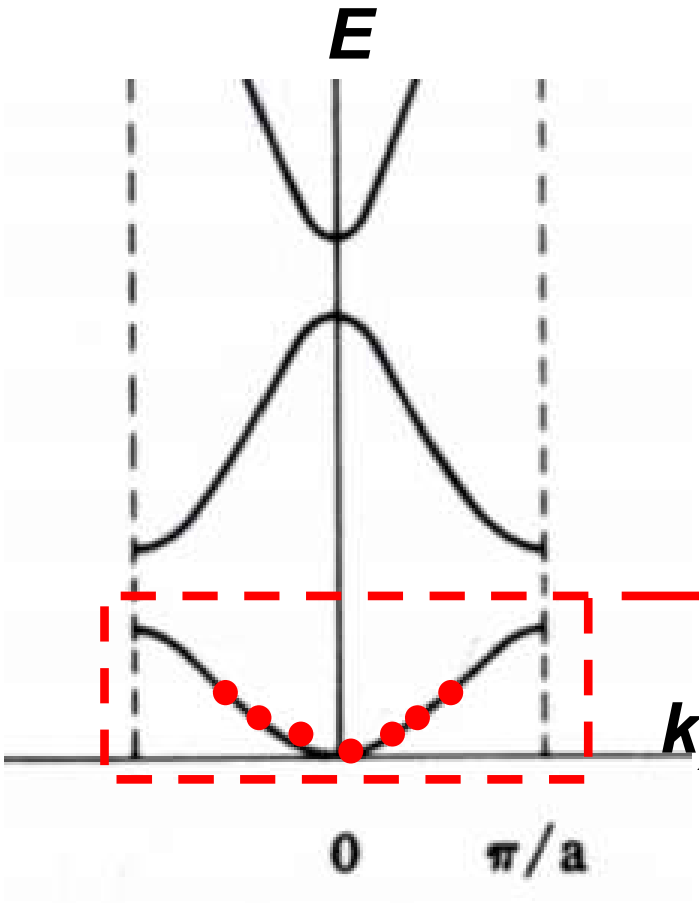
$N = 2n$
= total number of states

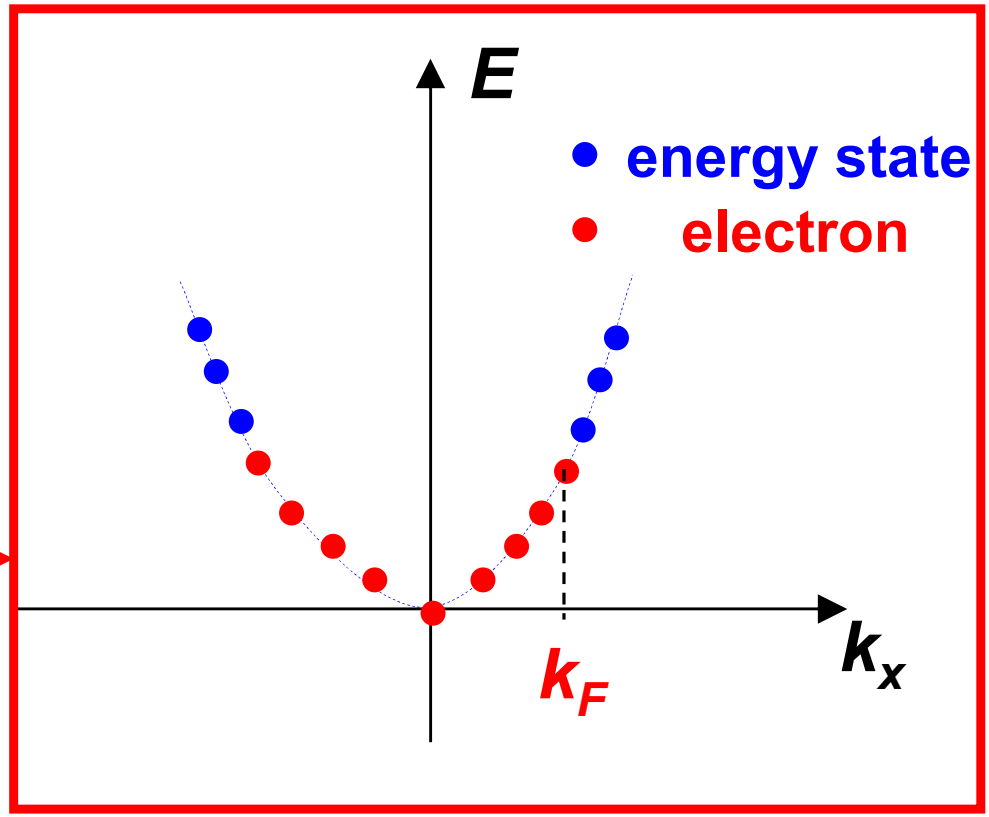
$n = L/a$
= number of primitive cells
= number of valence electrons



Electrons only fill half of the first band

1D Chain of *Monovalent* Atoms





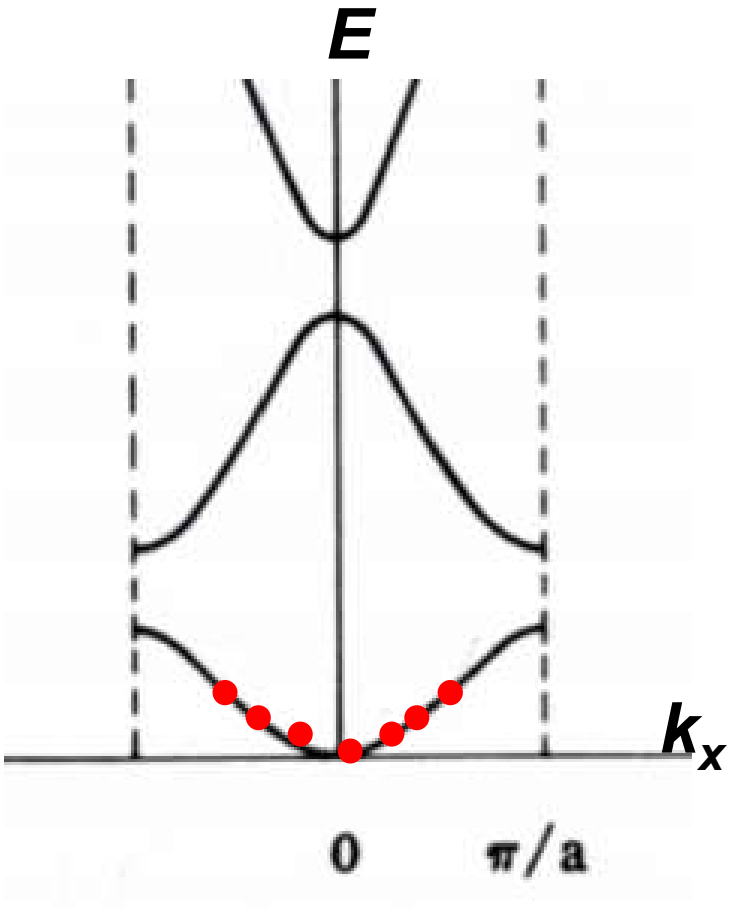
Electrons only fill half of the first band

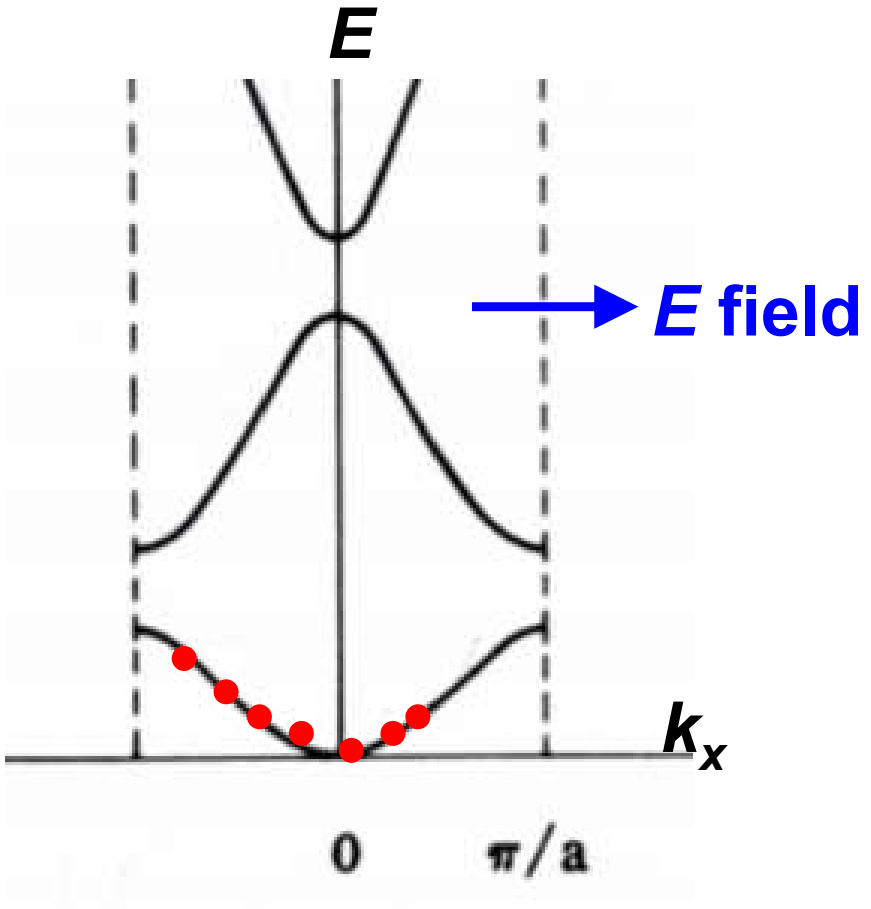
parabolic function

Free Electrons

Conductor

1D Chain of *Monovalent* Atoms





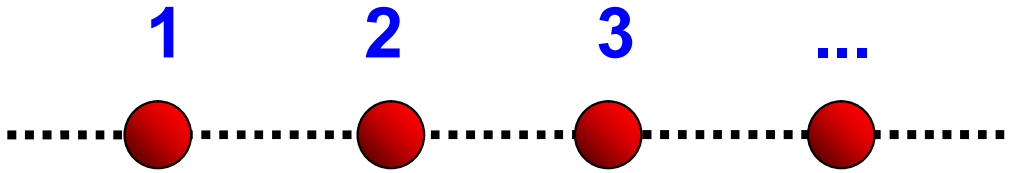
when $E = 0$, $v = 0$
no current

when $E \neq 0$, $v > 0$
electric current

$$\mathbf{j} = \sigma \mathbf{E}$$

1D Chain of *Divalent* Atoms

Each atom has *two* valence electrons (Mg, Ca, ...)

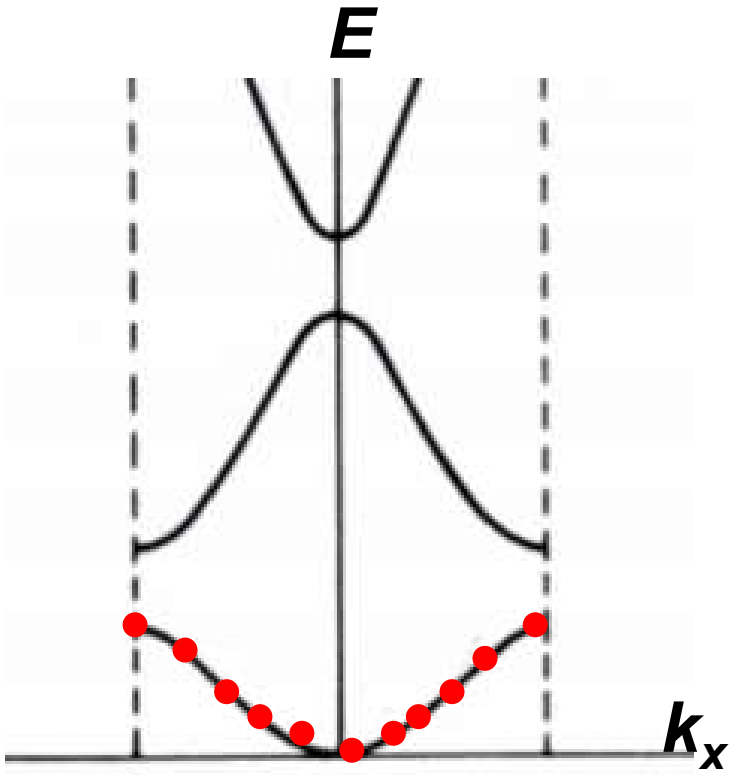


$N = 2n$

= total number of states

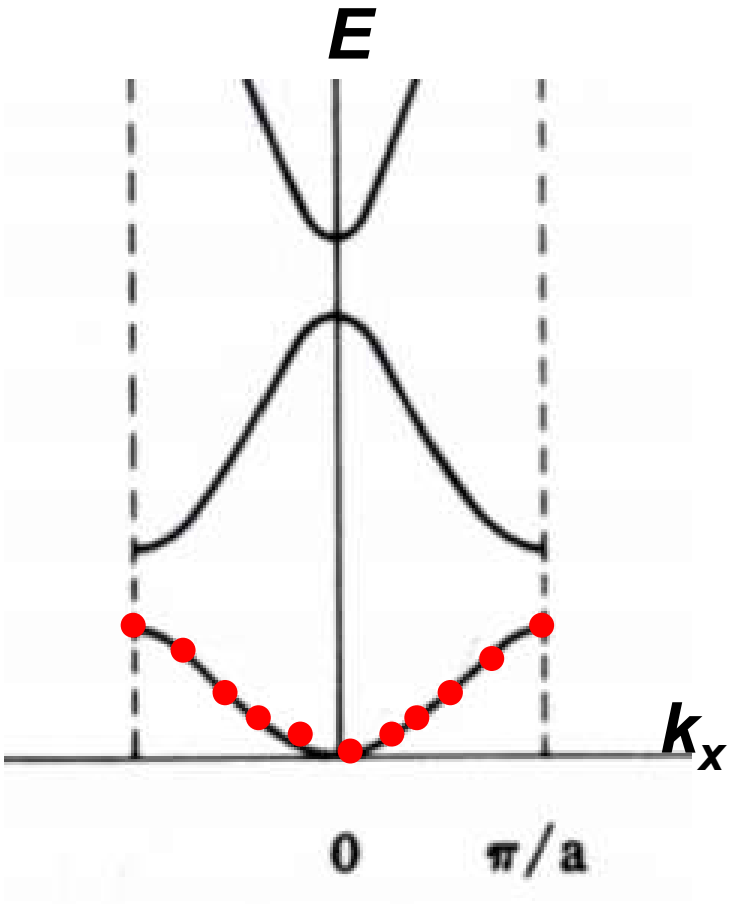
number of valence electrons

$= 2L/a = 2n$



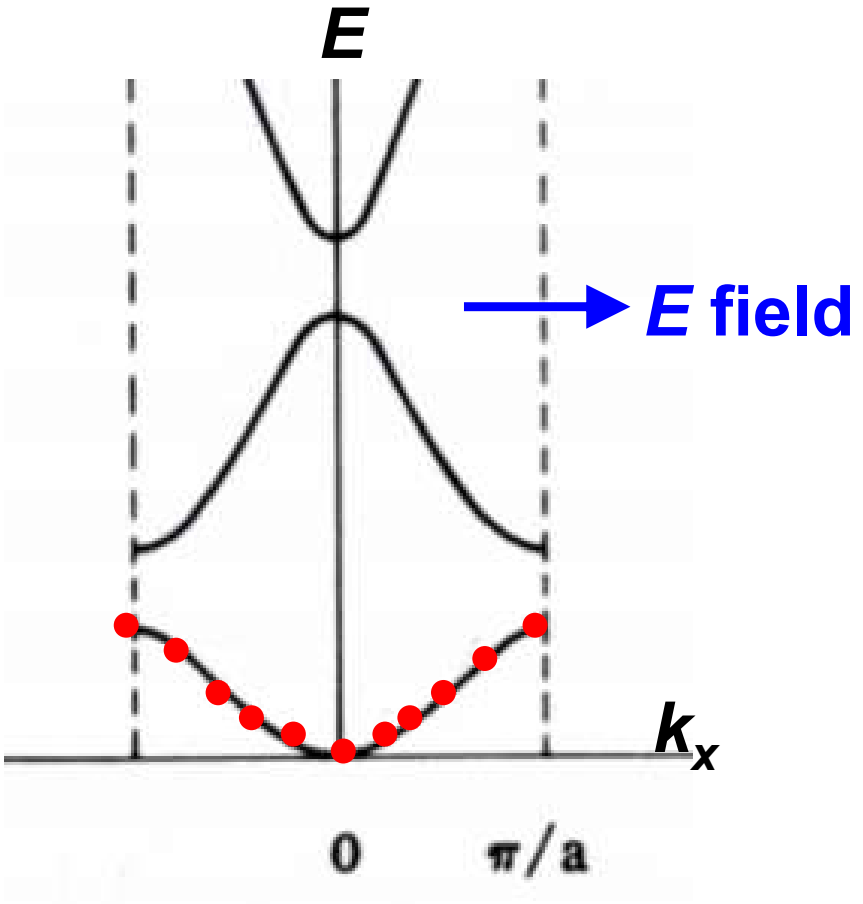
Electrons fill the entire band

1D Chain of *Divalent* Atoms



when $E = 0$, $v = 0$

no current



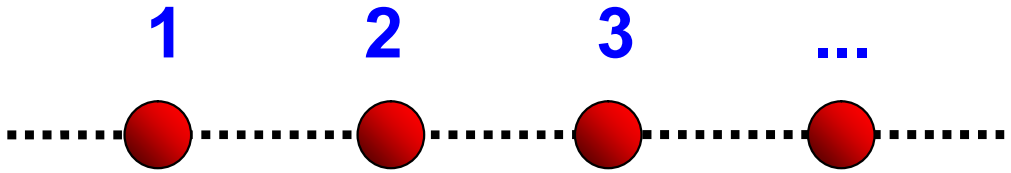
when $E \neq 0$, $v = 0$

no current

Electrons fill the entire band → *Insulator (at T = 0 K)*

1D Chain of *Trivalent* Atoms

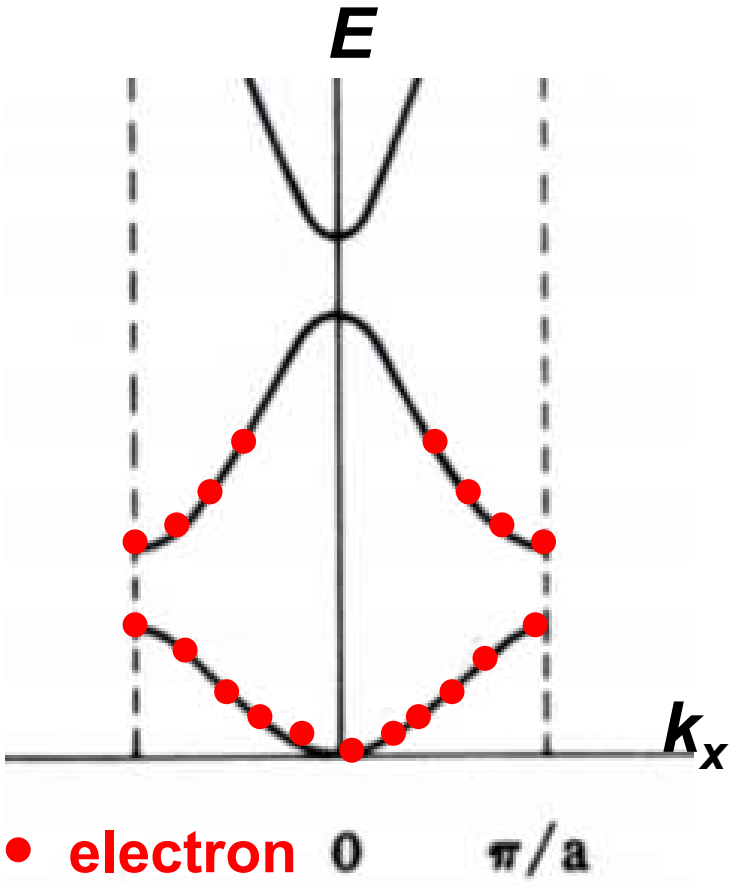
Each atom has *three* valence electrons (Al, Ga, ...)



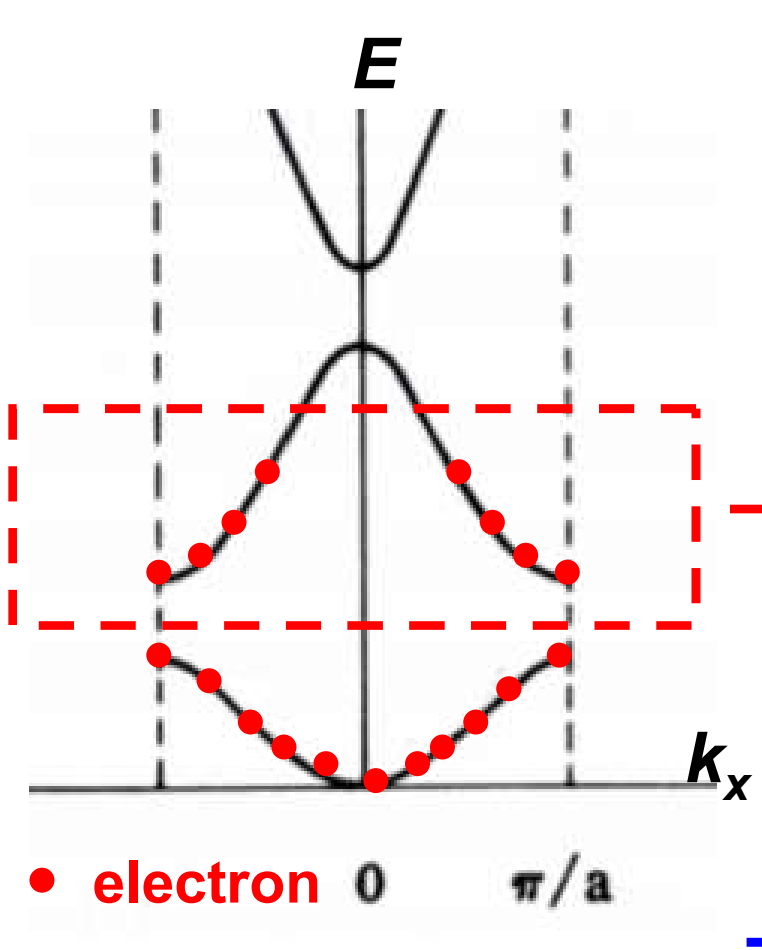
$N = 2n$
= total number of states

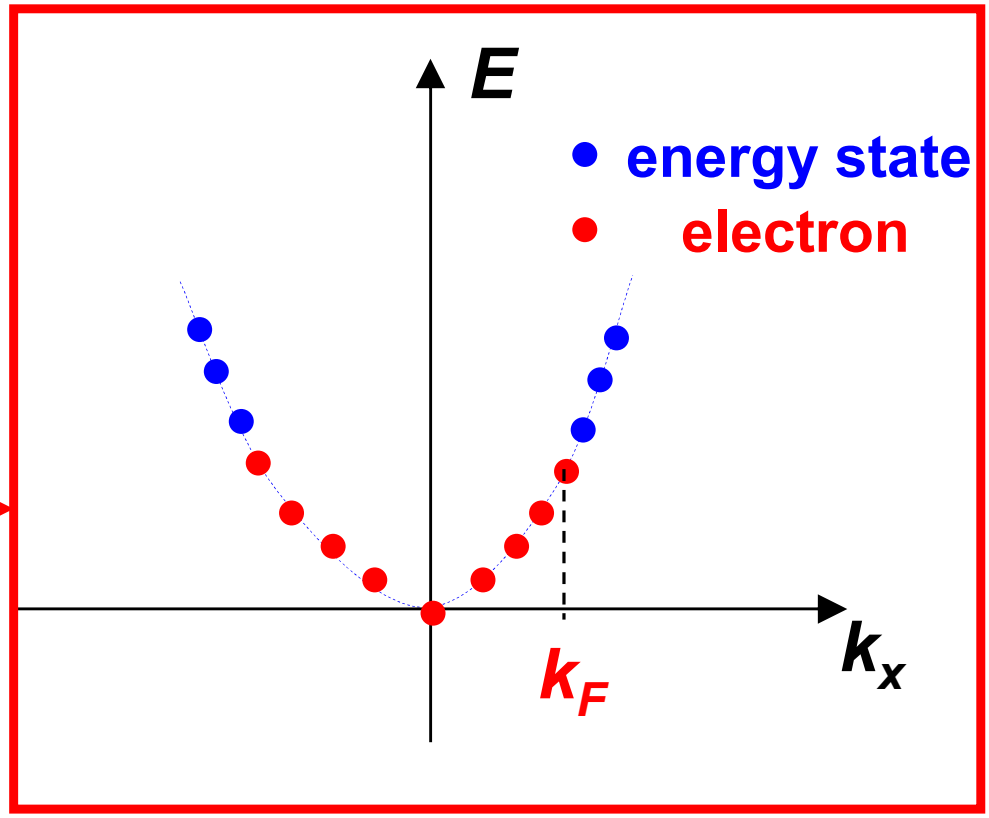
number of valence electrons
$= 3L/a = 3n$

Electrons start to fill the second band



1D Chain of *Trivalent* Atoms



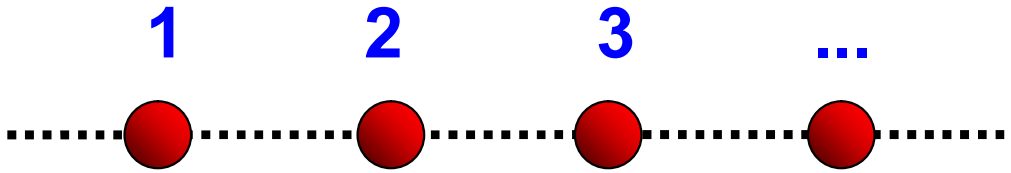


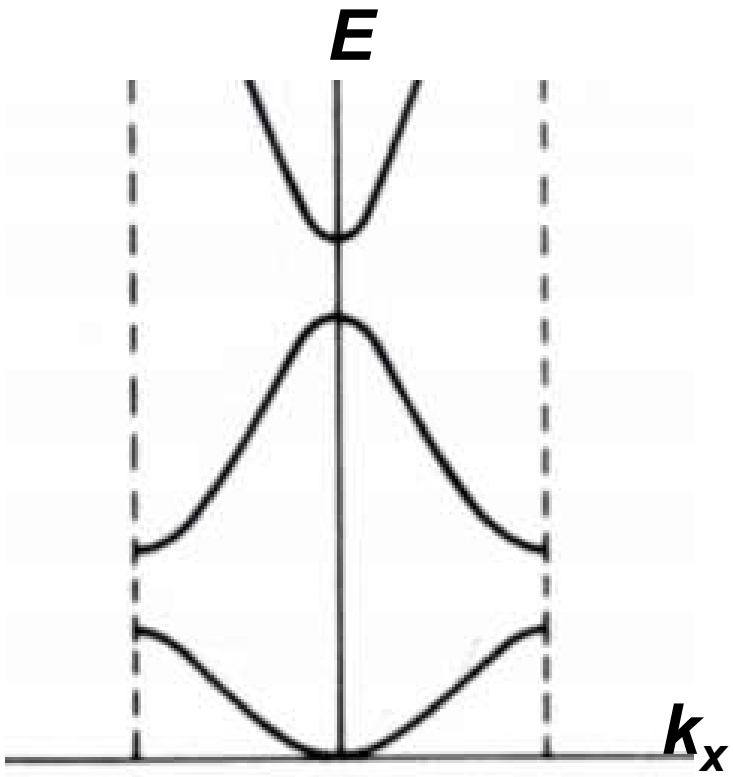
Free Electrons

Conductor

1D Chain of *Quadrivalent* Atoms

Each atom has *four* valence electrons (C, Si, ...)



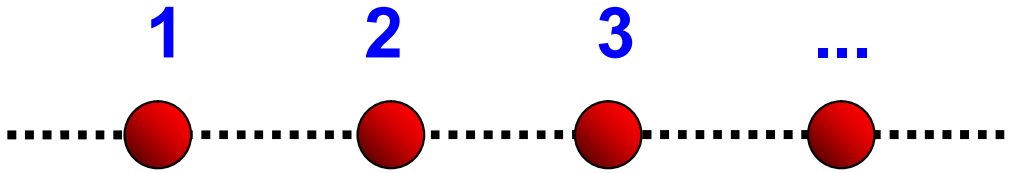


Q: How do electrons fill the bands?
Is it a conductor, or an insulator?

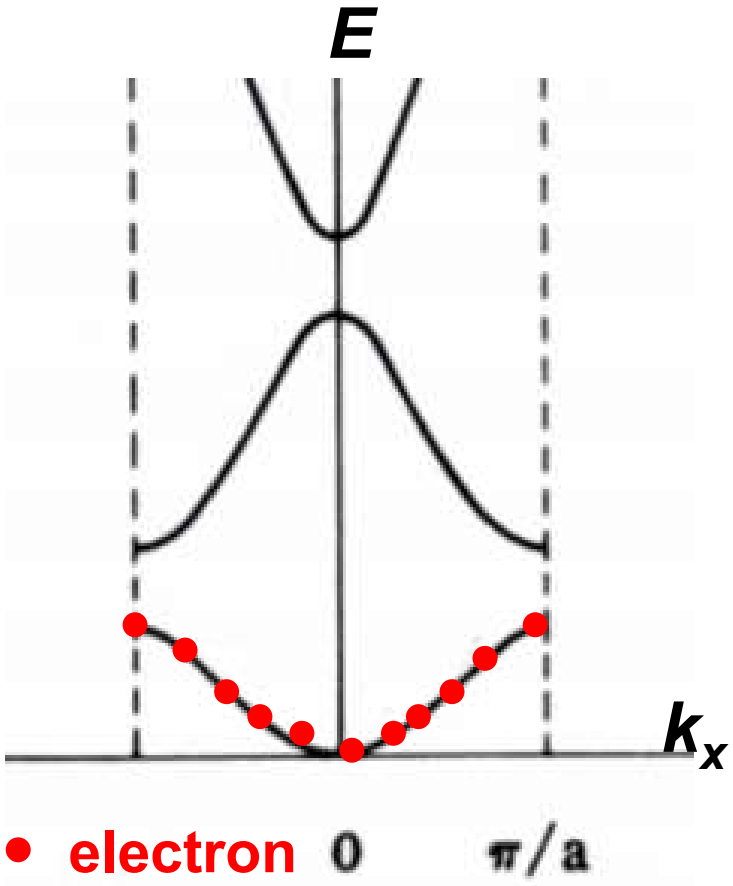
- electron

1D Chain of *Divalent* Atoms

Each atom has *two* valence electrons (Mg, Ca, ...)



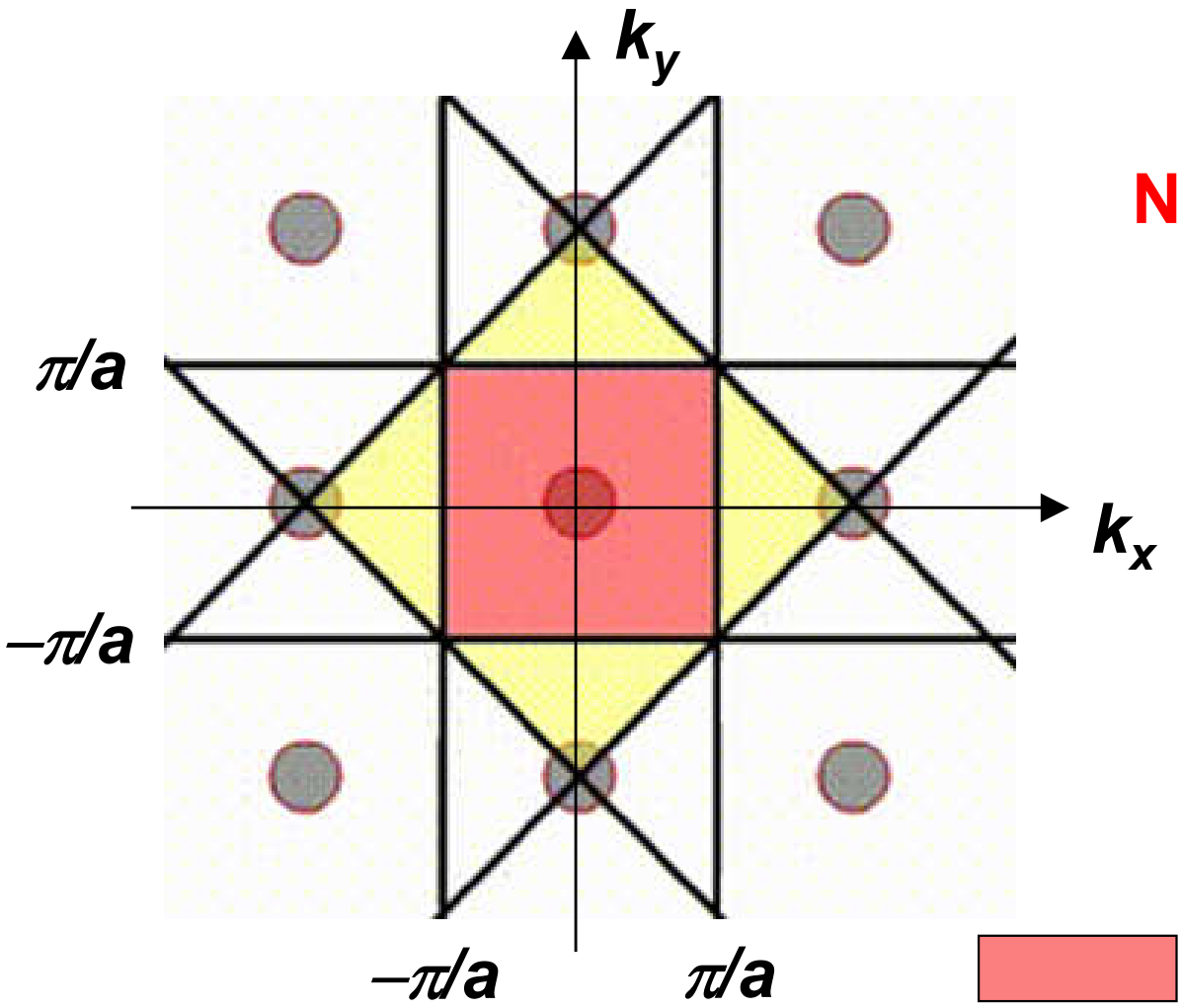
Electrons fill the entire band
--->
insulator



But we know metals like Mg and Ca are conductors, why?

2D case

Assume square lattice, in the reciprocal space



Number of states in each Brillouin zone

$N = 2n$

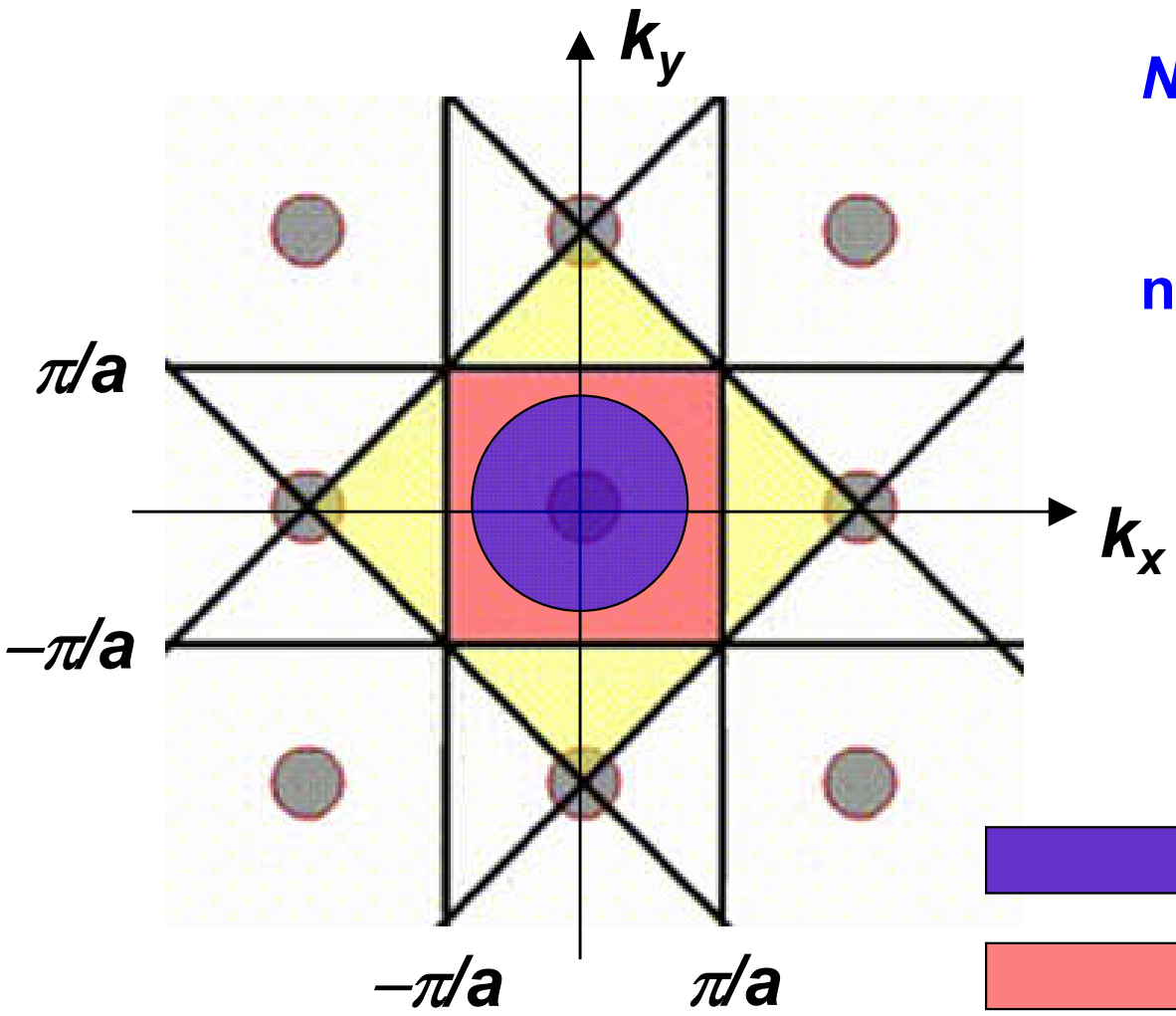
= total number of states

First BZ

Second BZ

2D case of *Monovalent* Atoms

Each atom has *one* valence electrons (Na, K, ...)



$N = 2n$
= total number of states

number of valence electrons
= $A/a/a = n$

FBZ is not full

↓

Conductor

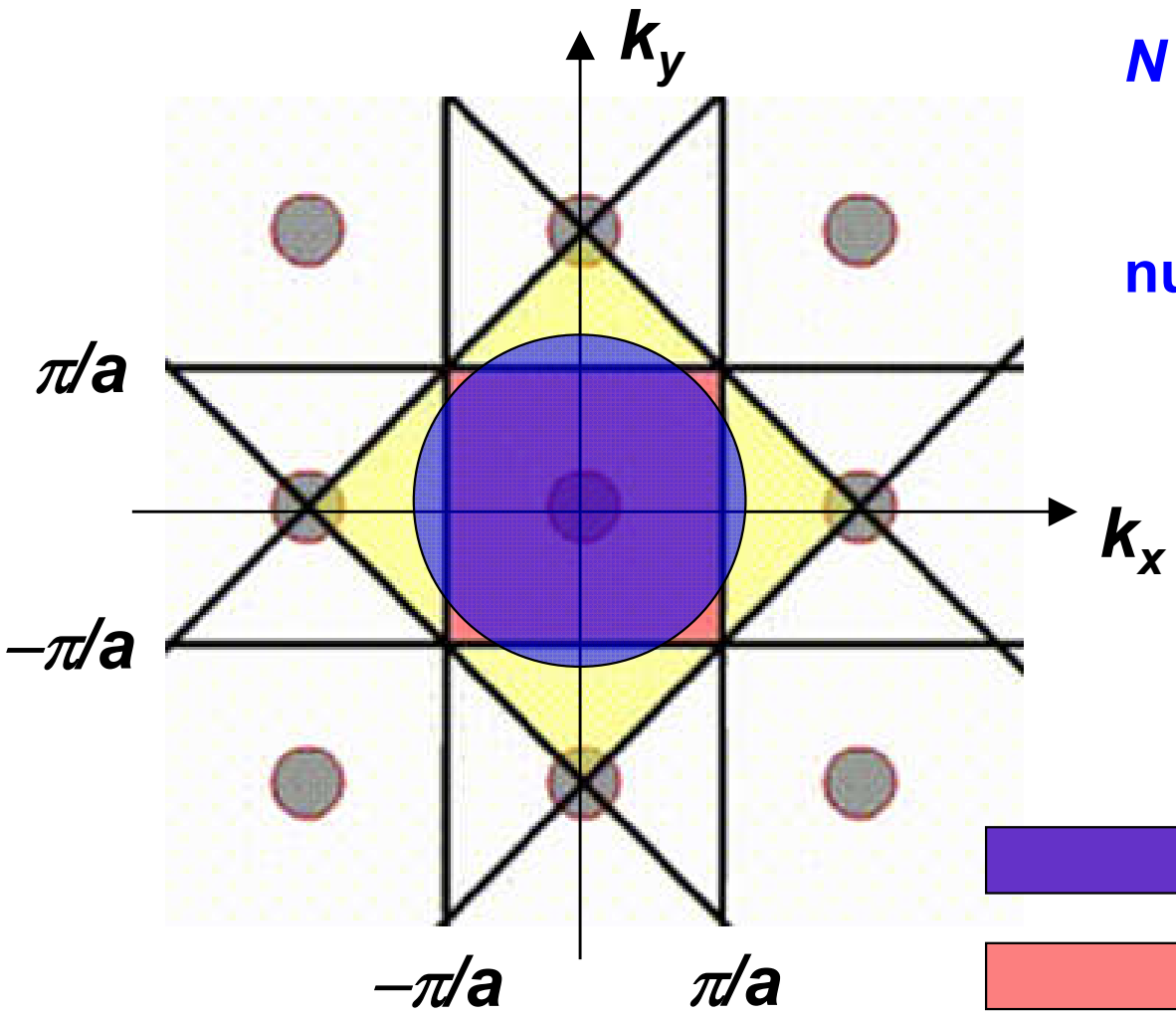
electrons

First BZ

Second BZ

2D case of *Divalent* Atoms

Each atom has *two* valence electrons (Mg, Ca, ...)



$N = 2n$
= total number of states

number of valence electrons
$= 2A/a/a = 2n$

start to fill SBZ, but FBZ is not full

Conductor (semimetal)

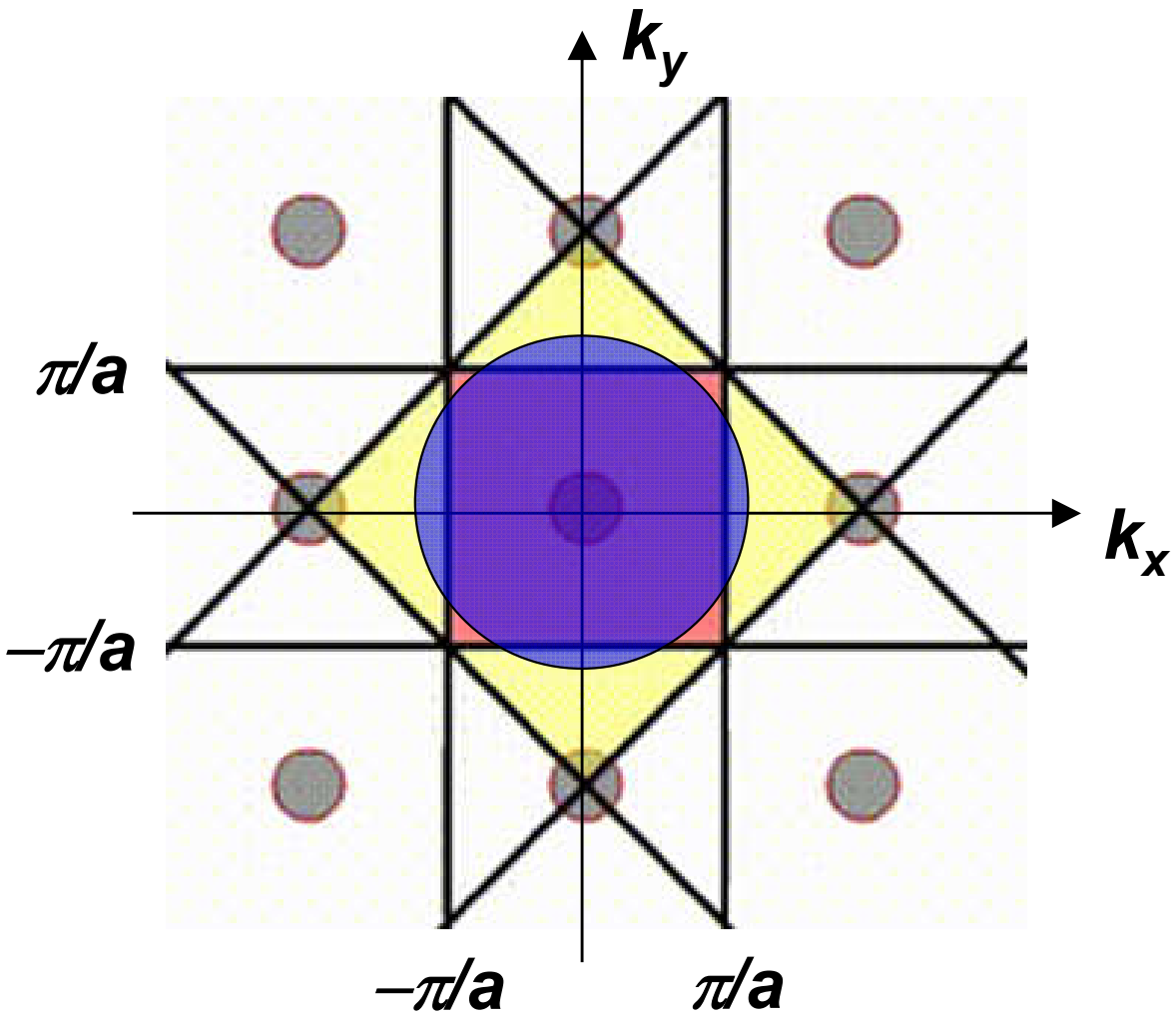
electrons

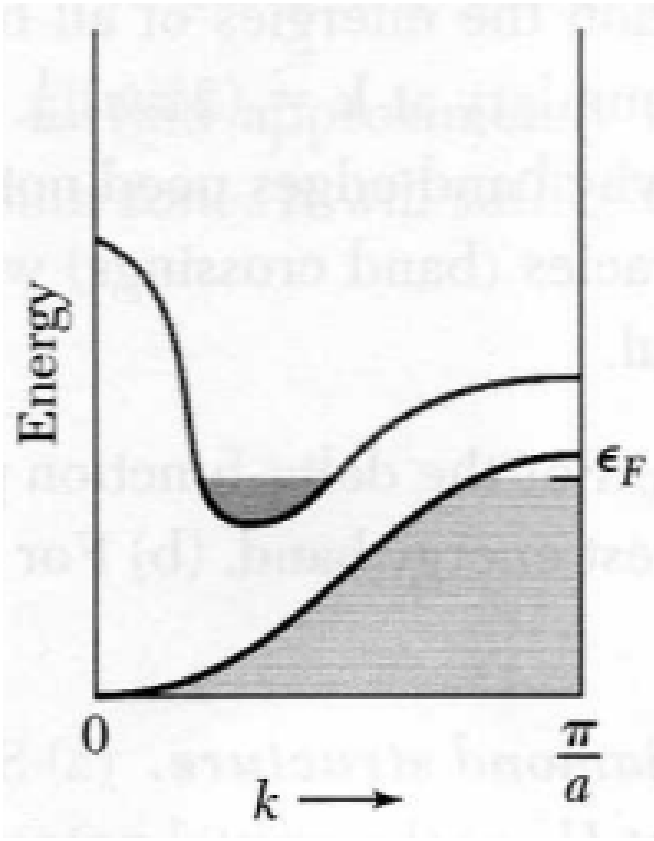
First BZ

Second BZ

2D case of *Divalent* Atoms

Each atom has *two* valence electrons (Mg, Ca, ...)

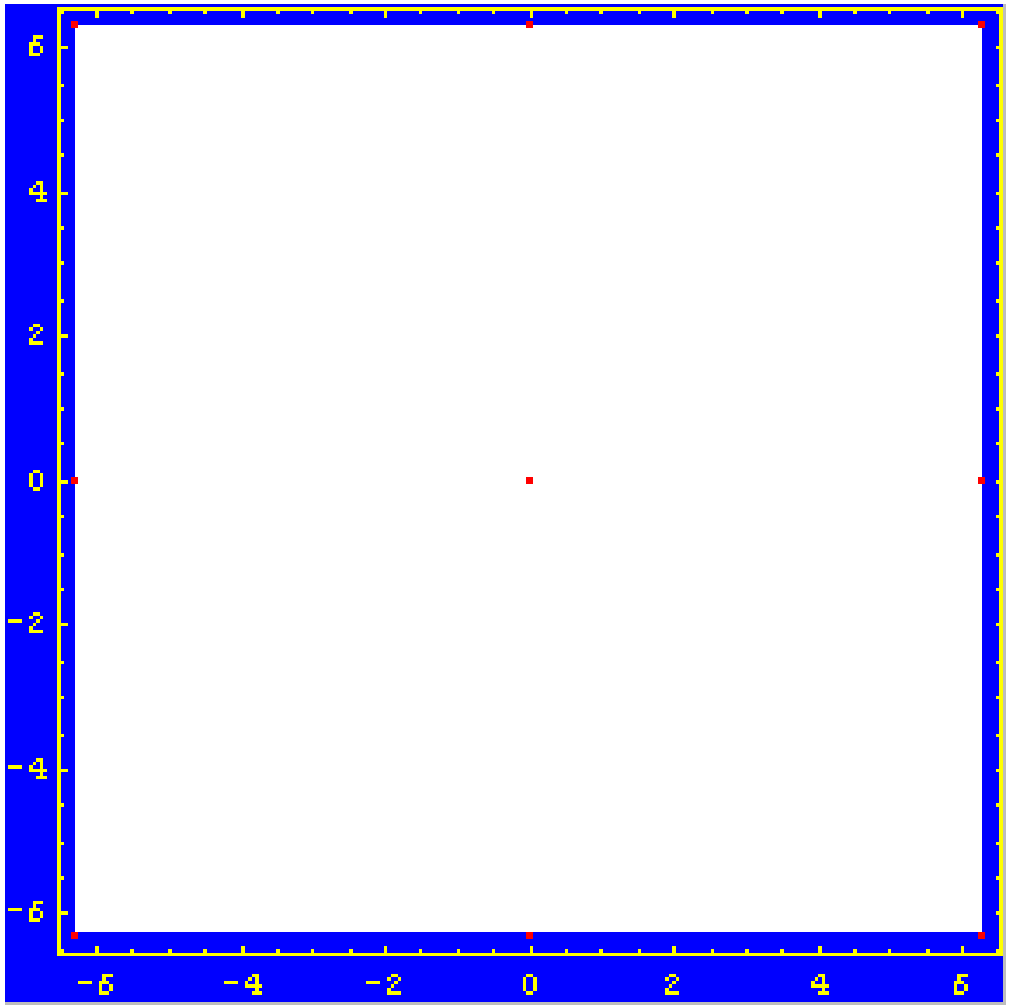




semimetal 半金属

2D Fermi Surface

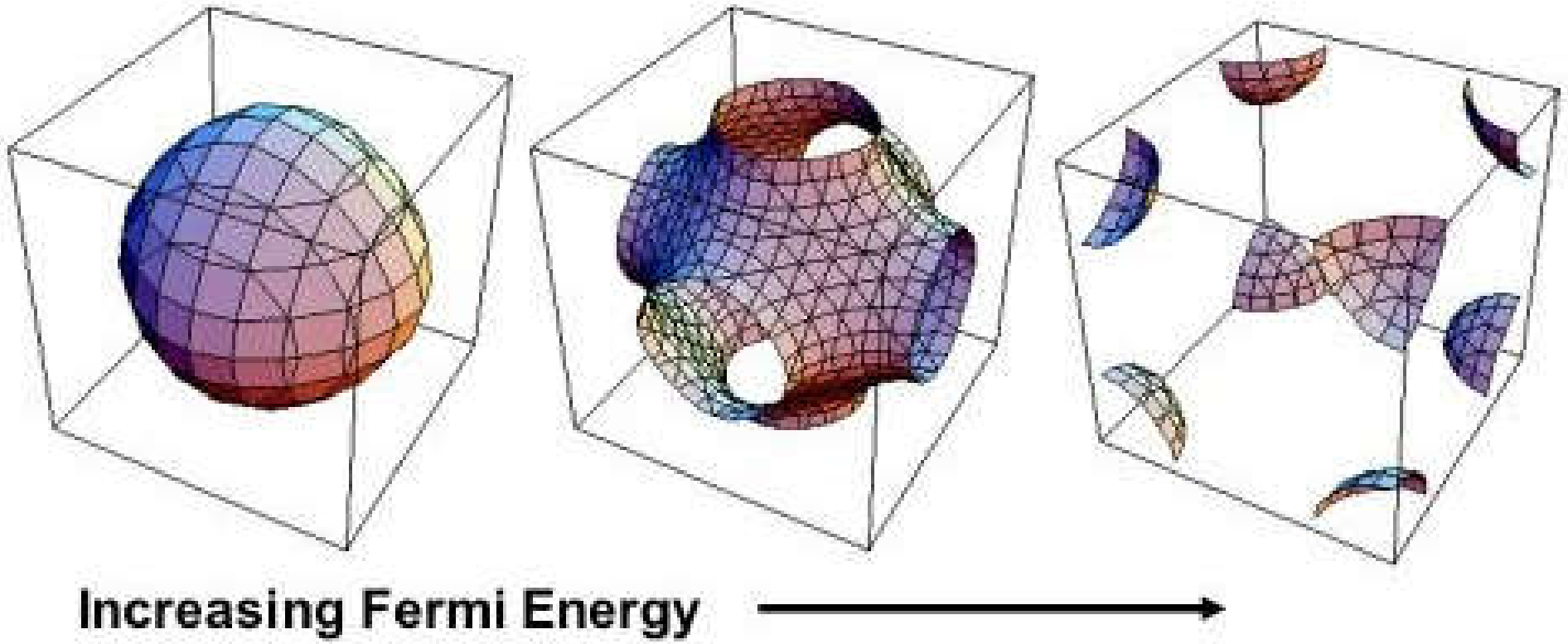
simple square



https://www.physics.upenn.edu/~mele/archives/webpage518/phys518.s03/log.html

3D Fermi Surface

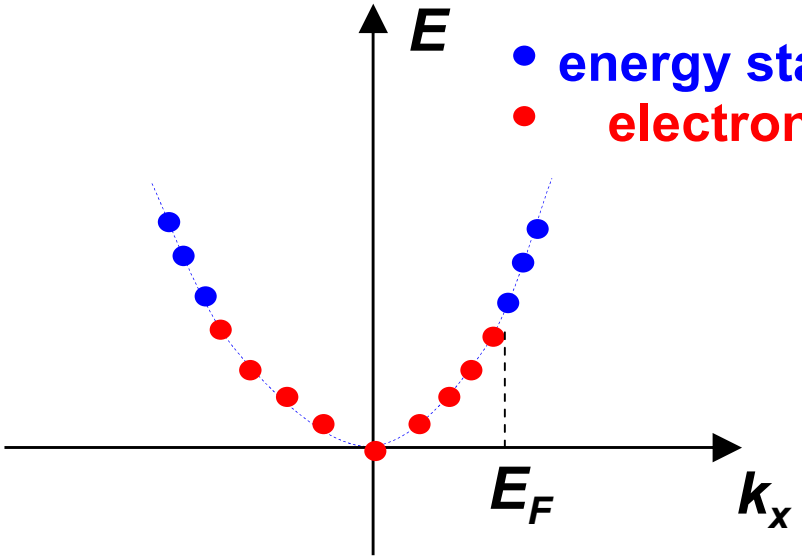
simple cubic

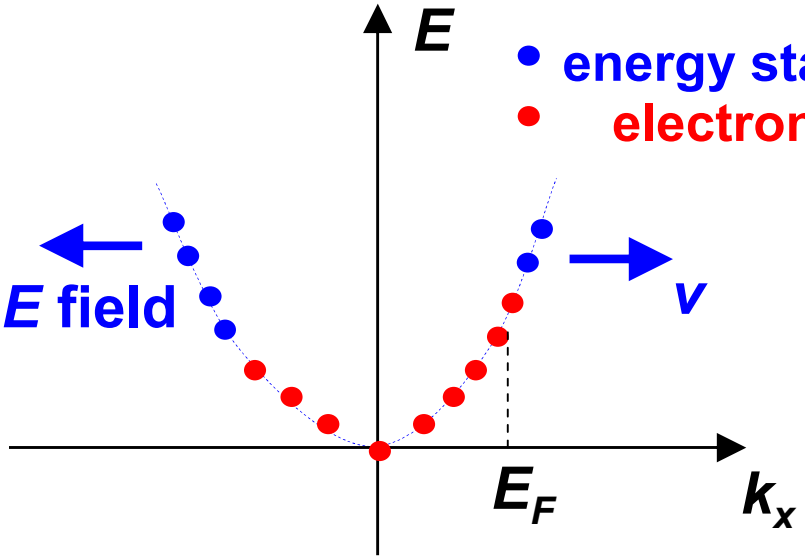


generated with a tight binding model:
http://home.cc.umanitoba.ca/~loly/fermisurf2.html

Electrical Conductivity - Revisit

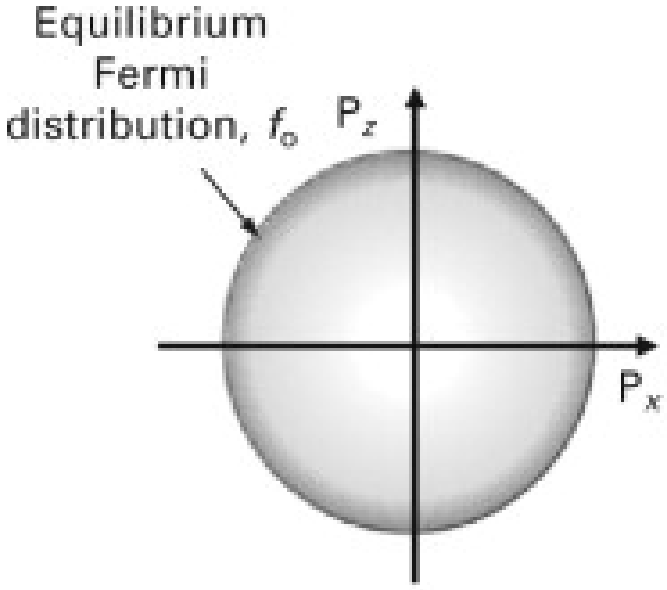
1D

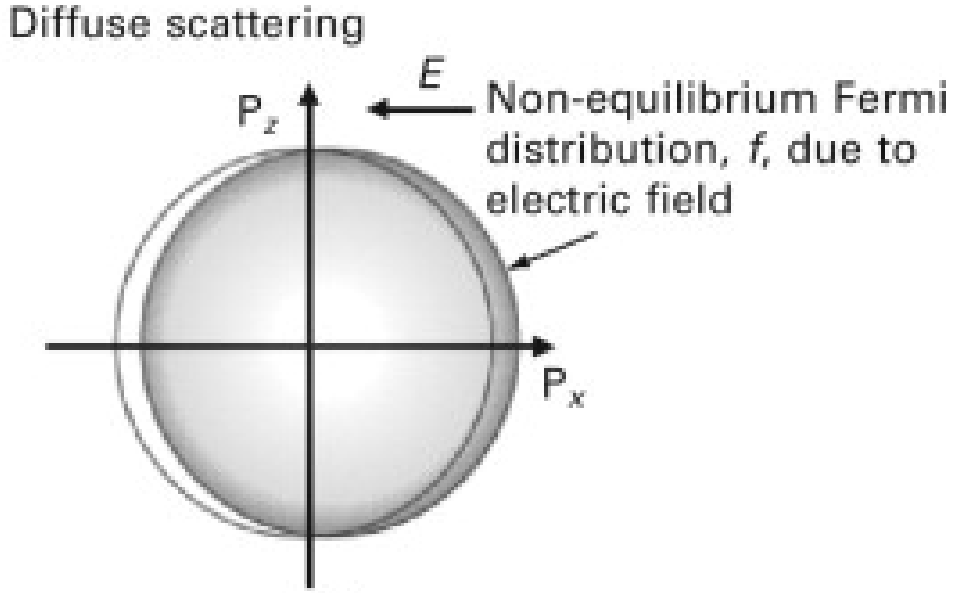




2D

3D



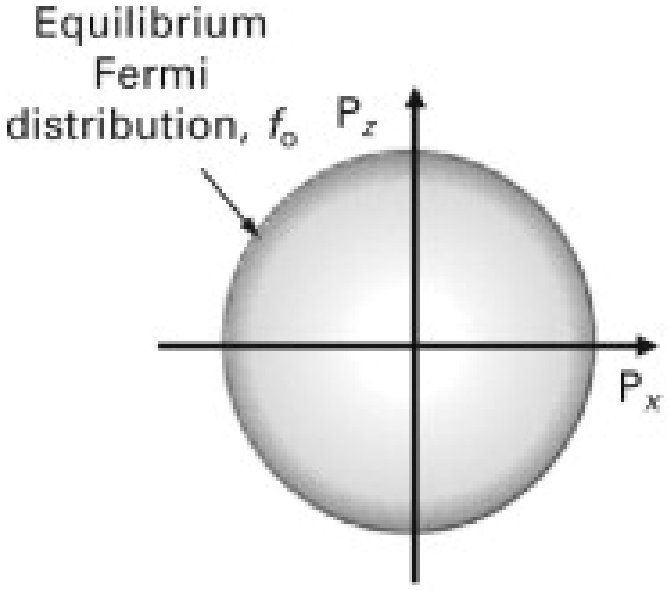


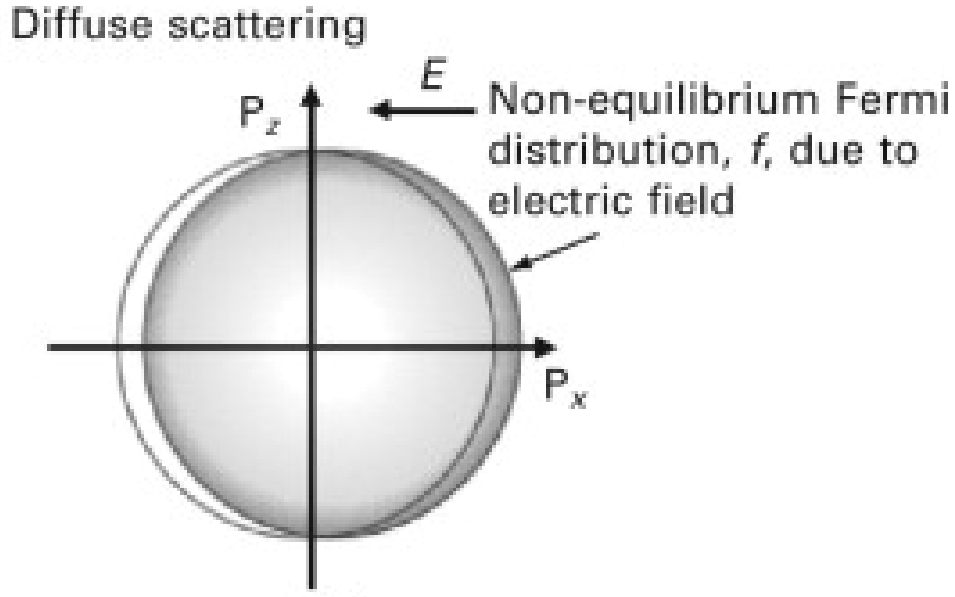
Electrical Conductivity - Revisit

- **Only electrons near the Fermi surface contribute to electrical (and thermal) conductivity in metals**

$$\boldsymbol{\sigma} = e^2 \cdot \tau(E_F) \cdot \int_{\substack{\text{occupied} \\ \text{levels}}} \frac{2d\mathbf{k}}{(2\pi)^3} \cdot \frac{1}{\mathbf{M}^*(\mathbf{k})}$$

Ashcroft & Mermin, Chap.13



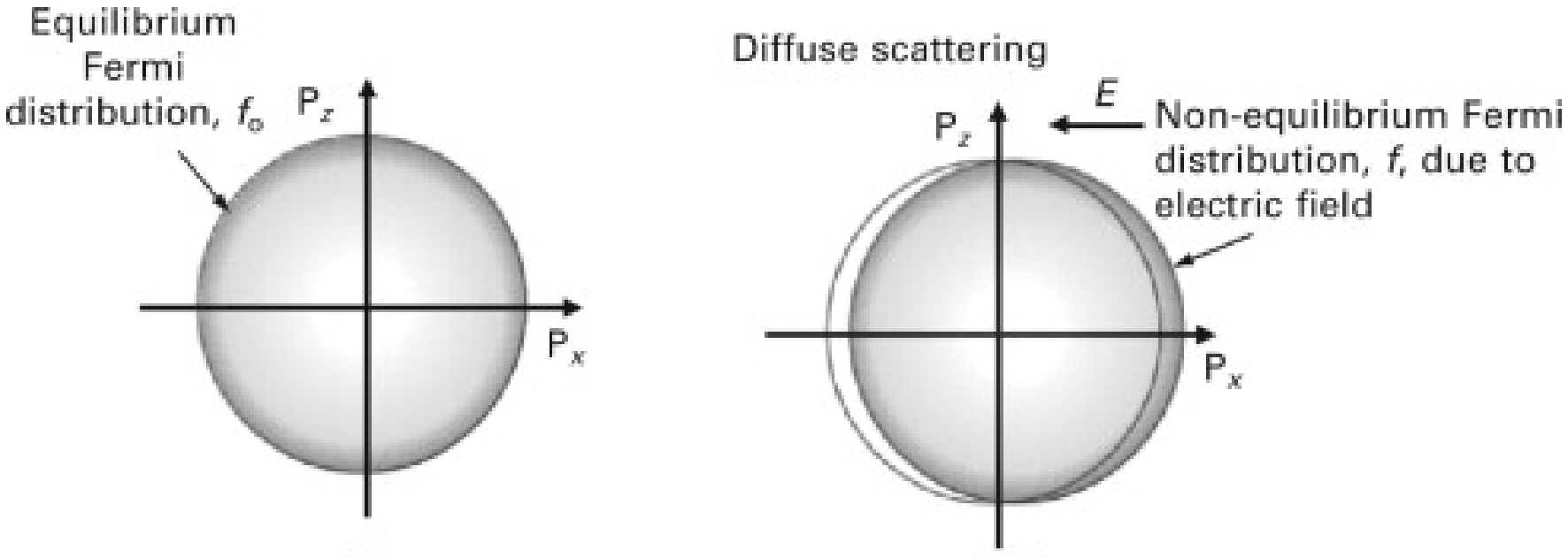


Electrical Conductivity - Revisit

- **Only electrons near the Fermi surface contribute to electrical (and thermal) conductivity in metals**

compare

$$\sigma = ne\frac{v}{E} = ne\mu = \frac{ne^2\tau}{m^*}$$



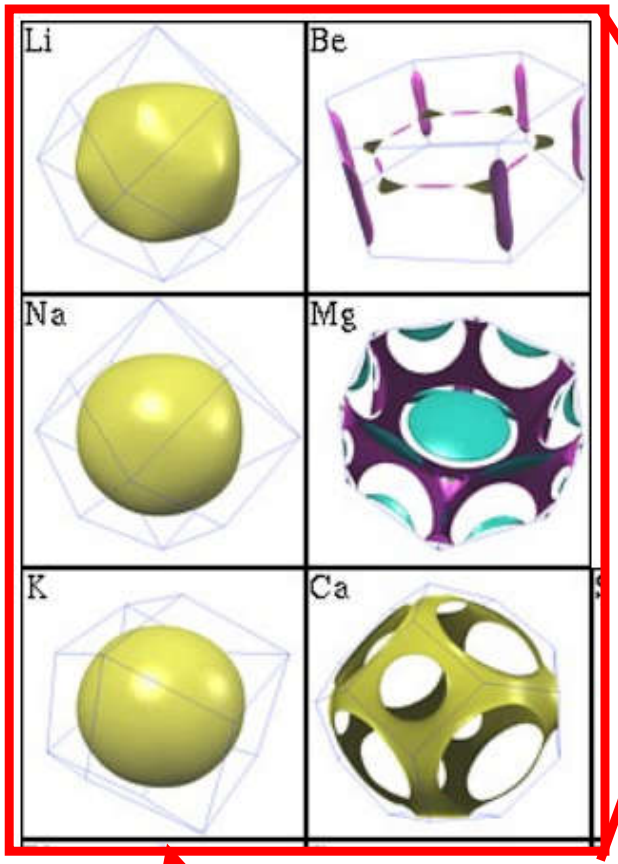
Electrical Conductivity - Revisit

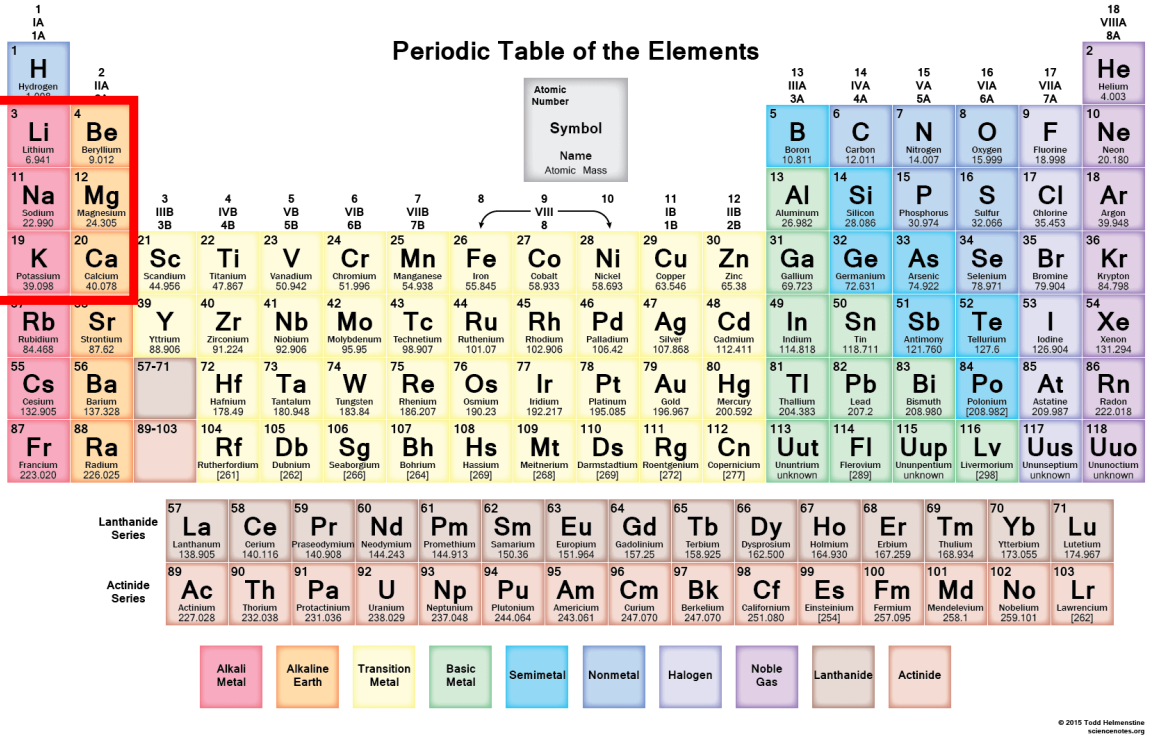
$$\sigma = ne\frac{v}{E} = ne\mu = \frac{ne^2\tau}{m^*}$$

	Classical	Quantum
electron density n	all valence electrons	electrons near Fermi surface (depend on *E* field)
μ τ		
velocity v	average (depend on temperature)	Fermi velocity v_F
mass m	free electron m_0	effective mass m^*

3D Fermi Surface

IA IIA



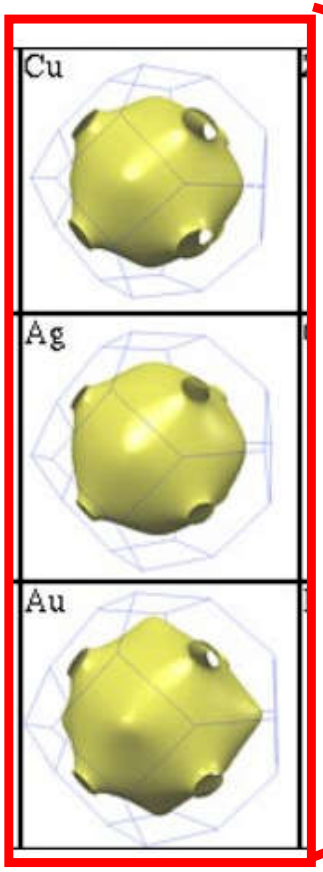


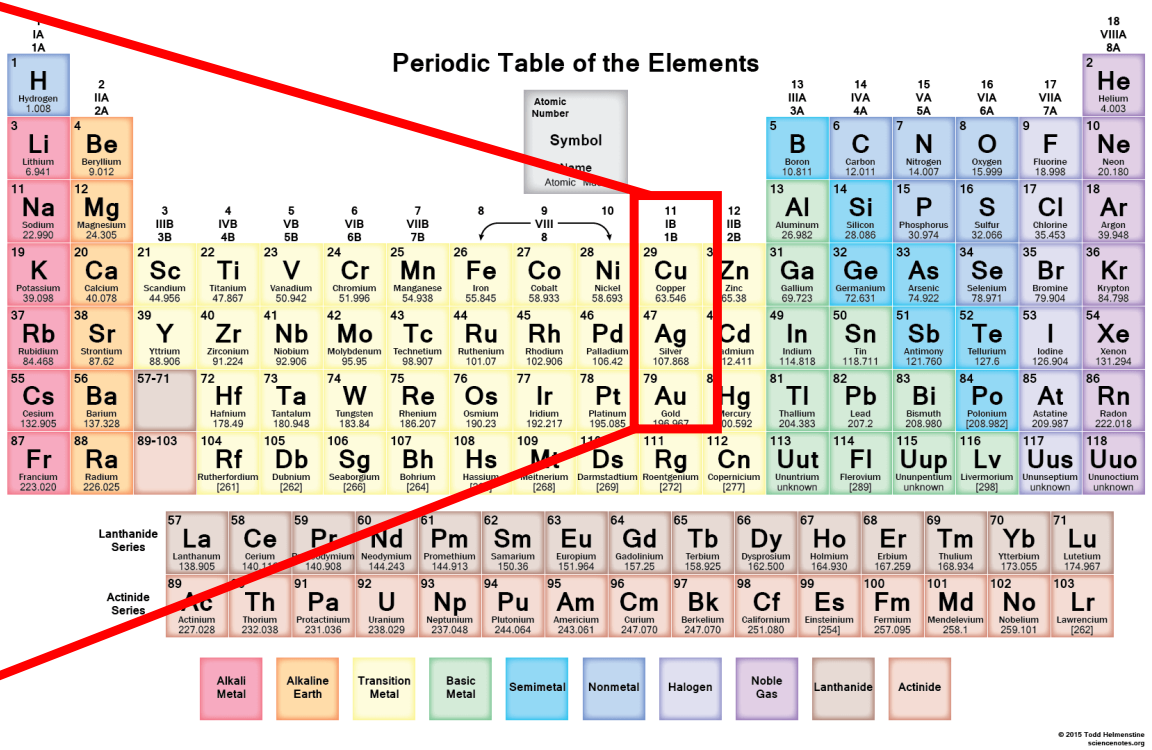
nearly free electrons

http://www.phys.ufl.edu/fermisurface/

3D Fermi Surface

IB



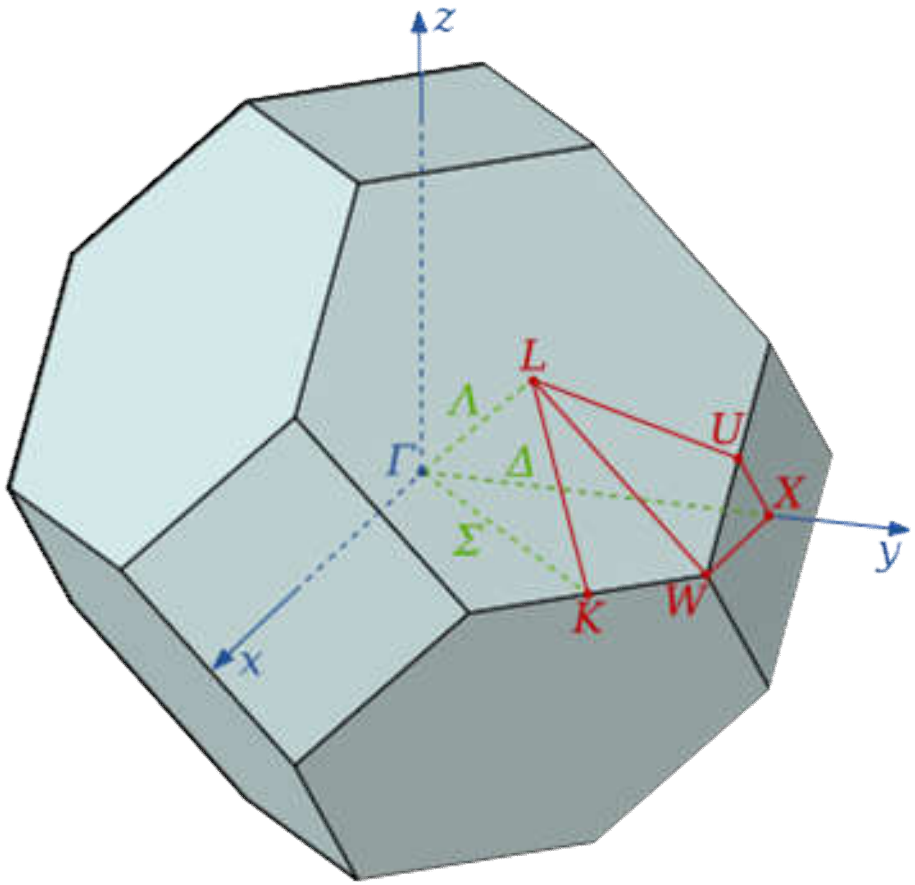


nearly free electrons

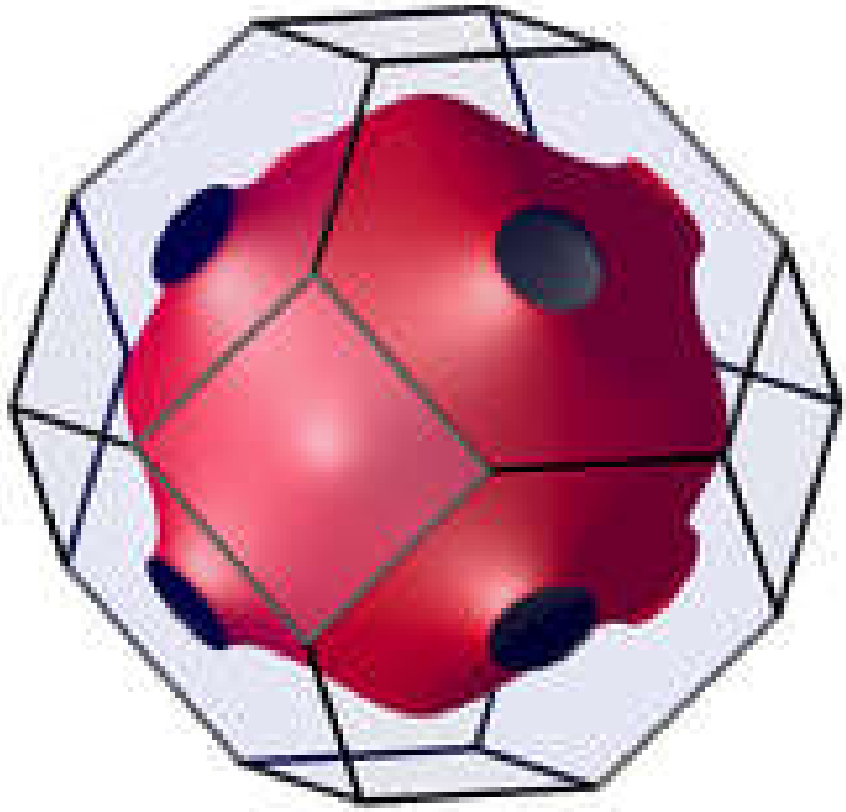
http://www.phys.ufl.edu/fermisurface/

3D case

copper (FCC)



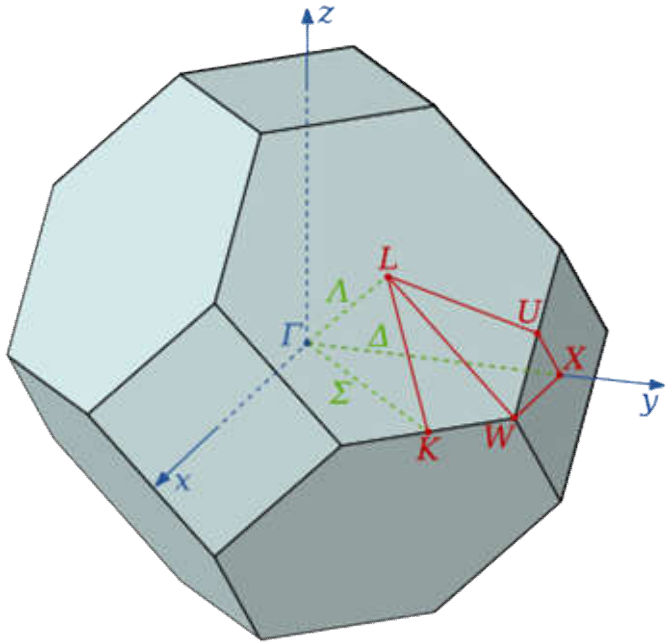
First BZ



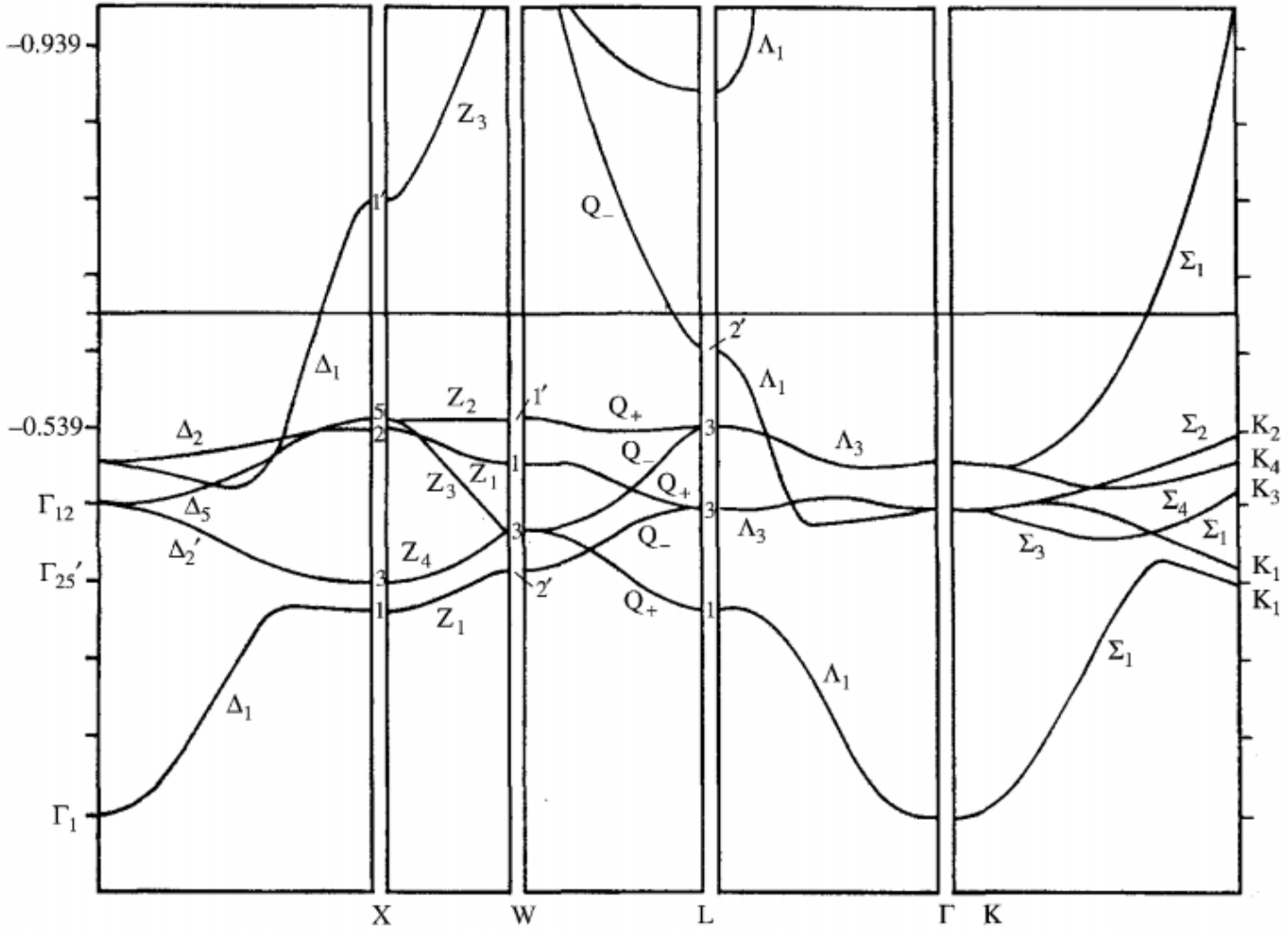
Fermi Surface

3D case

copper (FCC): band structure

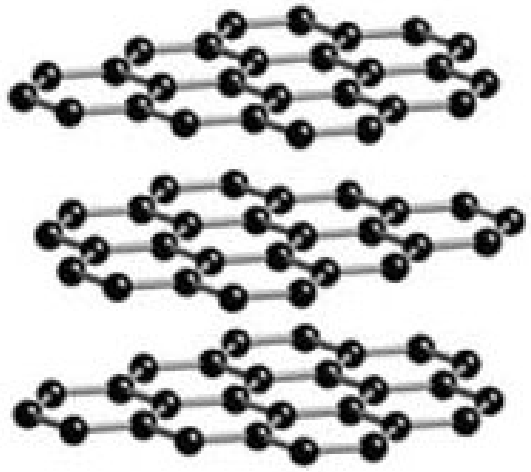


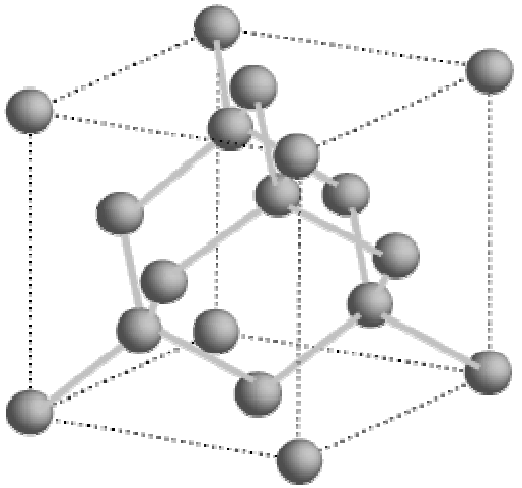
First BZ



G. A. Burdick, *Phys. Rev.* **129,** 138 (1963)

Example - Carbon

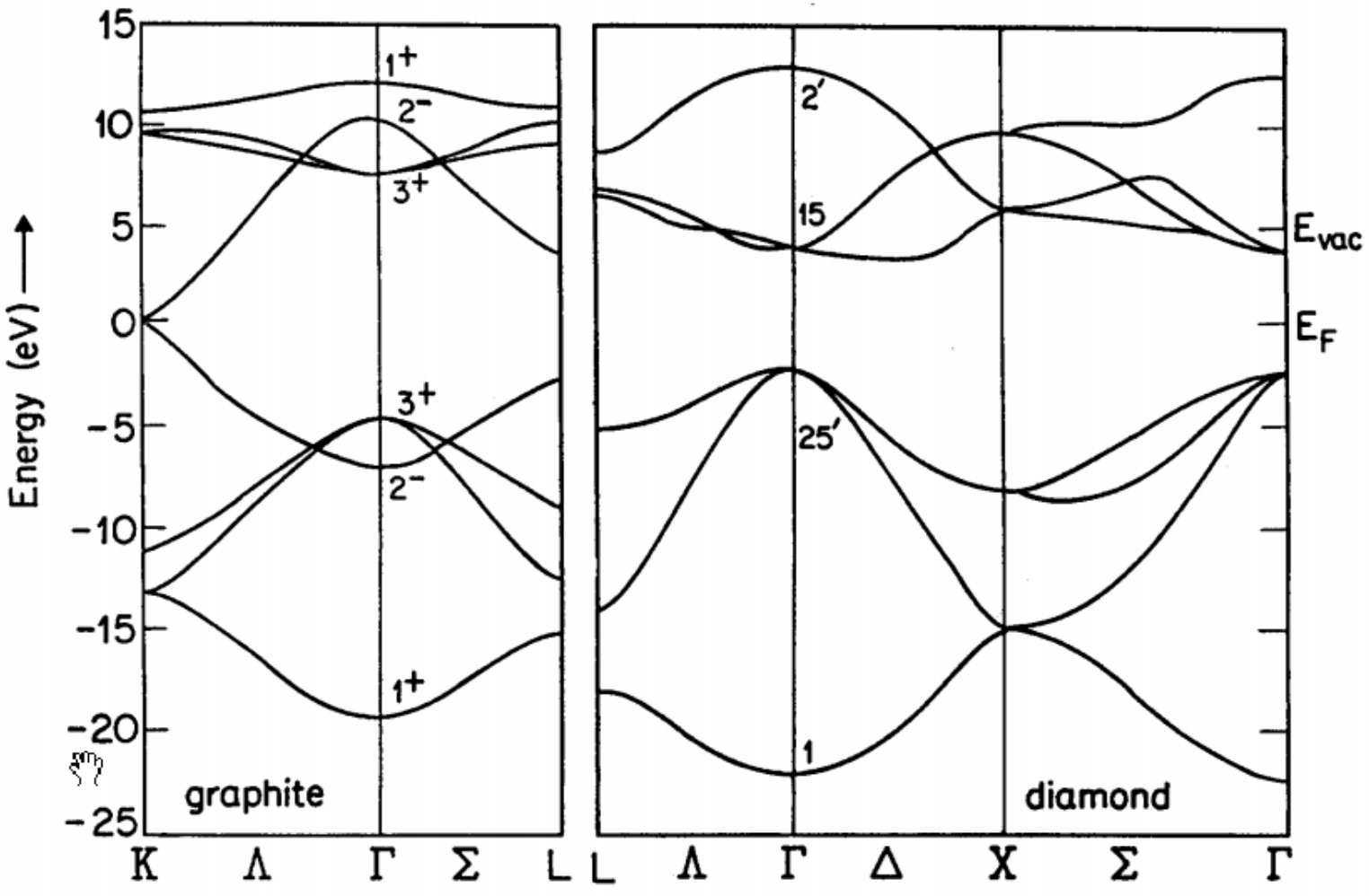




graphite
σ ~ 10^{5} S/m

diamond
σ ~ 10^{-13} S/m

Example - Carbon



graphite
conductor

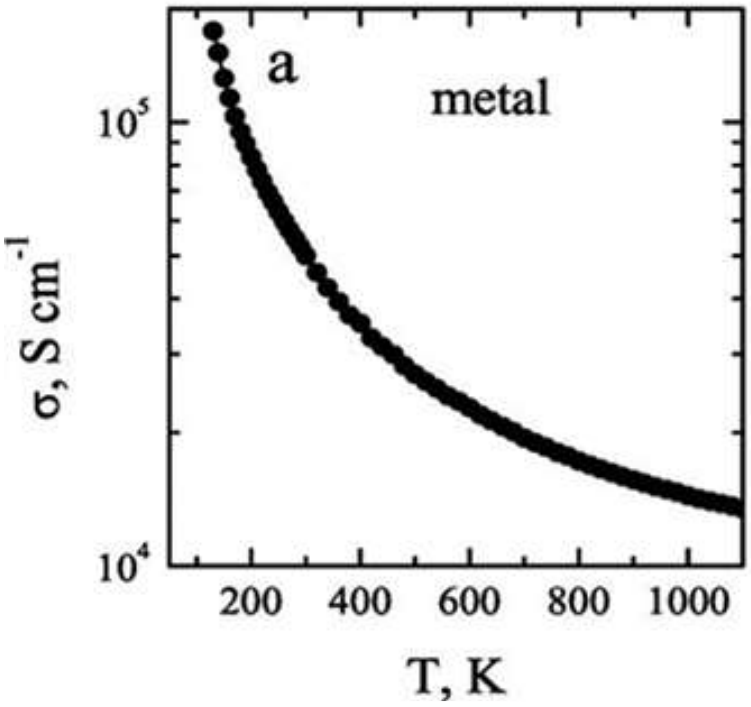
diamond
insulator (E_g = 5.5 eV)

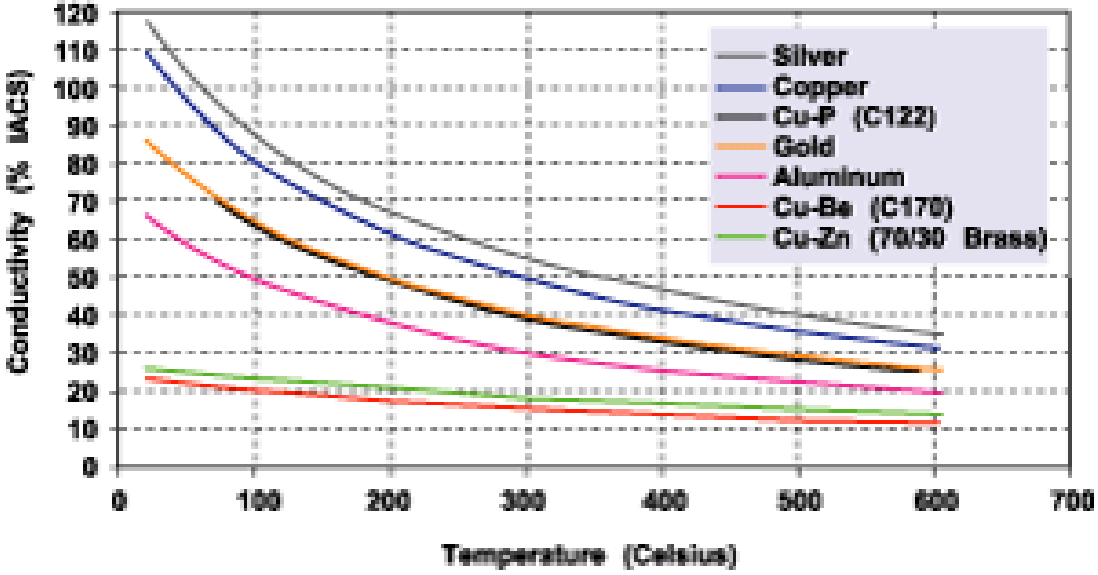
J. Robertson, *Prog.Solid St. Chem* **21,** 199 (1991)

Temperature Dependence of σ

- **For metals**
  - ***n*** **and** ***m**** **have weak dependence on** ***T***
  - **t has a strong dependence on T**
  - **higher** ***T*** **---> shorter** τ **---> smaller** μ **---> smaller** σ

$$\sigma = ne\mu = \frac{ne^2\tau}{m^*}$$





https://www.thefabricator.com/

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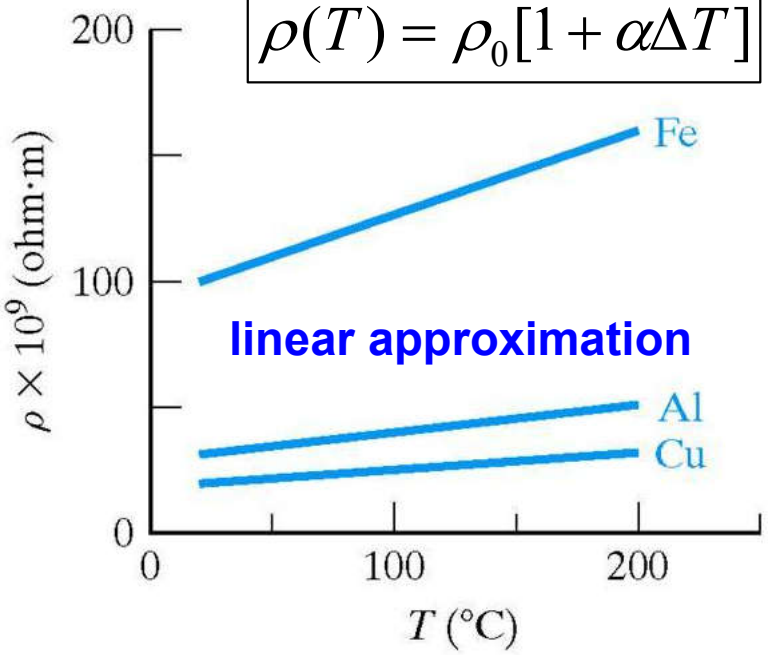
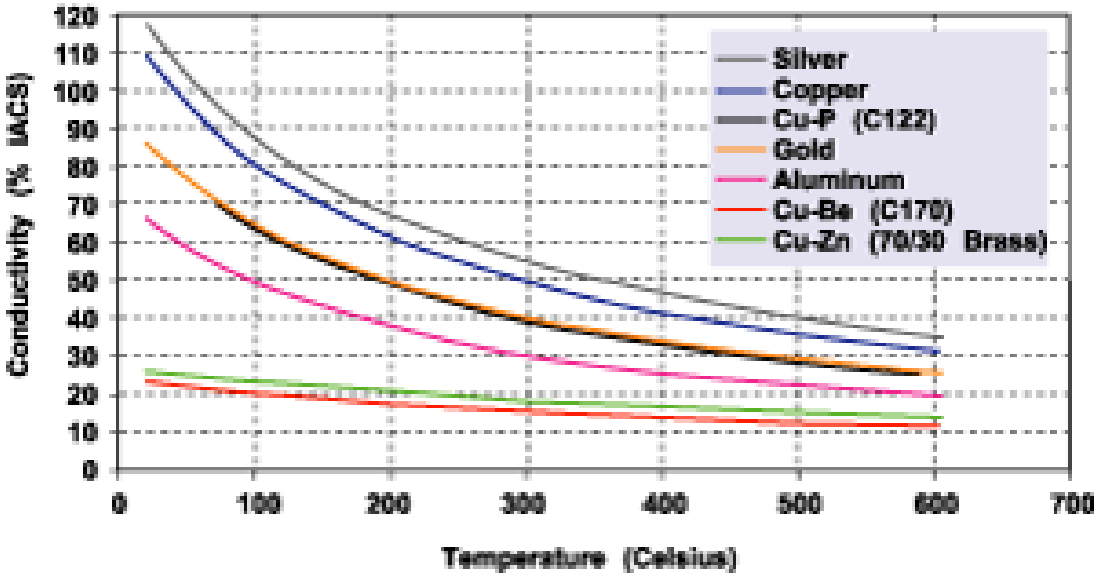
$$\rho(T) = \rho_0[1 + \alpha\Delta T]$$



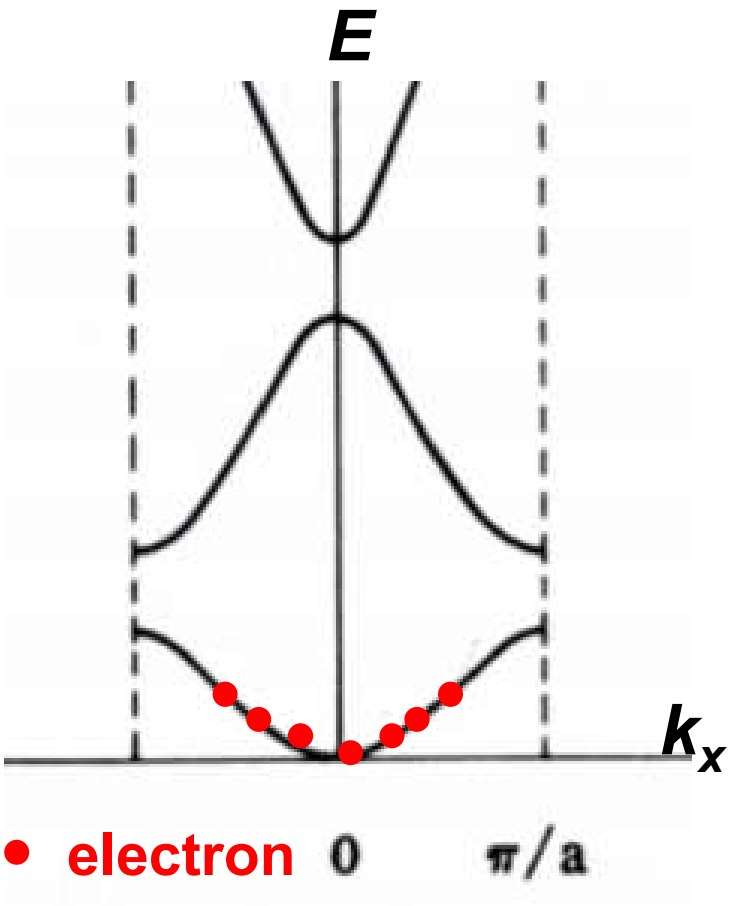


https://fog.ccsf.edu/~wkaufmyn/ENGN45/Course%20Handouts/15_ElectricalProps/05_TemperatureConductivityConductor.html

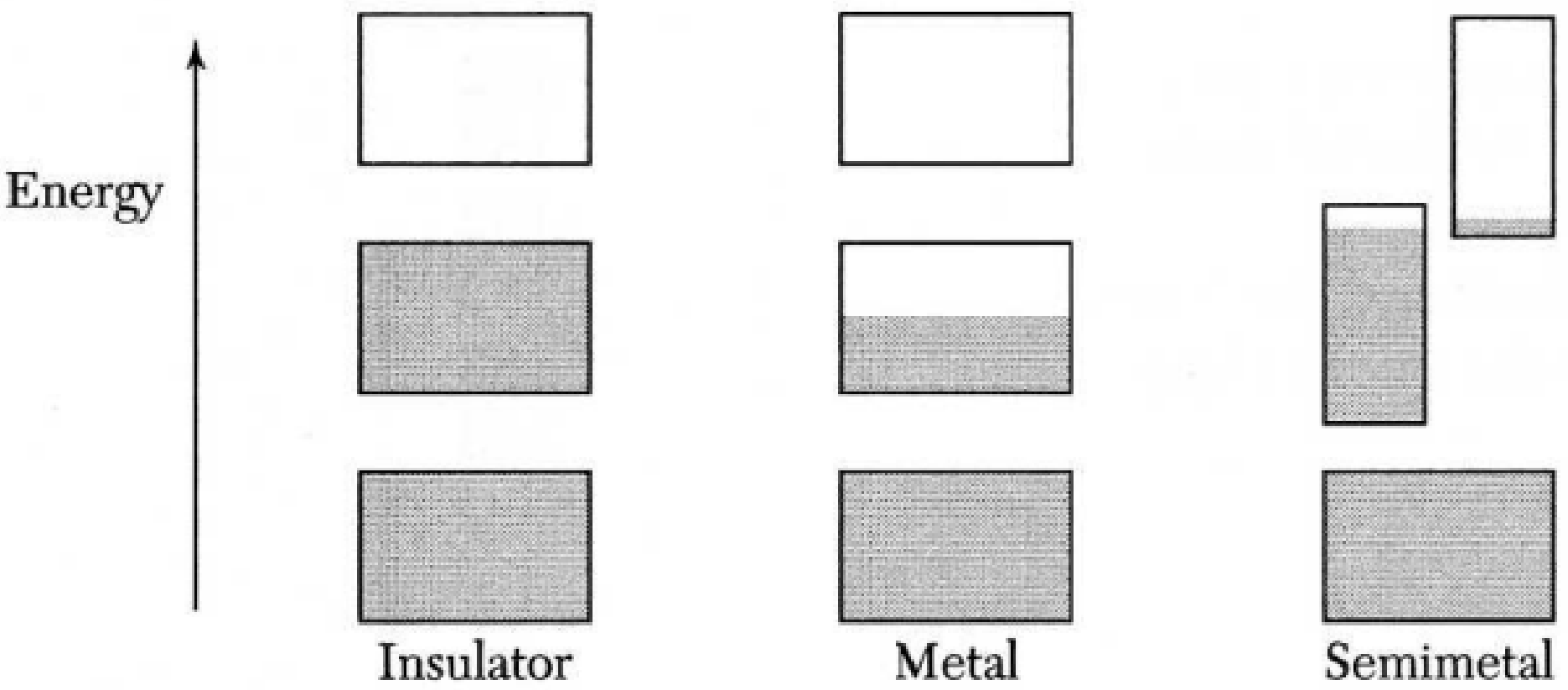
https://www.thefabricator.com/

Summary

- Electronic properties of solids depend on
  - band structure
  - electron density
  - defects
  - temperature
  - electric field
  - ...



Summary



Thank you for your attention