Fundamentals of Solid State Physics

Metals and Insulators

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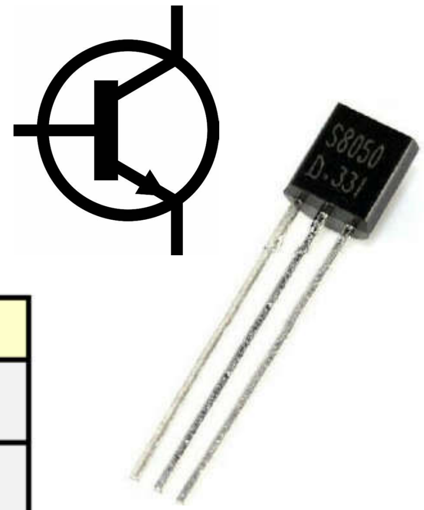
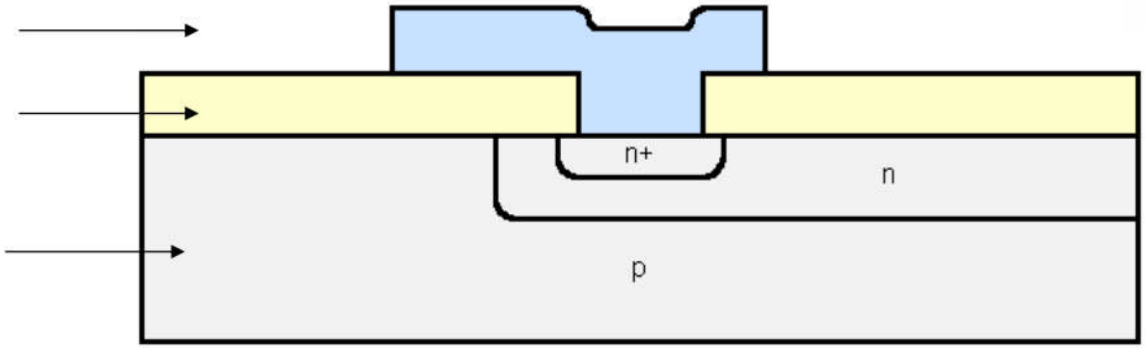
Electronic Properties of Materials

CMOS transistor
- Complementary Metal-Oxide-Semiconductor



conductor Al
insulator SiO_2
semiconductor Si

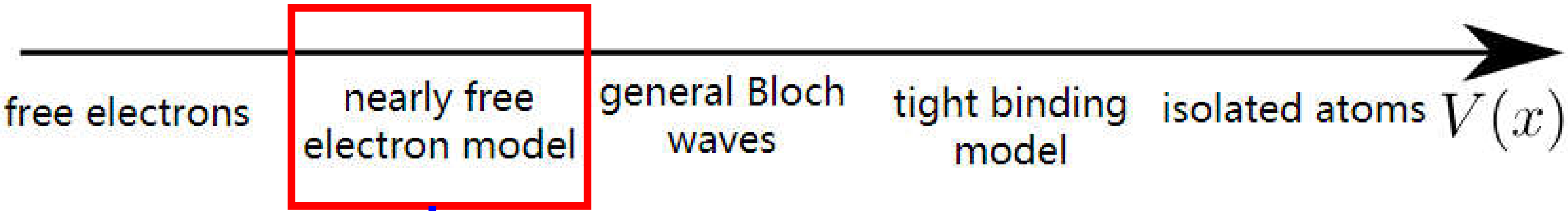


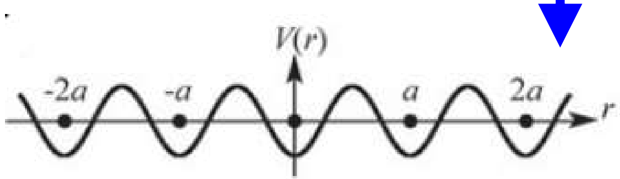
Metal

SiO_2

Silicon

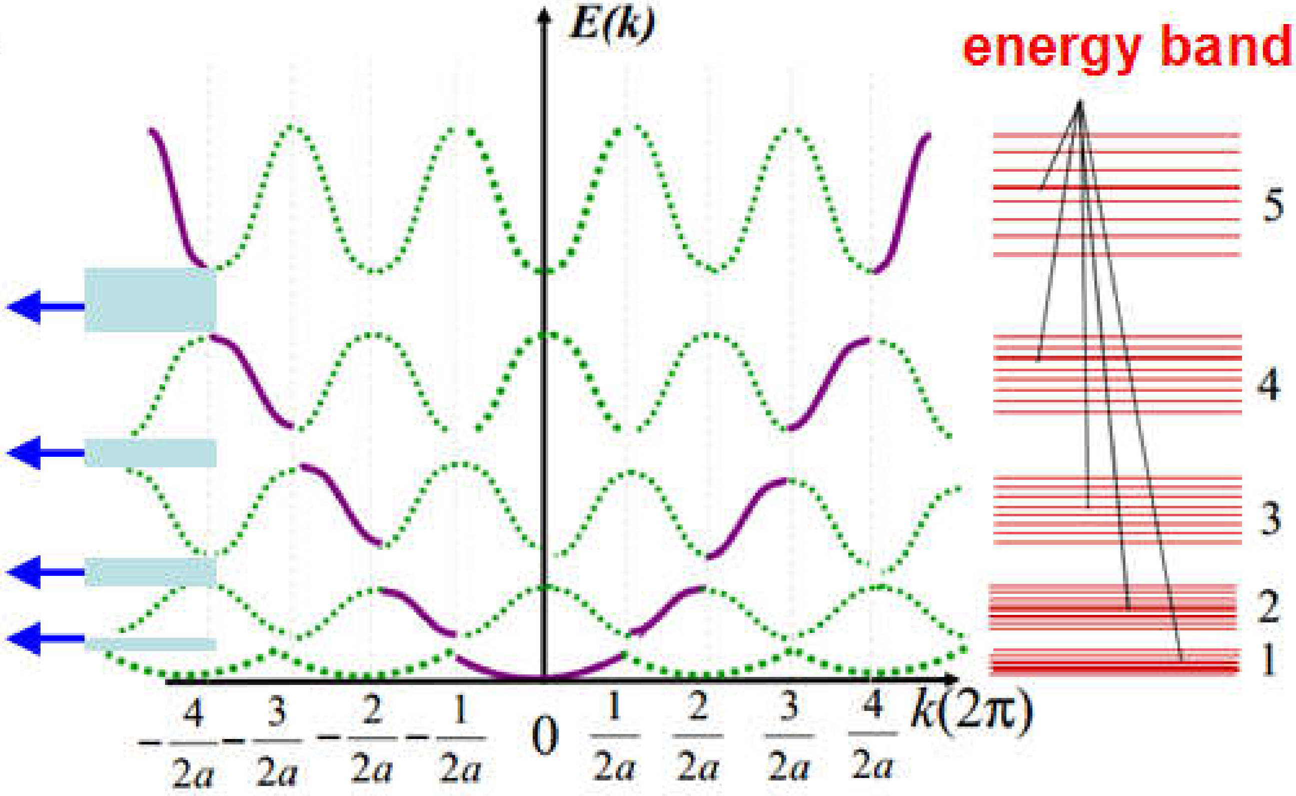
Formation of Band Gaps



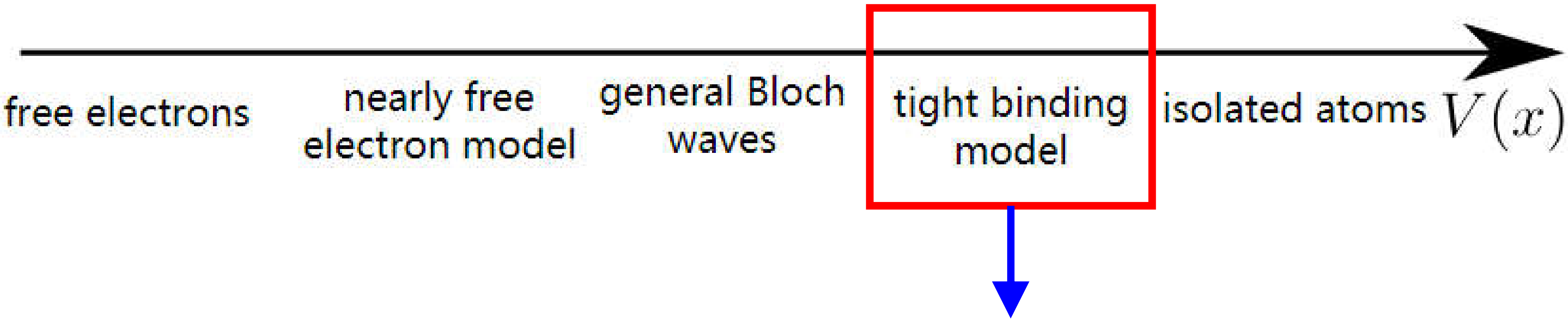


free electrons are perturbed by weak, periodic potentials

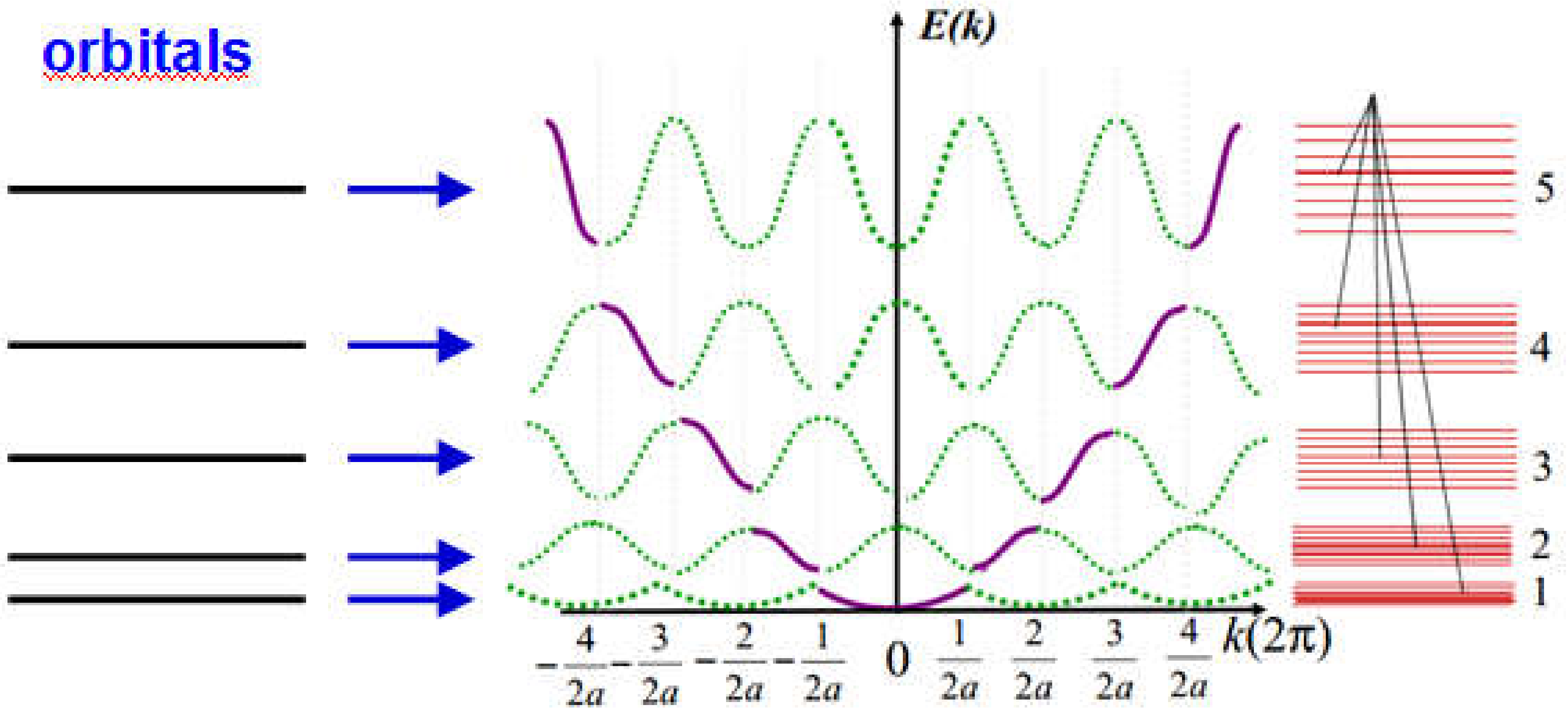
band gap



Formation of Band Gaps



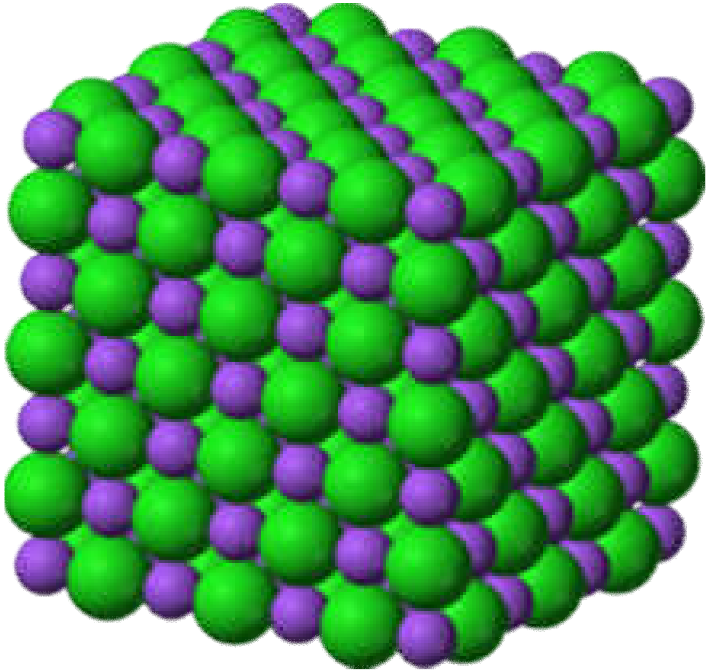
orbitals

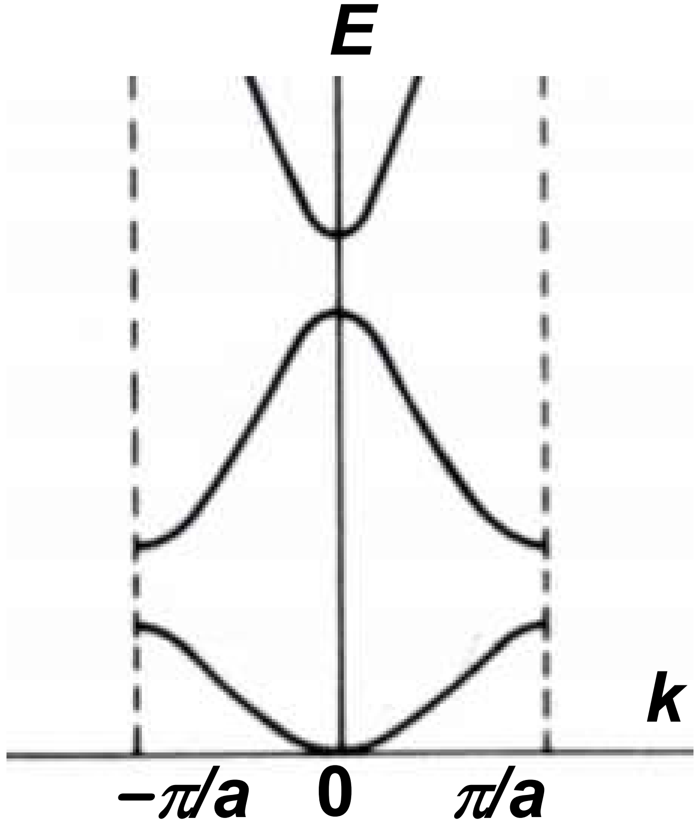


band structures and band gaps

discrete orbitals are combined to form quasi-continuous bands

Formation of Band Gaps





Fill electrons into these bands

Q: Is it a metal or insulator?

State vs. Electron

energy state / level / orbital
能态 / 能级 / 轨道

electron / phonon / ...
电子 / 声子 / ...

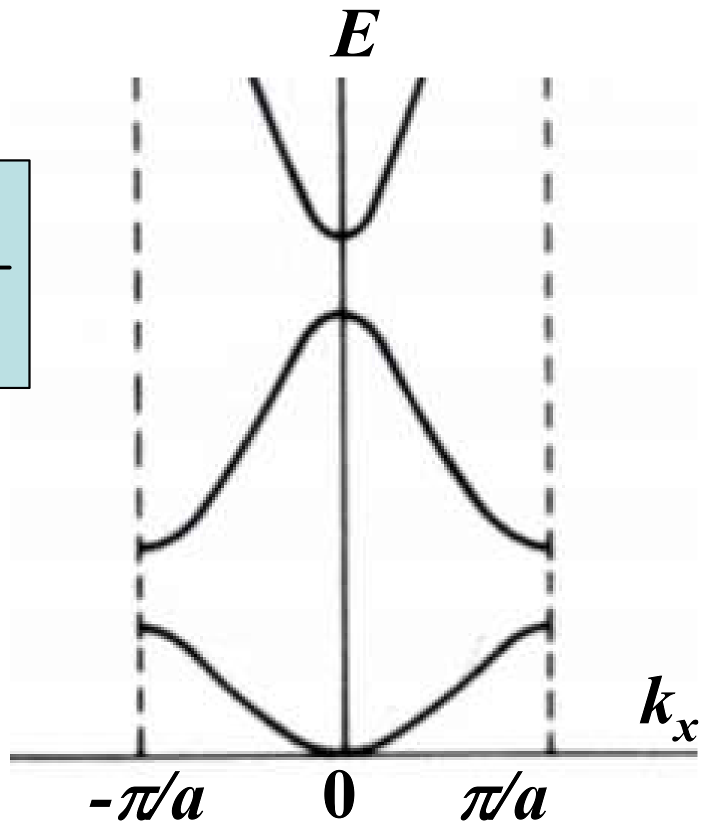
Number of states are infinite.
Number of electrons are finite.

Energy States

How many energy states in each band?

$$N = 2 \cdot \frac{\text{size of FBZ}}{\text{density of } k \text{ points}} = 2 \cdot \frac{2\pi / a}{2\pi / L_x} = 2 \frac{L_x}{a} = 2n$$

$$k_x = \frac{2\pi n_x}{L_x}$$

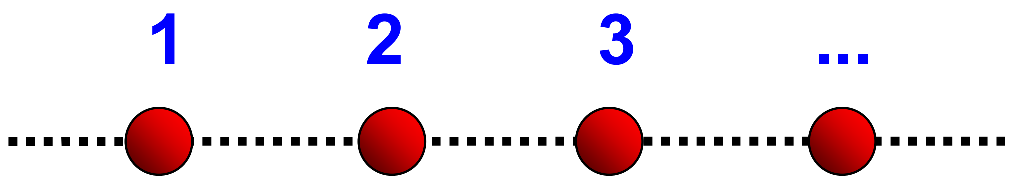


FBZ - First Brillouin Zone
N **- total number of states**
n = L/a **- number of primitive cells**
2 - spin up and down

Q: How about 2D and 3D cases?

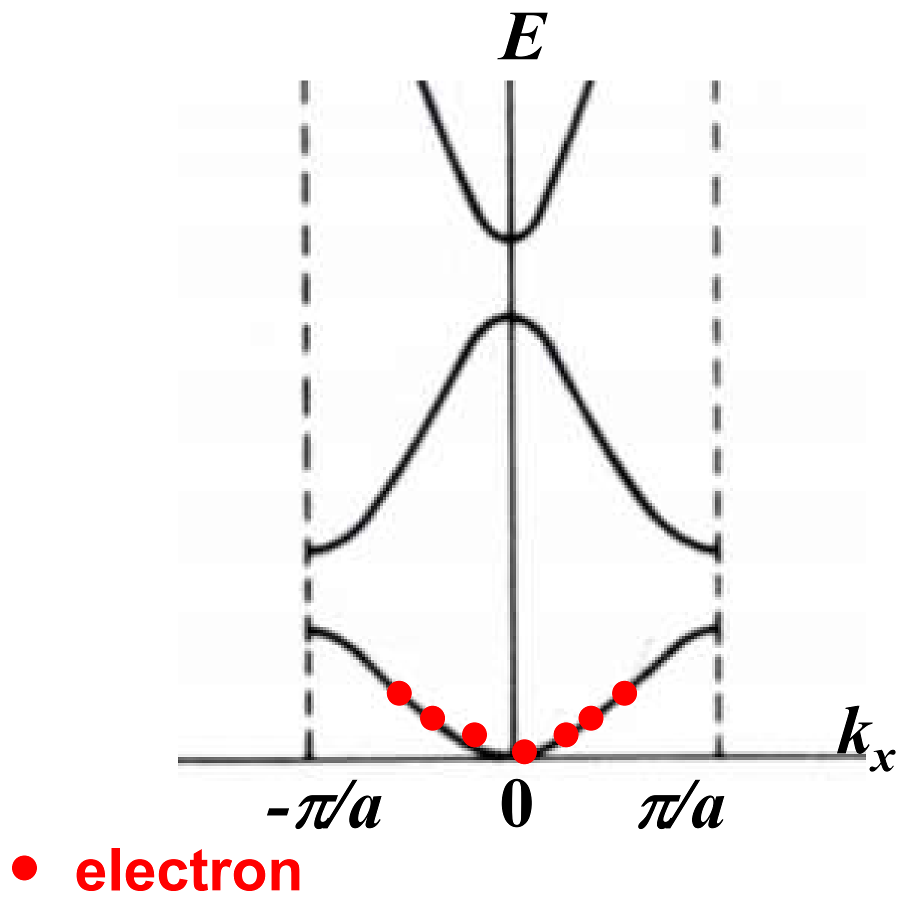
1D Chain of *Monovalent* Atoms

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



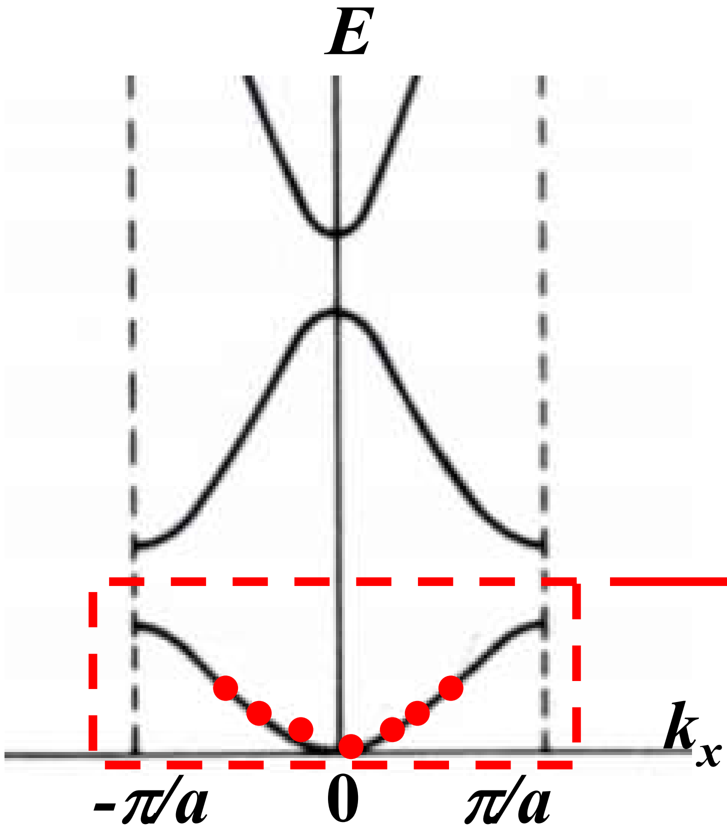
N = 2*n*
= total number of states

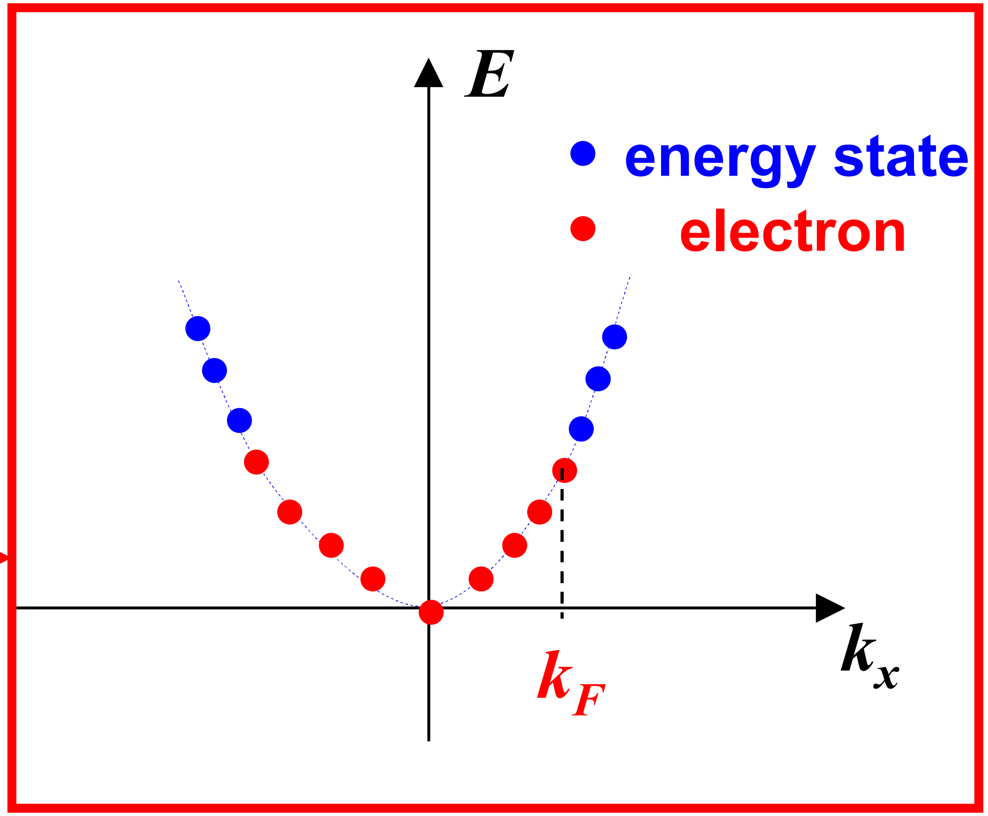
n = *L*/*a*
= number of primitive cells
= number of valence electrons



Electrons only fill half of the first band

1D Chain of *Monovalent* Atoms

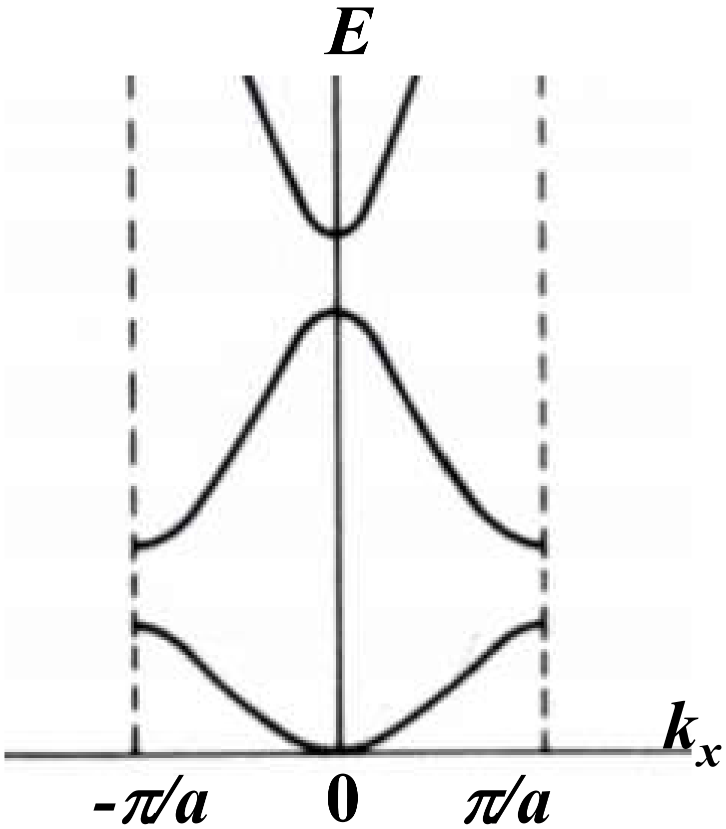


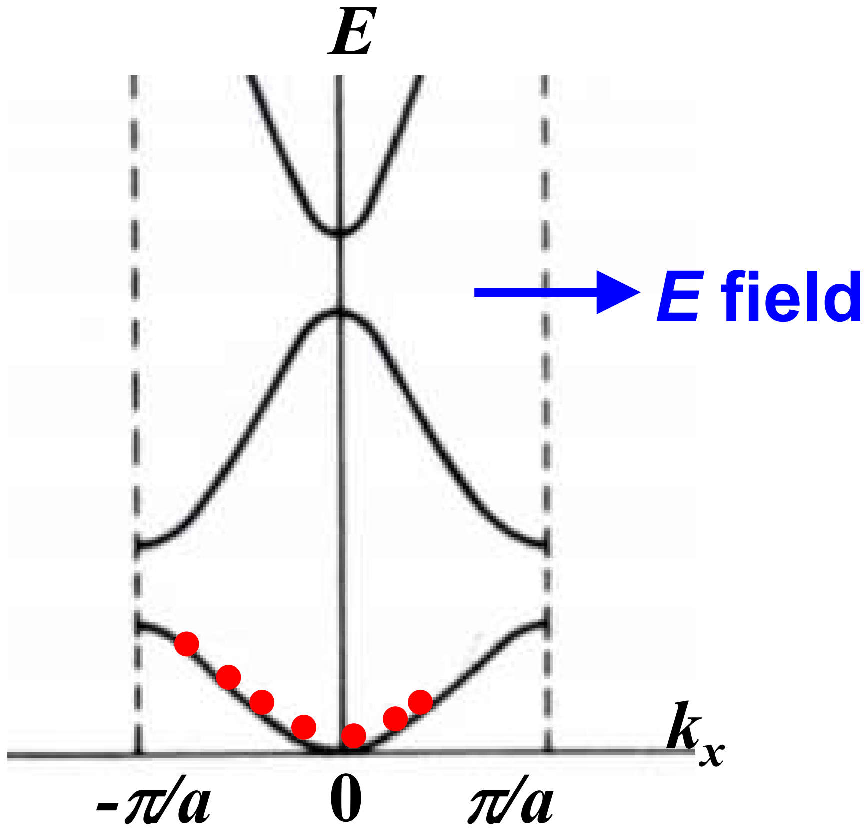


Electrons only fill half of the first band → ***Free Electrons*** → ***Conductor***

parabolic function

1D Chain of *Monovalent* Atoms





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

when *E ≠ 0, v > 0*
electric current

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

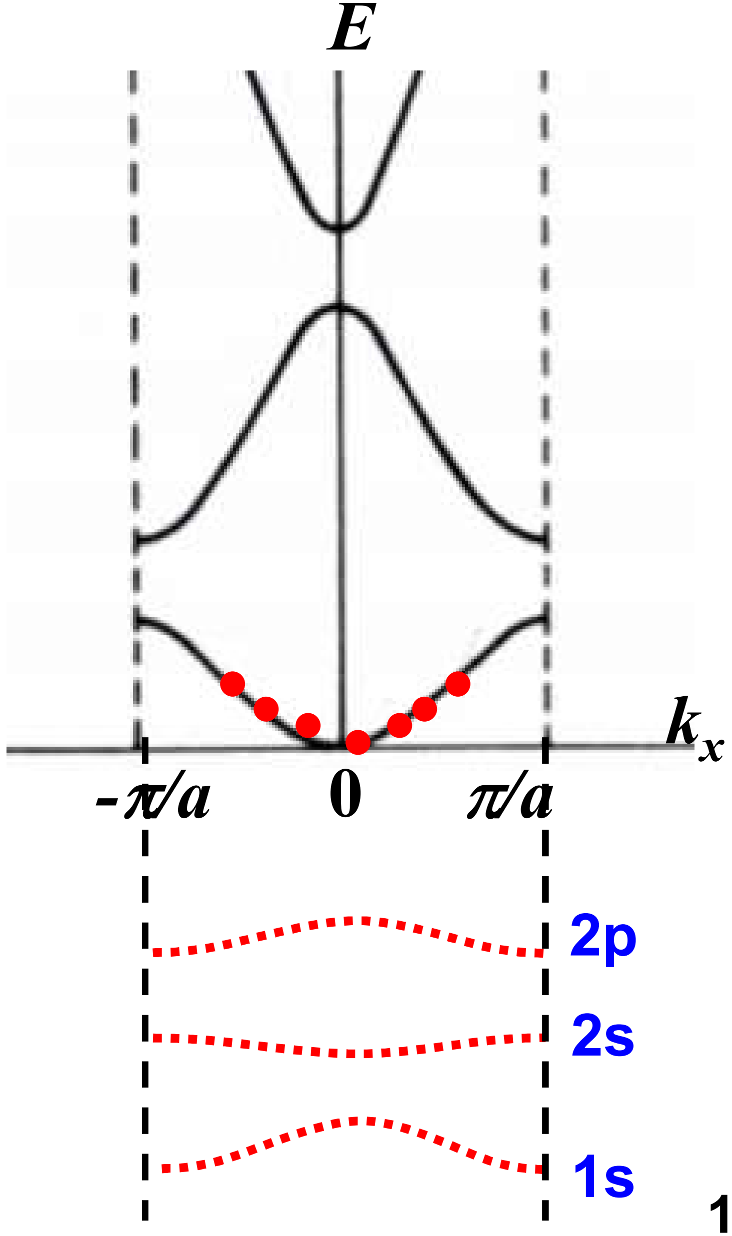
1D Chain of *Monovalent* Atoms

Question:

A Na atom has 11 electrons.
[$1s^2$ $2s^2$ $2p^6$] $3s^1$
Where are the rest 10 electrons?

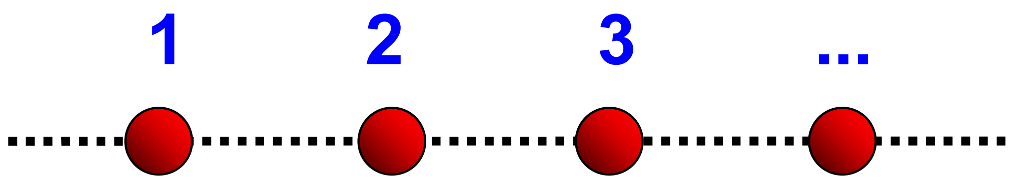
Answer:

Localized electrons have lower energies. All the lower bands are completely full. So they have no contribution to conductivity.



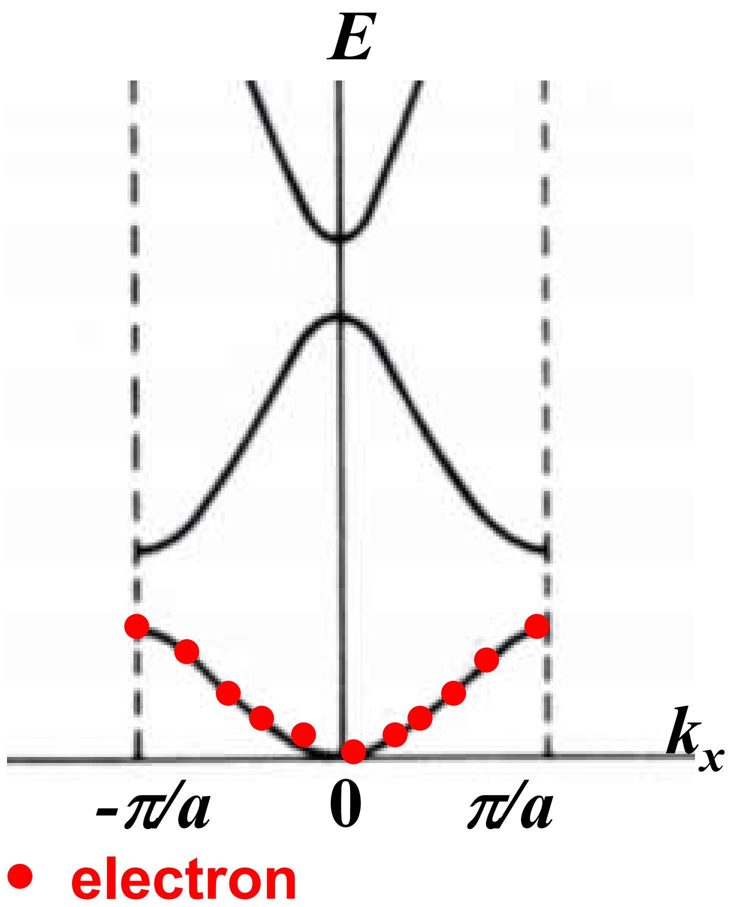
1D Chain of *Divalent* Atoms

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



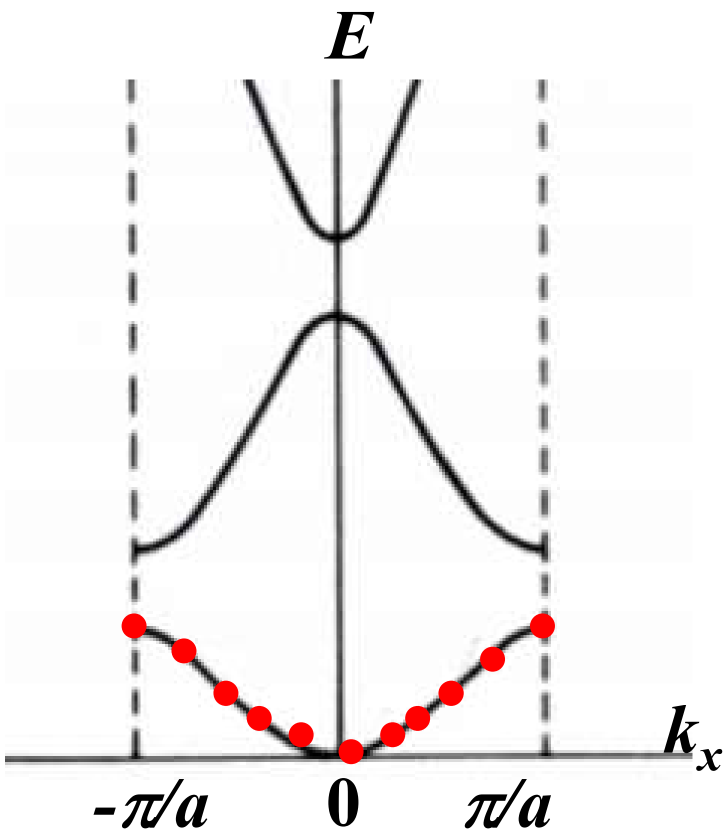
N* = 2*n
= total number of states

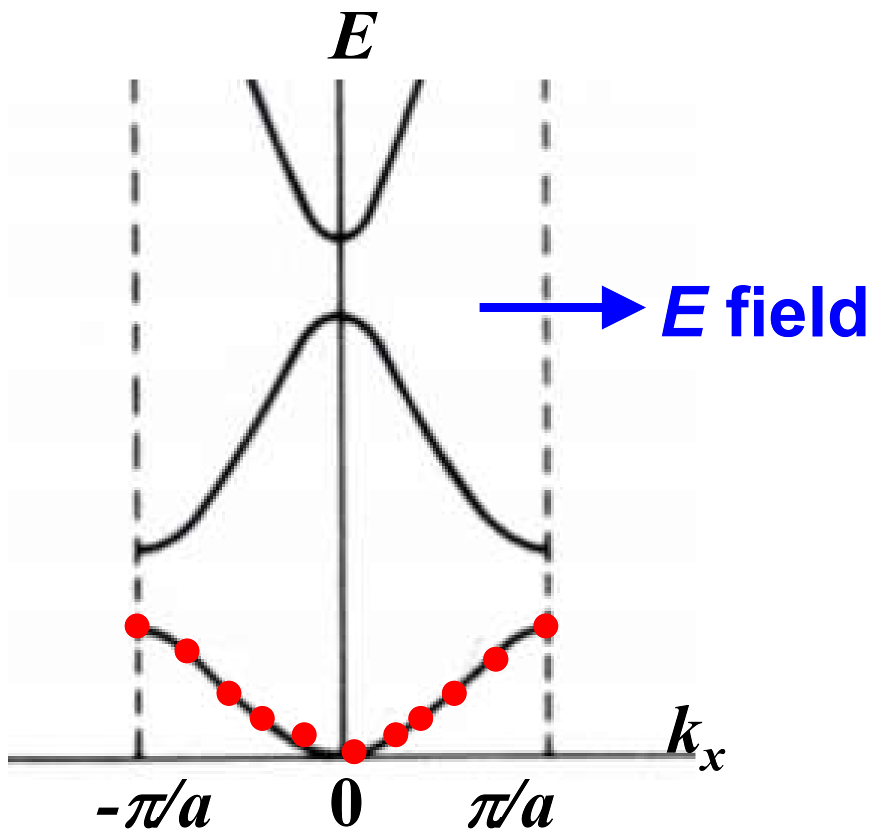
number of valence electrons
= 2*L*/*a* = 2*n*



Electrons fill the entire band

1D Chain of *Divalent* Atoms





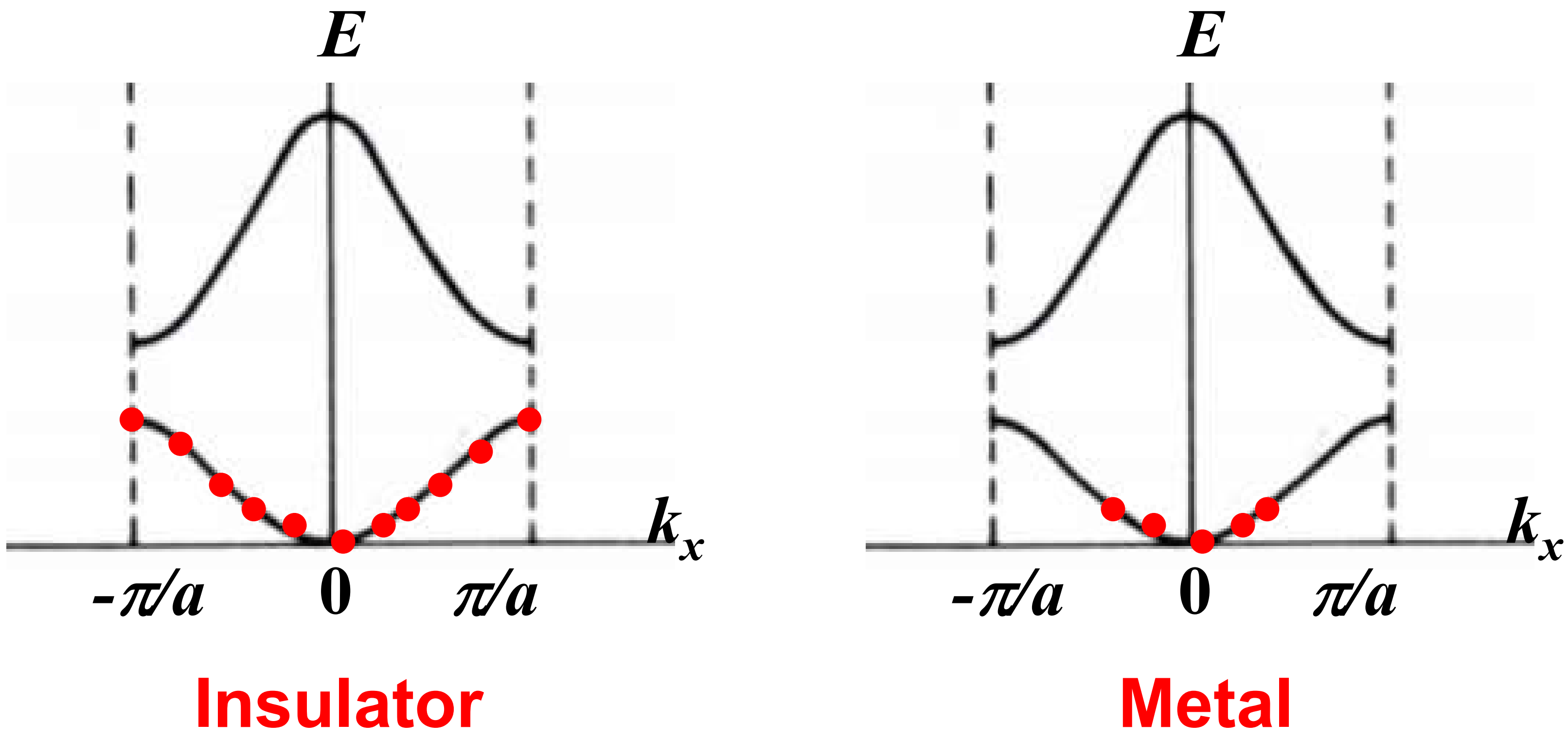
when $E = 0$, $v = 0$
no current

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

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

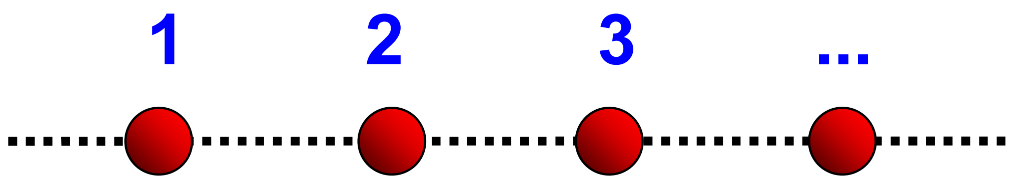
Metal vs. Insulator

- **Metals and Insulators are fundamentally different**
  - **Insulators are not just "bad" metals**
  - **An insulator has all bands completely filled or empty**
  - **A metal has partially filled bands**



1D Chain of *Trivalent* Atoms

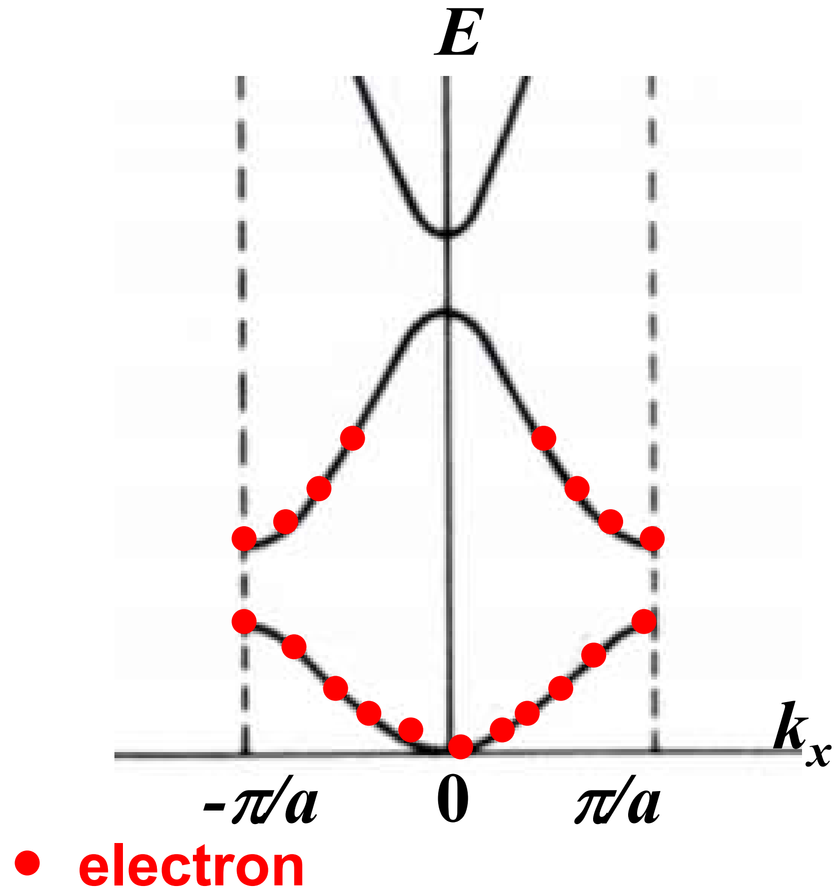
Each atom has *three* valence electrons (Al, Ga, ...)



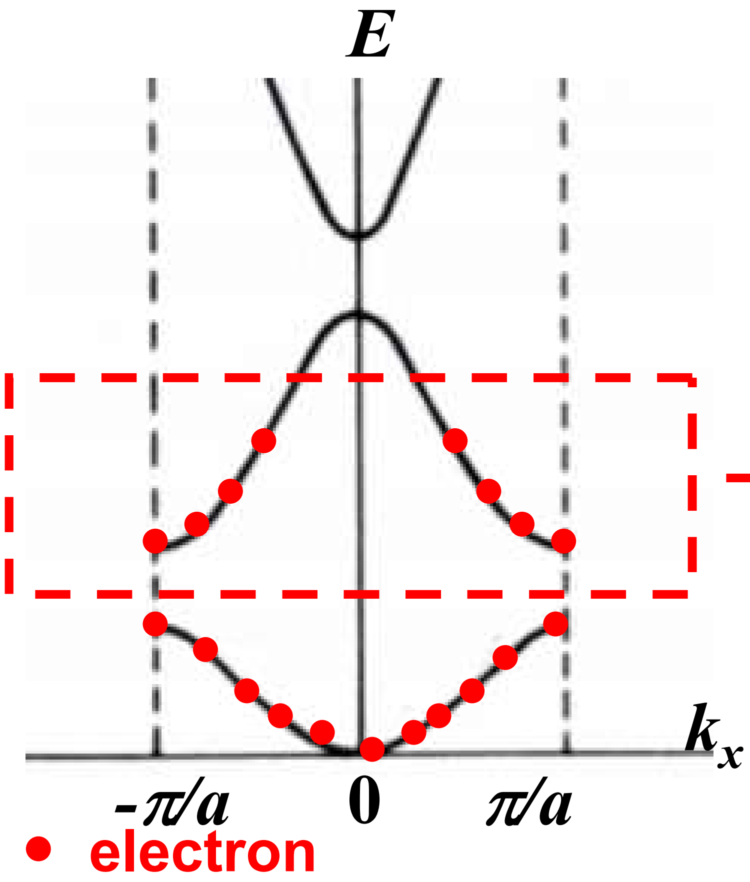
N* = 2*n
= total number of states

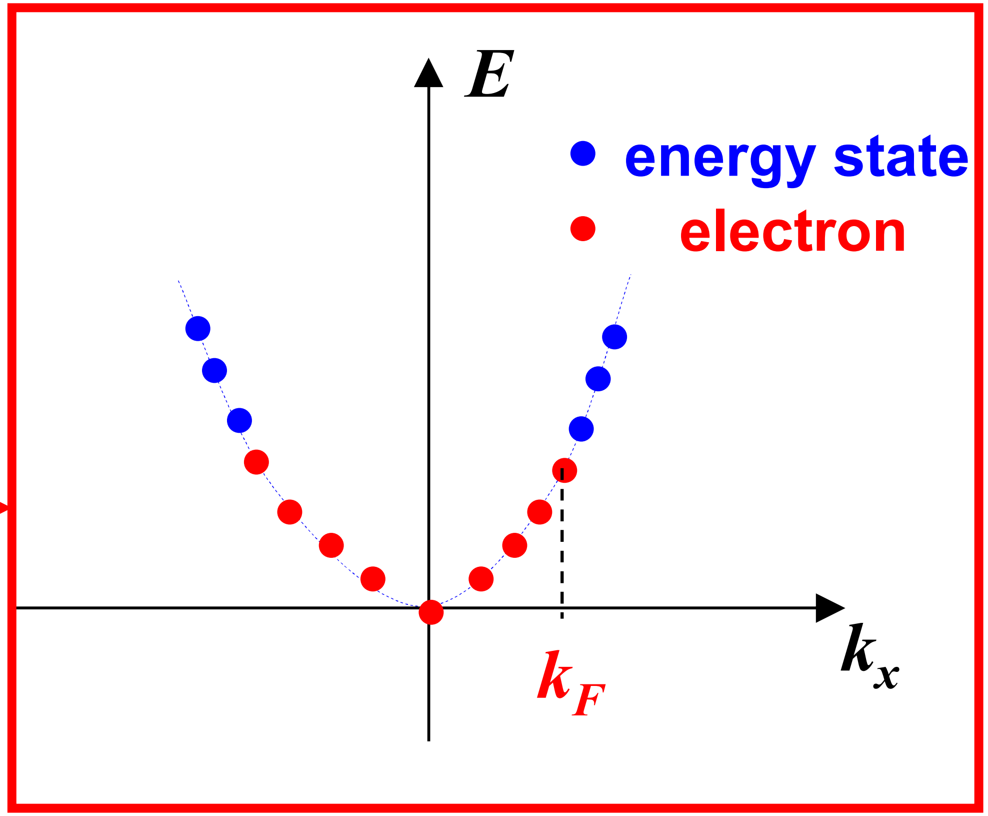
number of valence electrons
= 3*L*/*a* = 3*n*

Electrons start to fill the second band



1D Chain of *Trivalent* Atoms





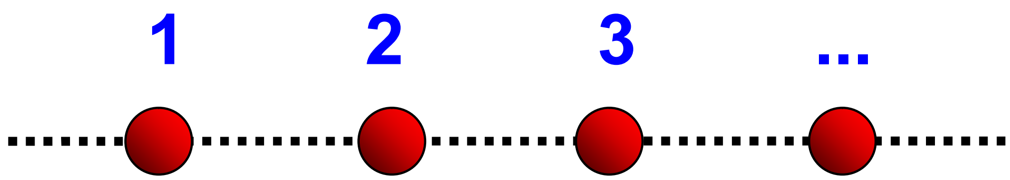
→ ***Free Electrons***

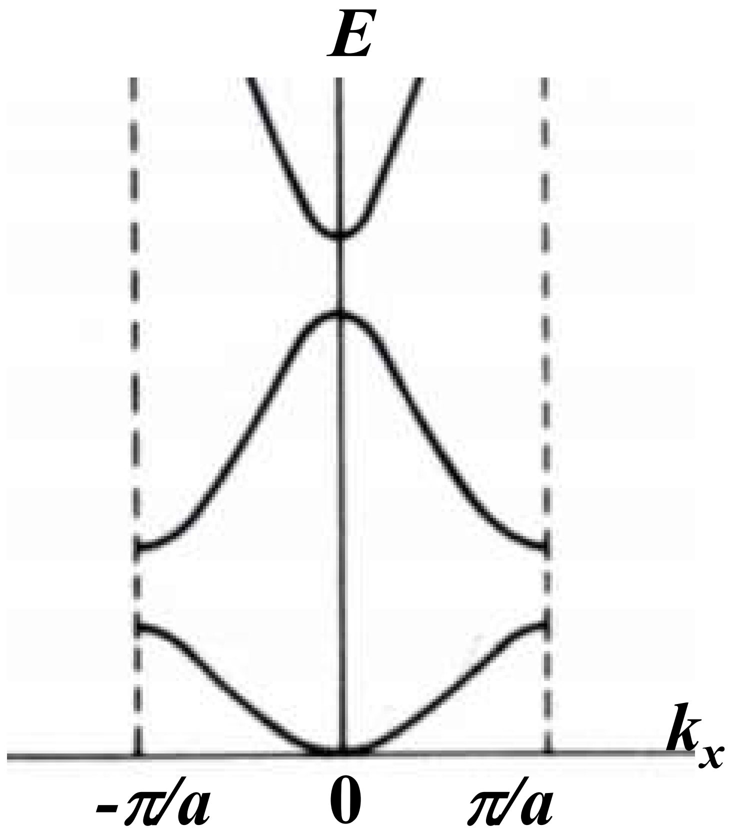
↓

Conductor

1D Chain of *Quadrivalent* Atoms

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



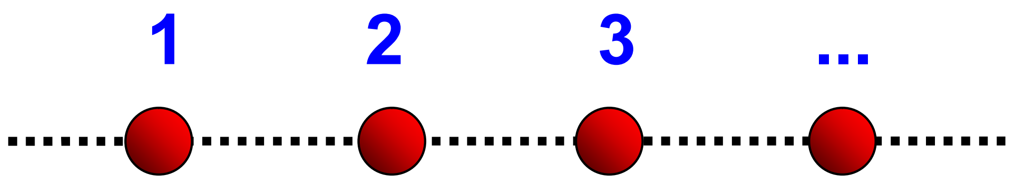


• electron

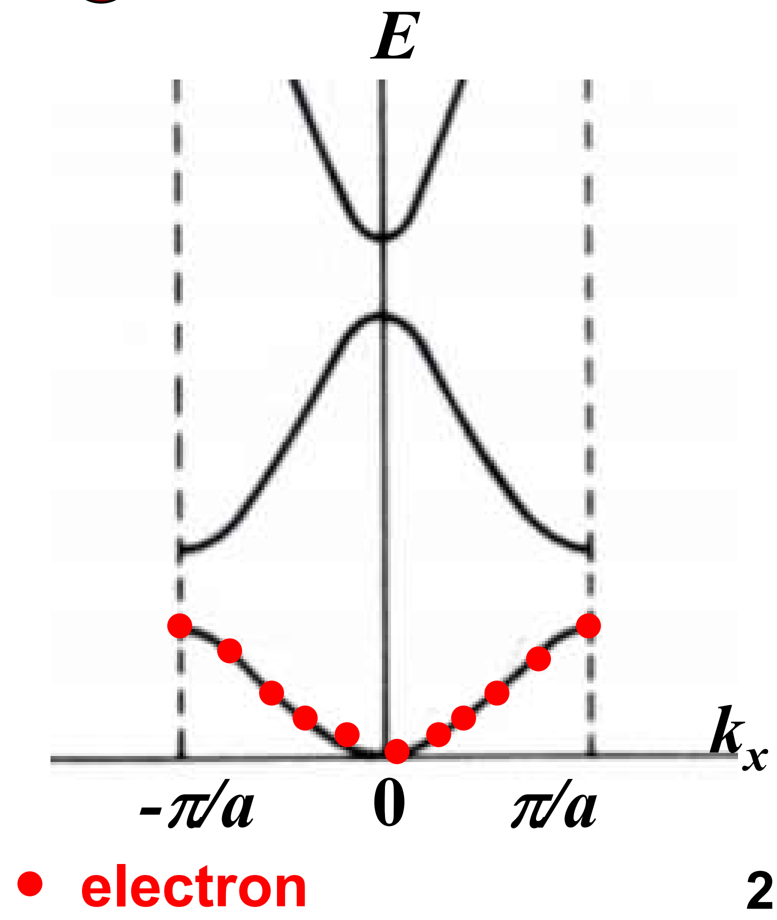
Q: How do electrons fill the bands?
Is it a conductor, or an insulator?

1D Chain of *Divalent* Atoms

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



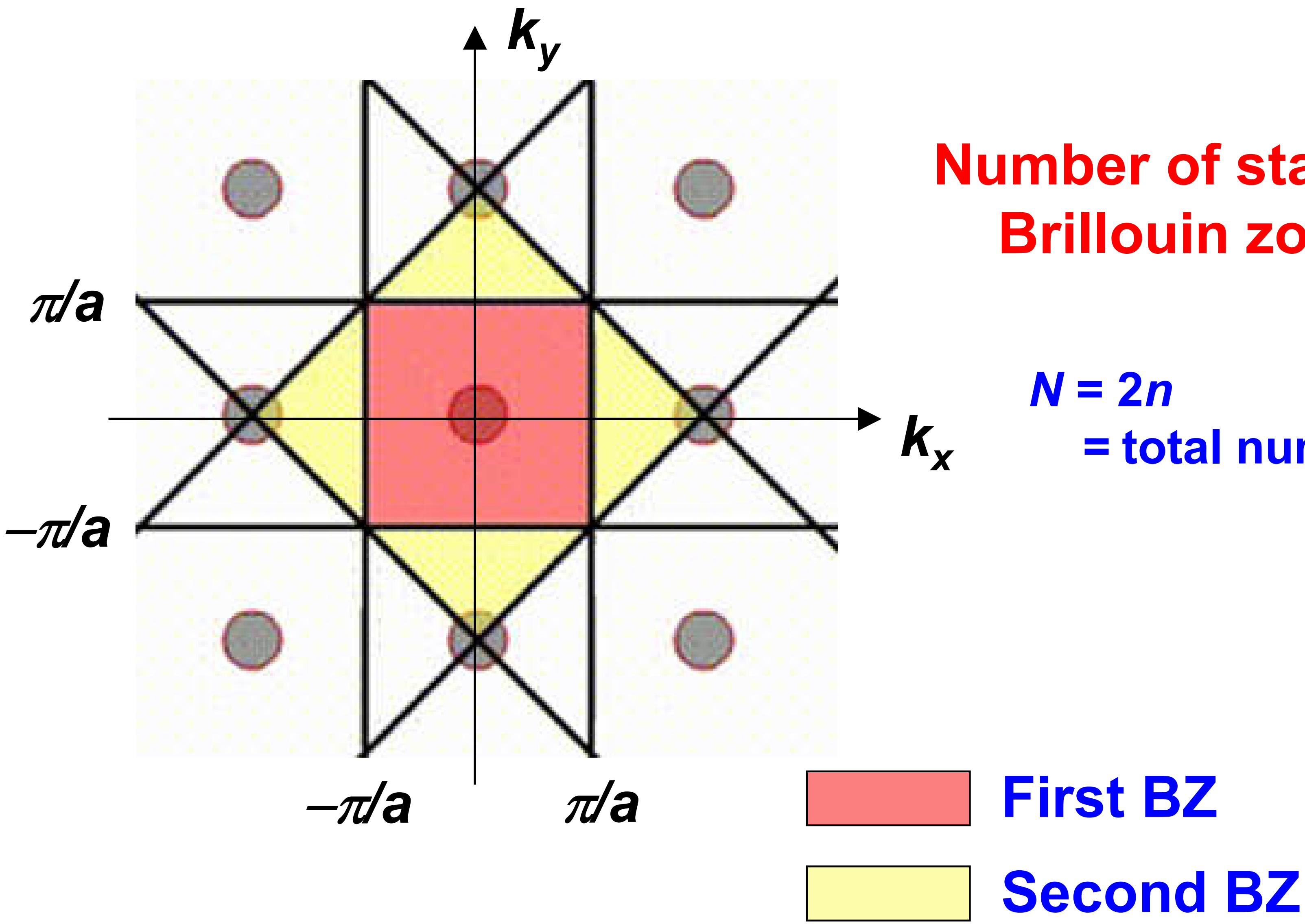
Electrons fill the entire band
--->
insulator



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

2D case

Assume a square lattice in the reciprocal space



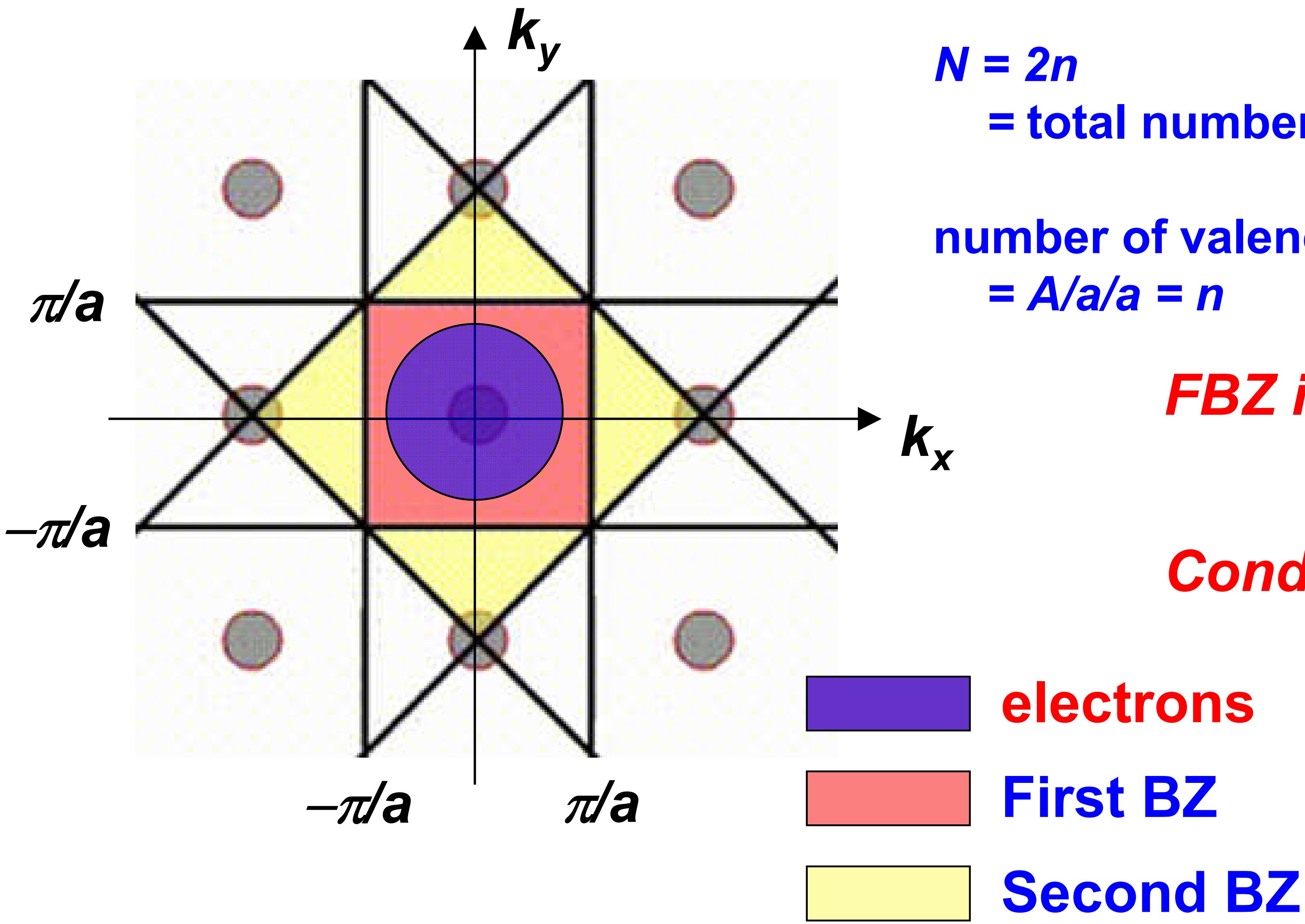
Number of states in each Brillouin zone

$N = 2n$

= total number of states

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*

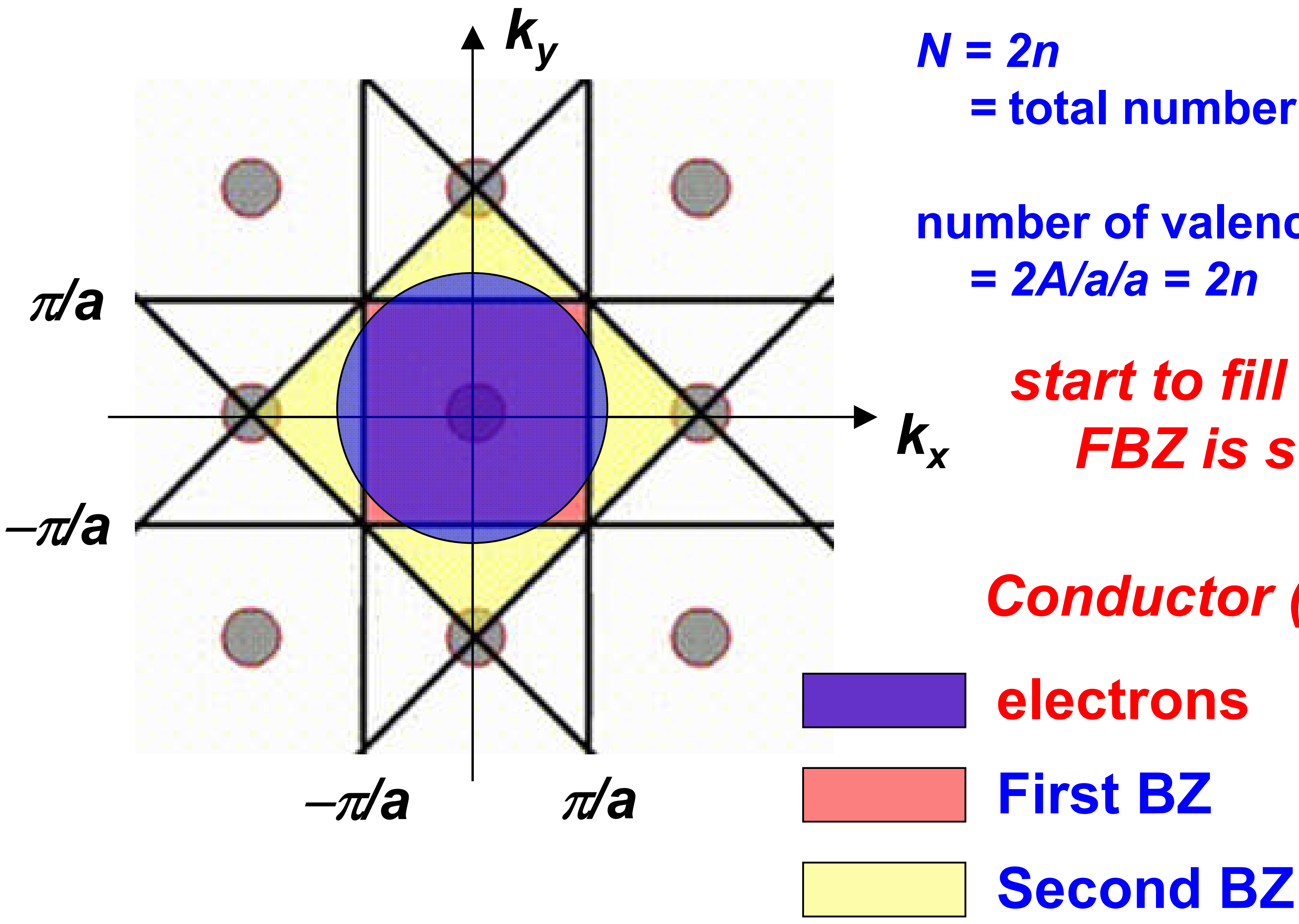
FBZ is not full

↓

Conductor

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*

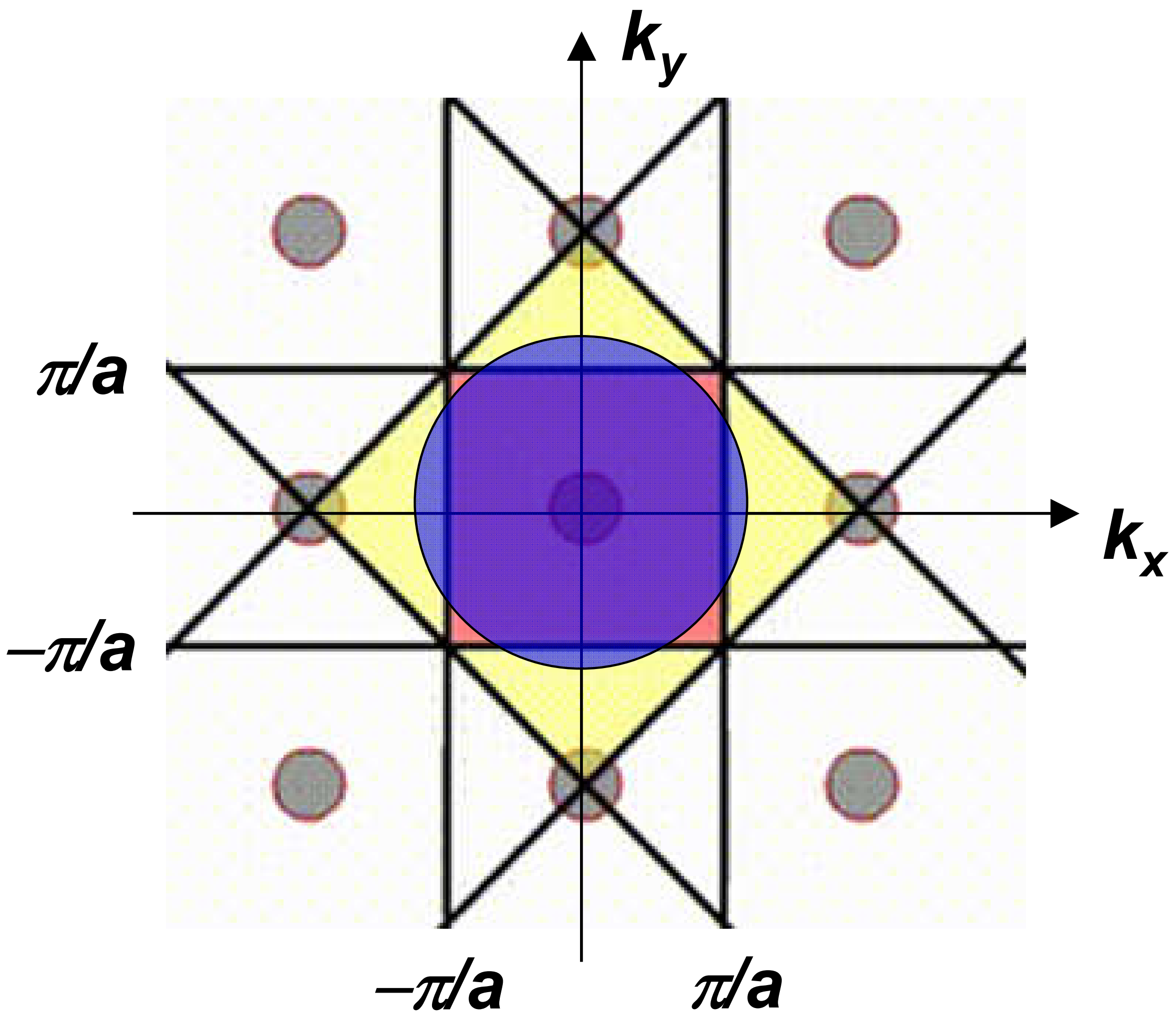
start to fill SBZ, but FBZ is still not full

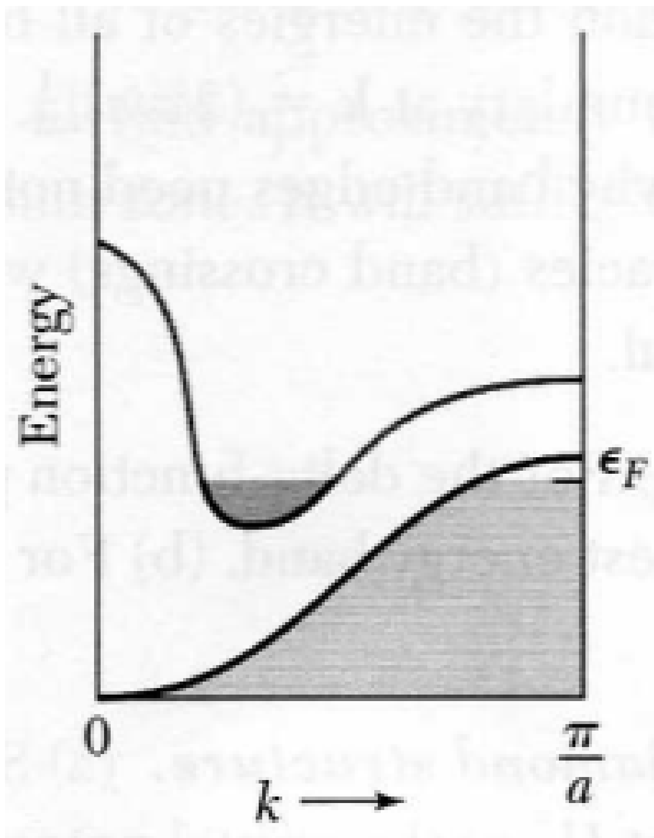
↓

Conductor (semimetal)

2D case of *Divalent* Atoms

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

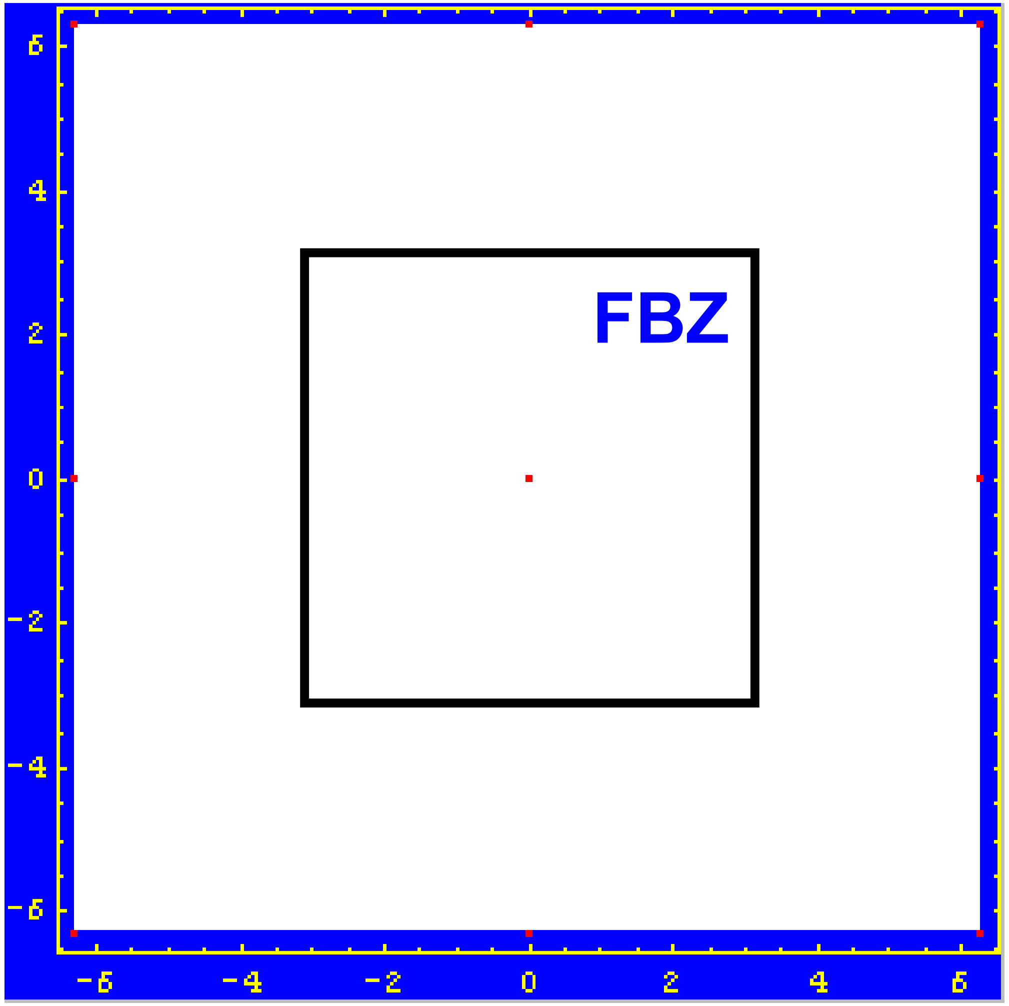




semimetal 半金属

2D Fermi Surface

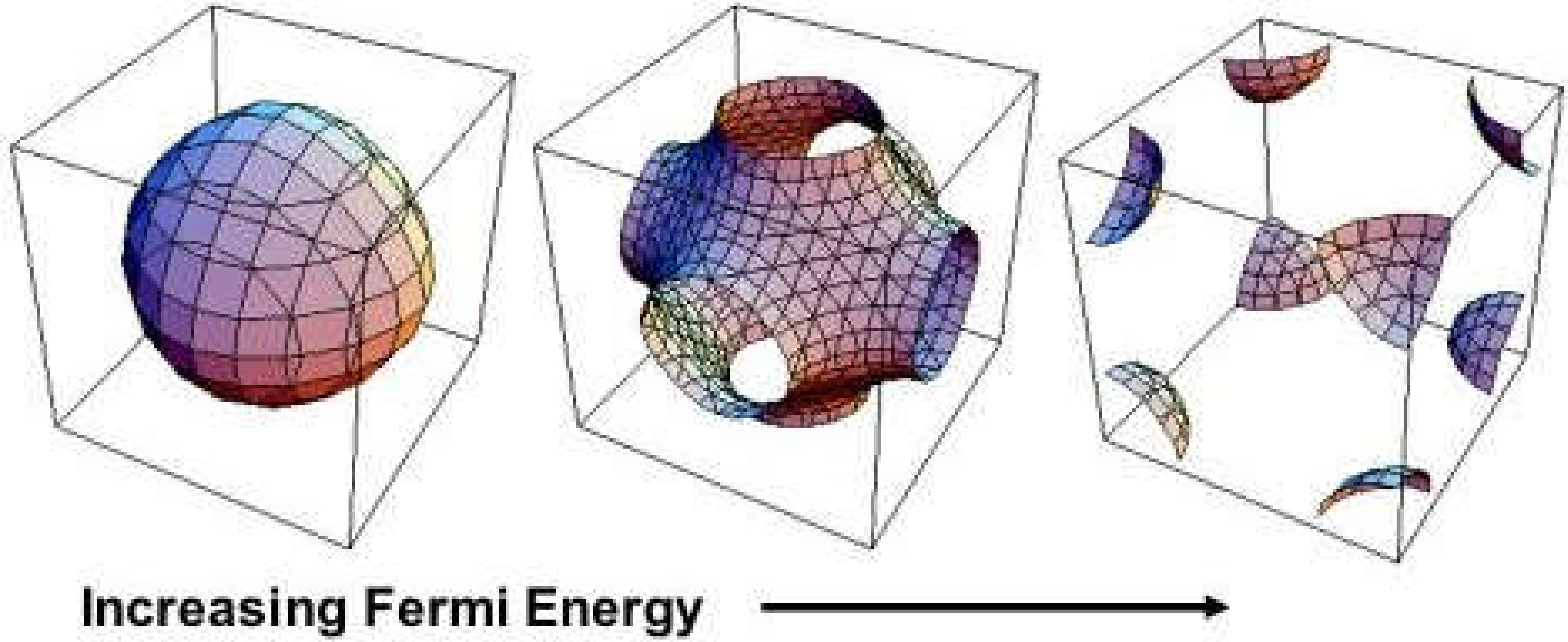
simple square



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

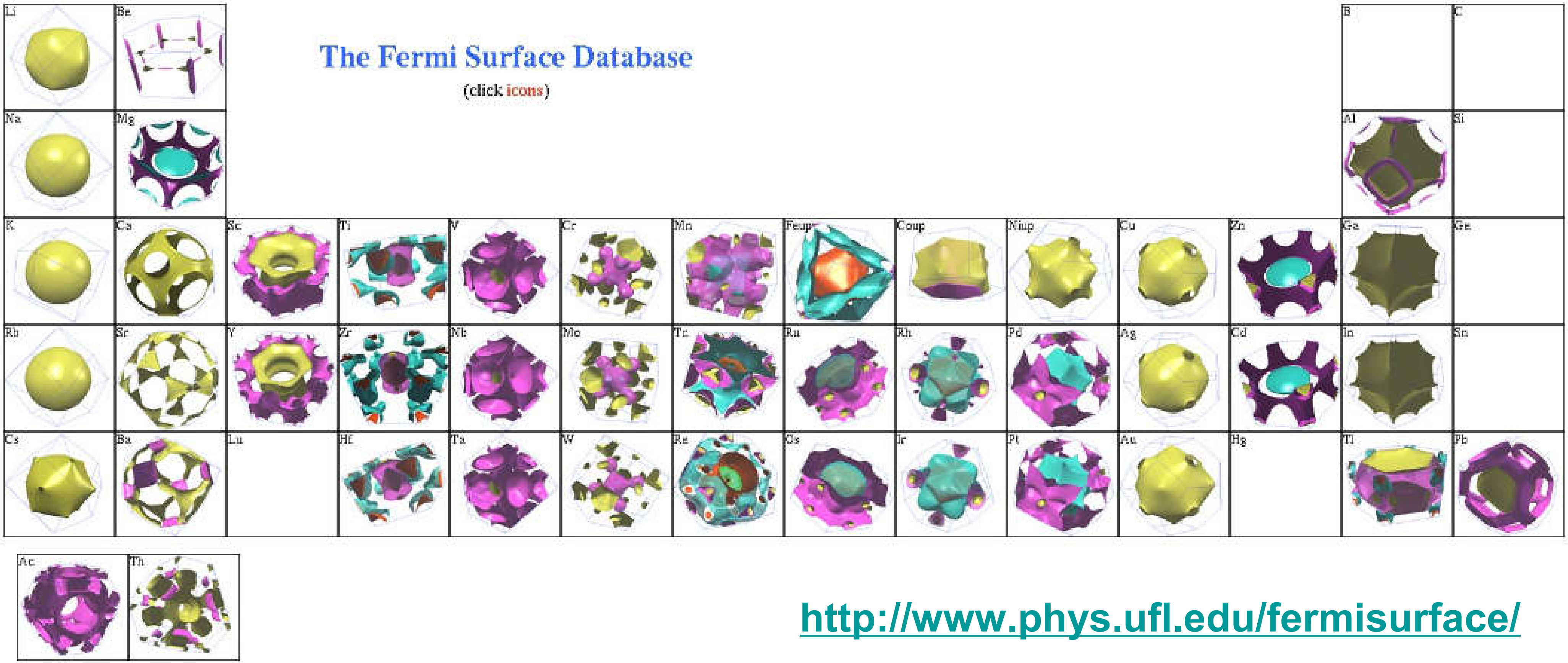
3D Fermi Surface

simple cubic



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

3D Fermi Surface – More Examples

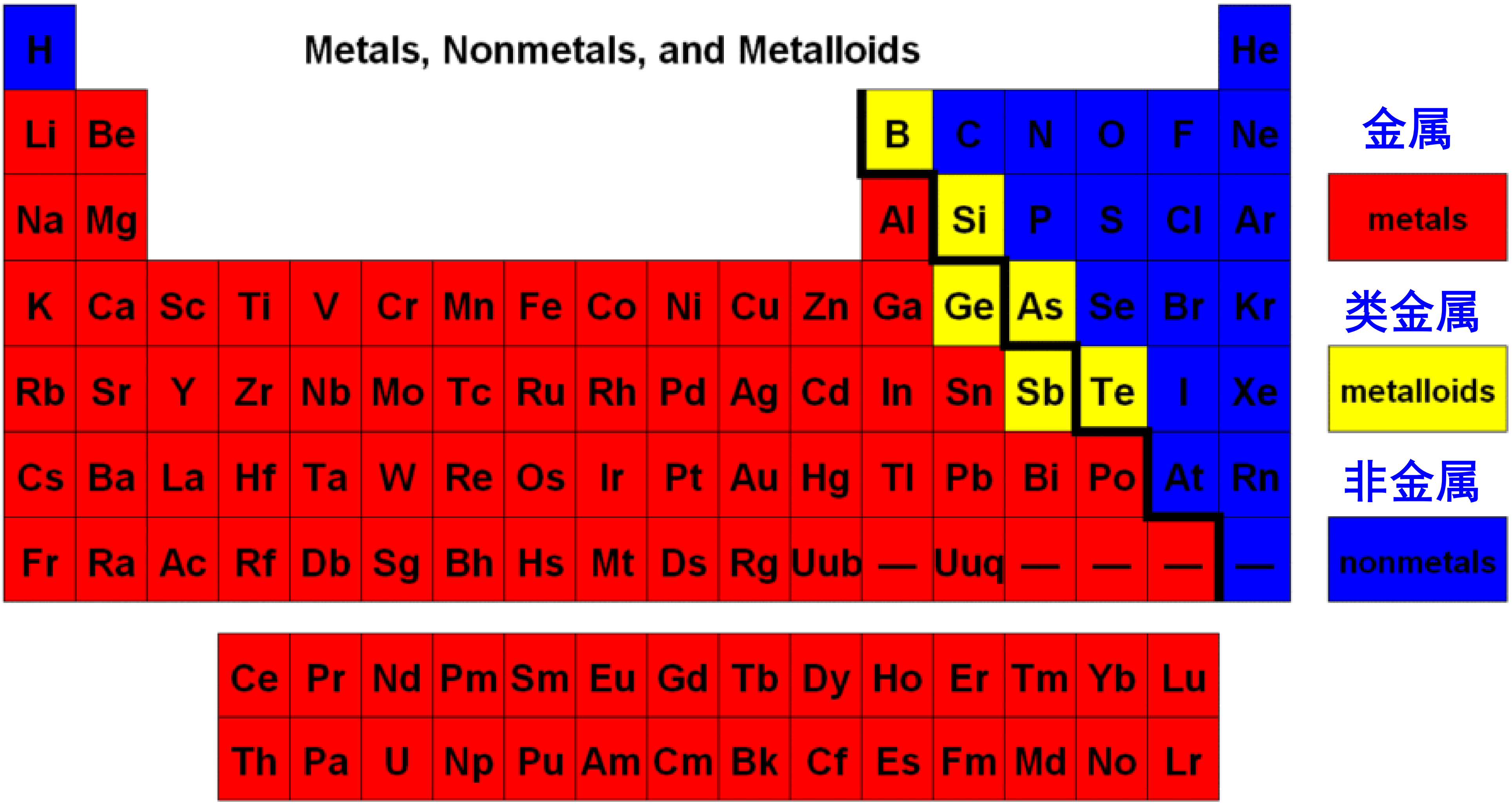


http://www.phys.ufl.edu/fermisurface/

Fermi surface is the surface in reciprocal space which separates occupied from unoccupied electron states at *T* = 0 K.

S. B. Dugdale, *Phys. Scr.* **91,** 053009 (2016)

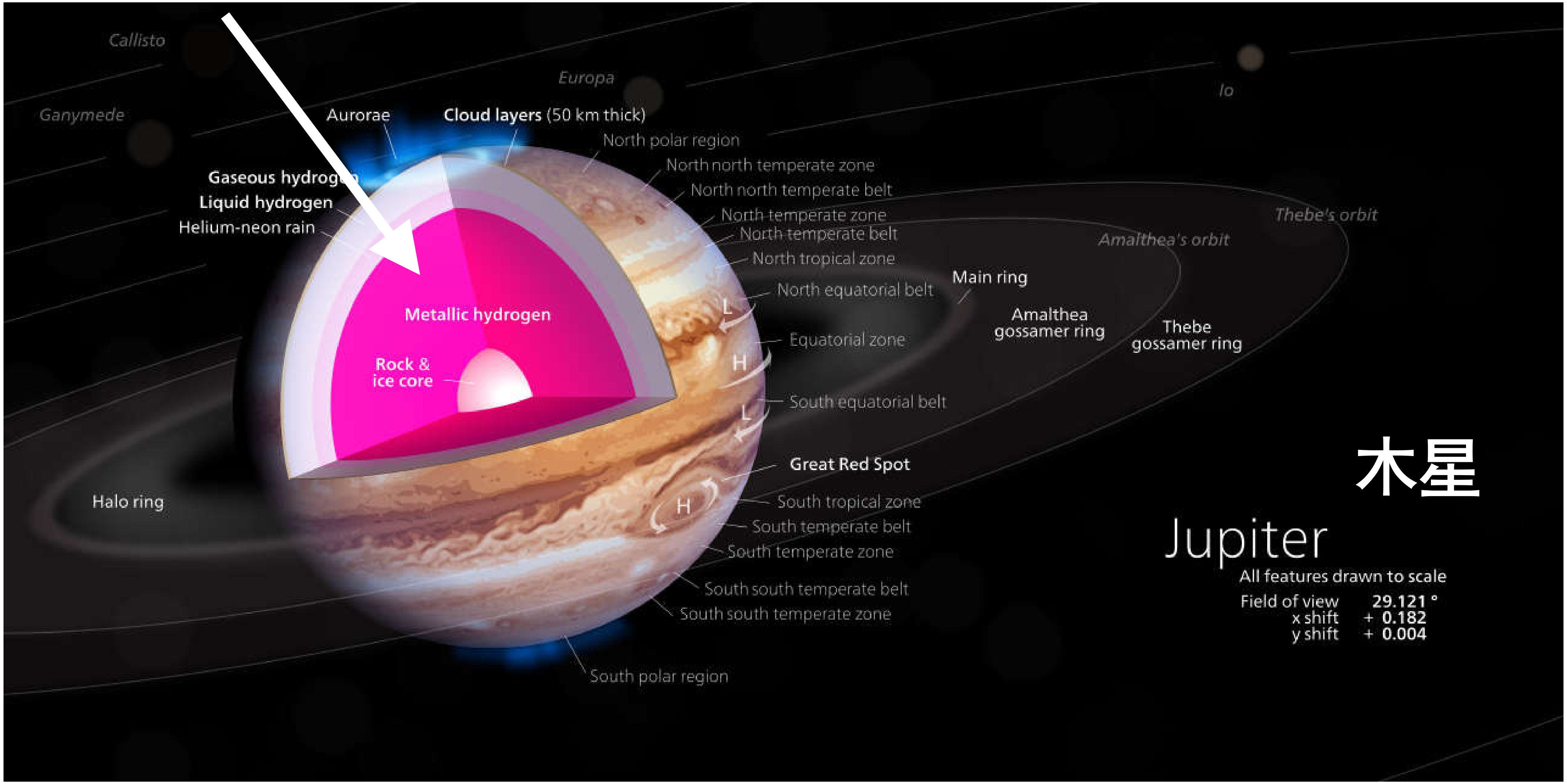
Metals in the Periodic Table



https://www.angelo.edu/faculty/kboudrea/periodic/physical_metals.htm

Solid Hydrogen is also Metallic

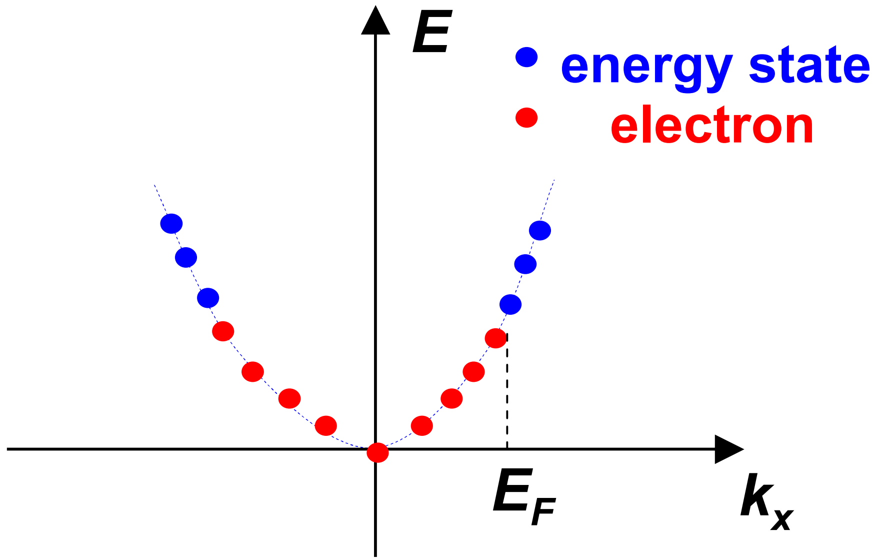
Metallic hydrogen only exists under very high pressure

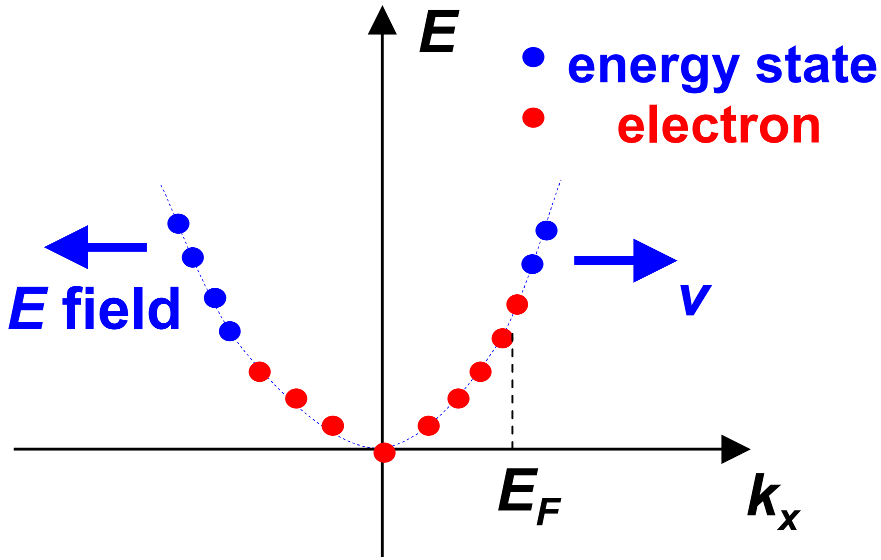


https://en.wikipedia.org/wiki/Metallic_hydrogen

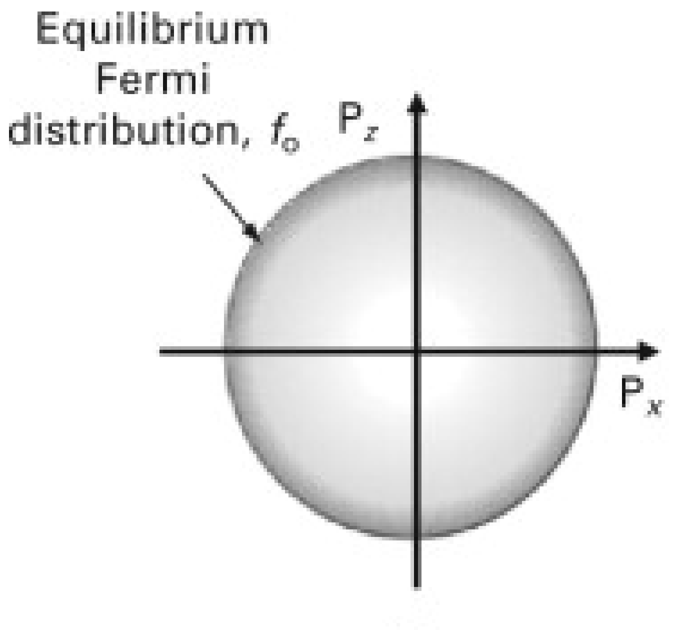
Electrical Conductivity - Revisit

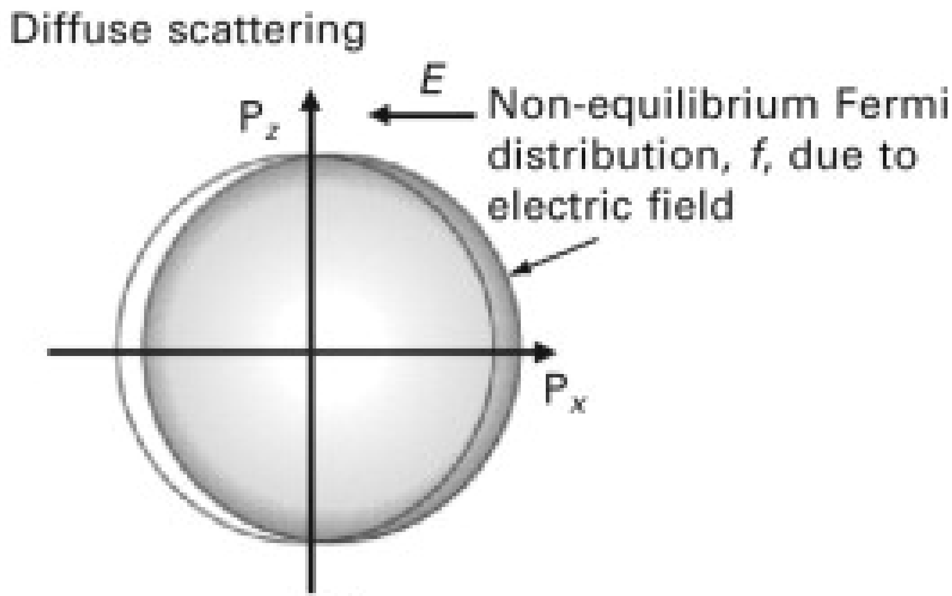
1D





2D
3D



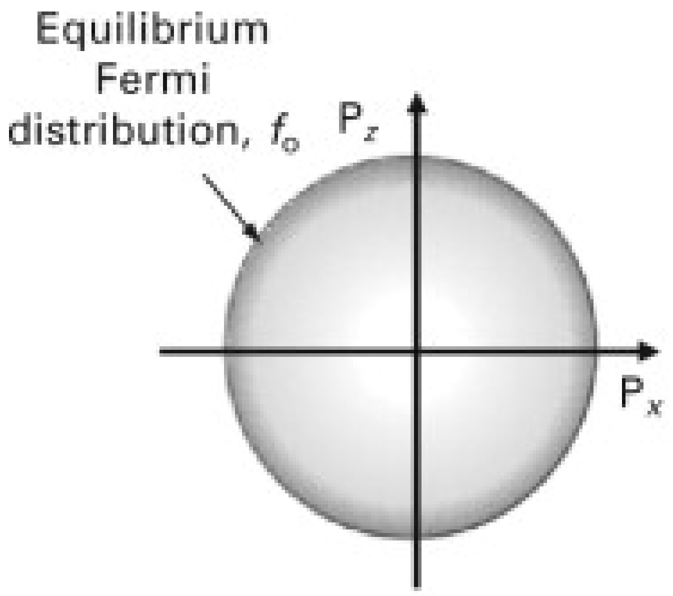


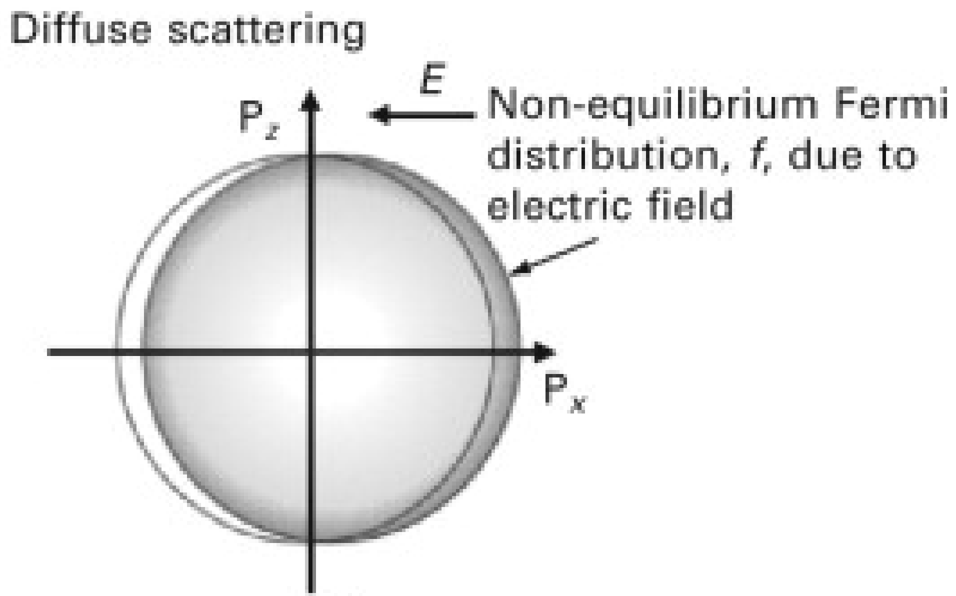
Electrical Conductivity - Revisit

- **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



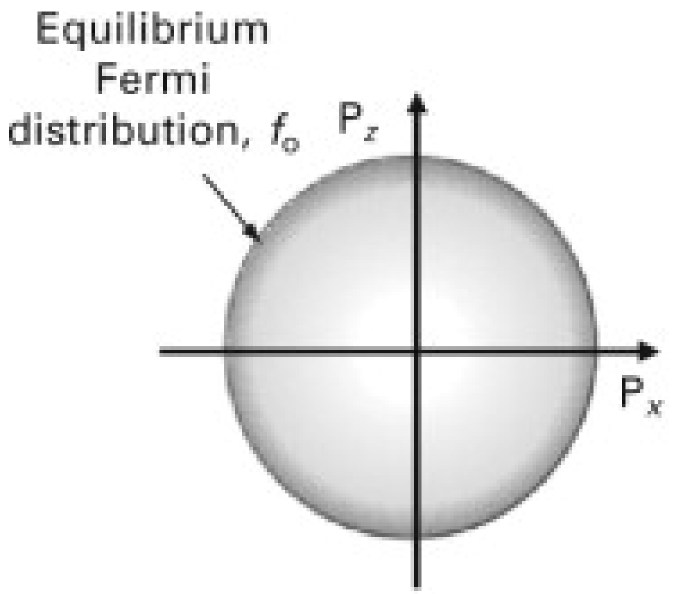


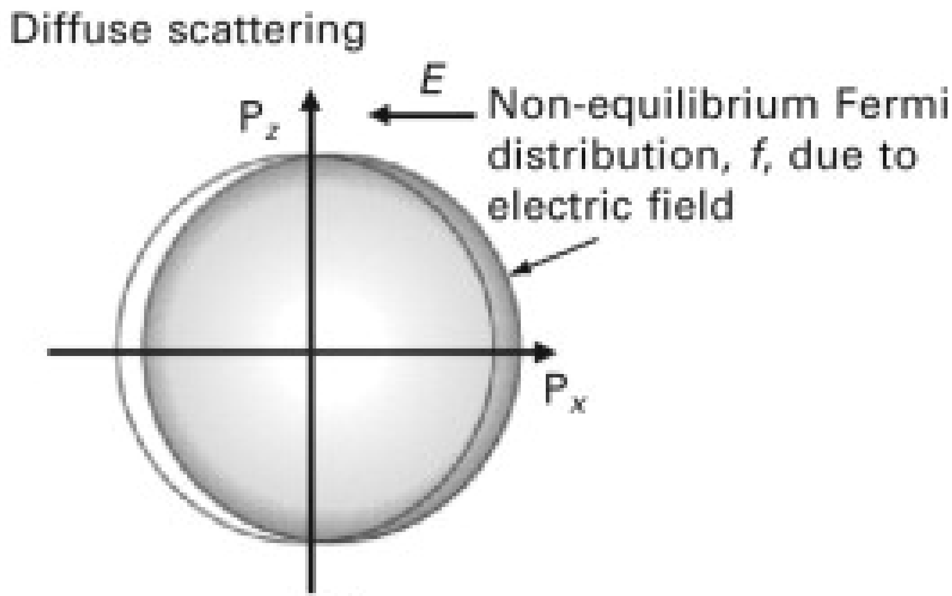
Electrical Conductivity - Revisit

- **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

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

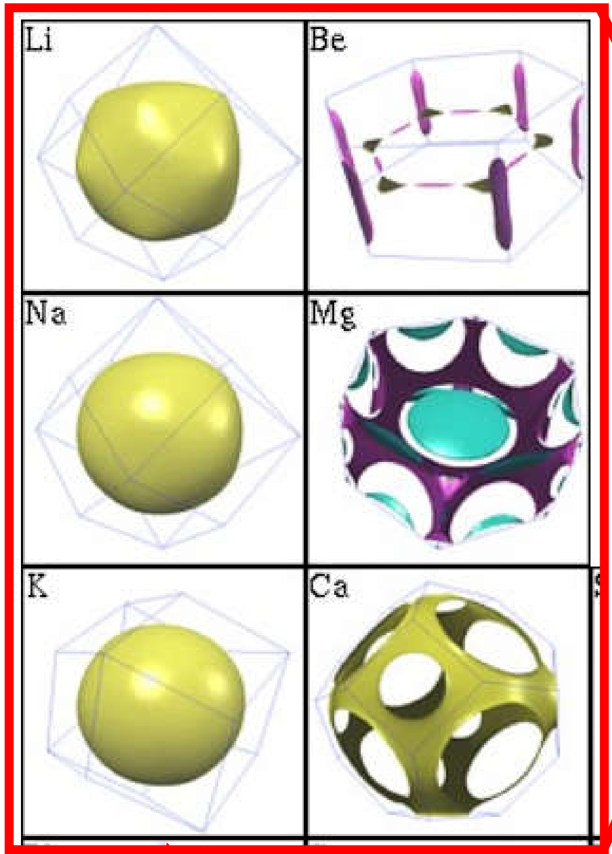
Electrical Conductivity - Revisit

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

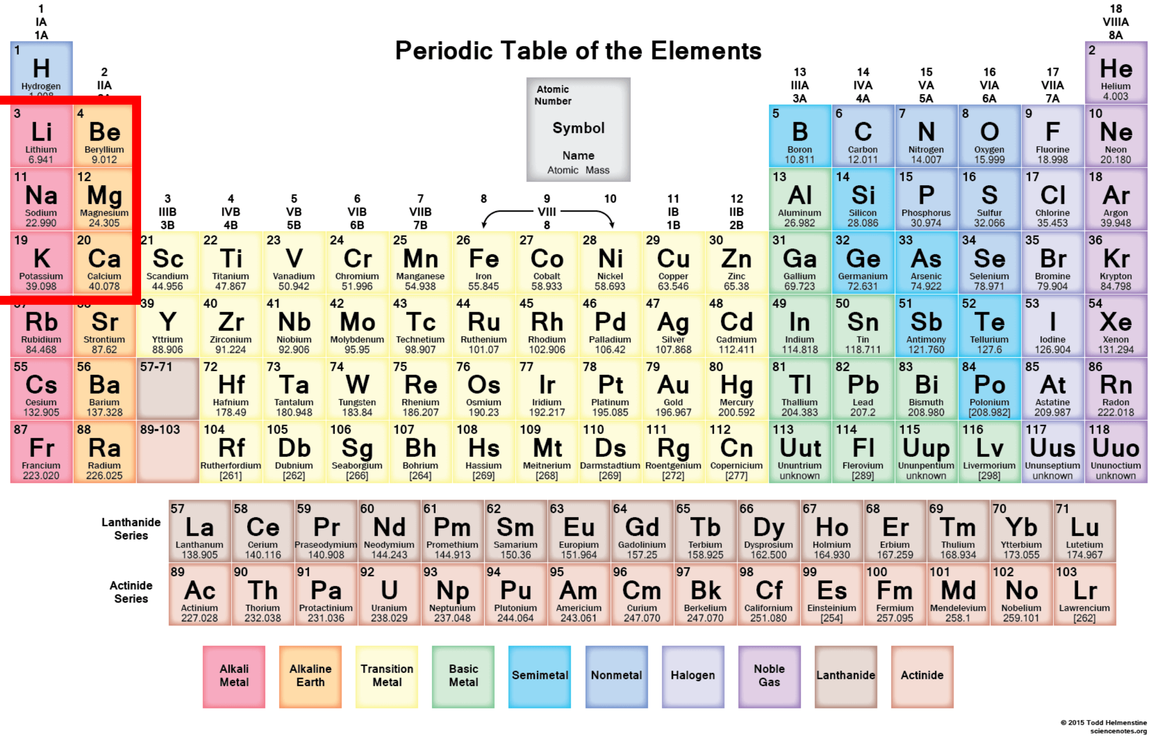
	Classical	Quantum
electron density n	all valence electrons	electrons near Fermi surface (depend on *E* field)
μ τ		
velocity v	average (depend on temperature)	Fermi velocity v_F
mass m	free electron m_0	effective mass m^*

3D Fermi Surface

IA **IIA**



Metals in Group IA and IIA have very different properties

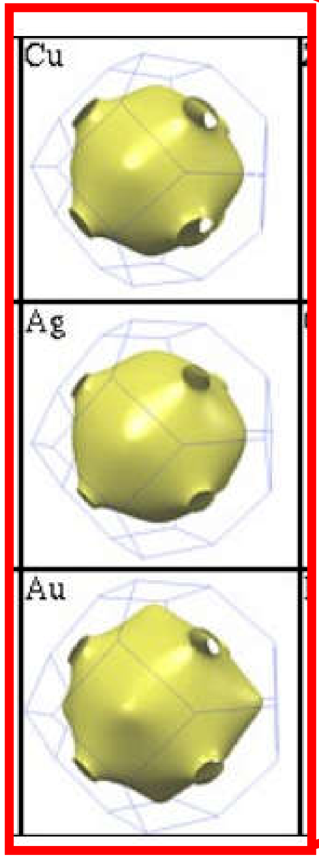


spherical shape
close to free electrons

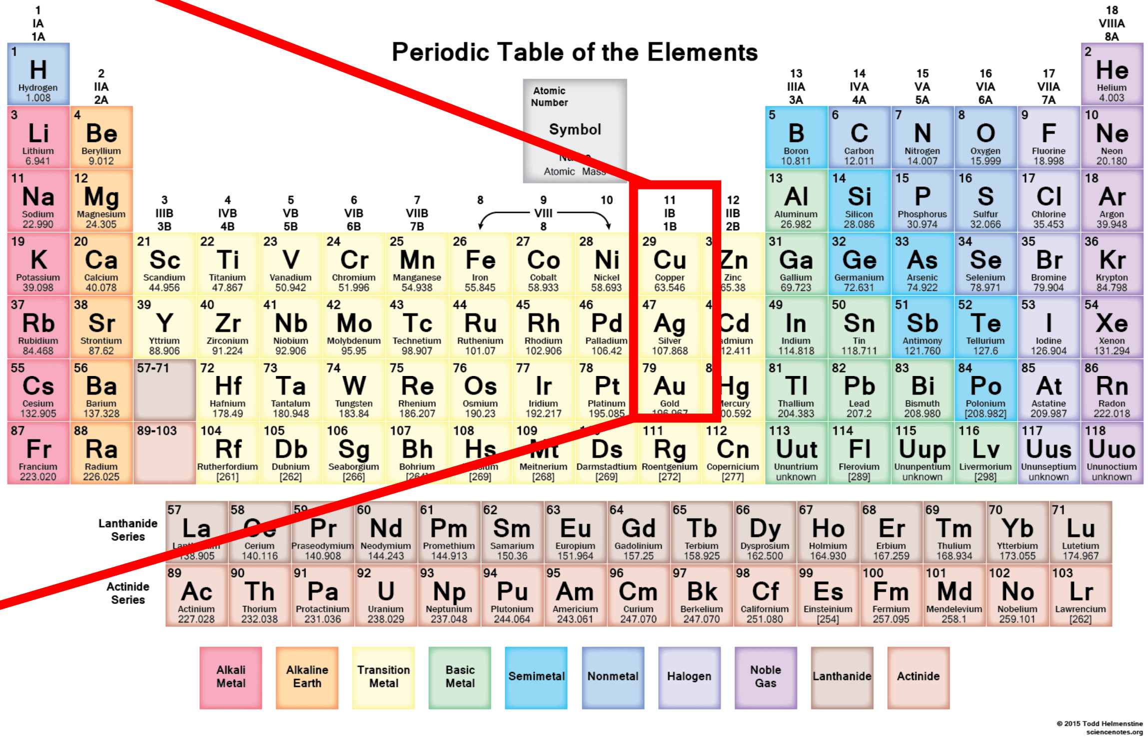
http://www.phys.ufl.edu/fermisurface/

3D Fermi Surface

IB



Metals in Group IB are very good conductors



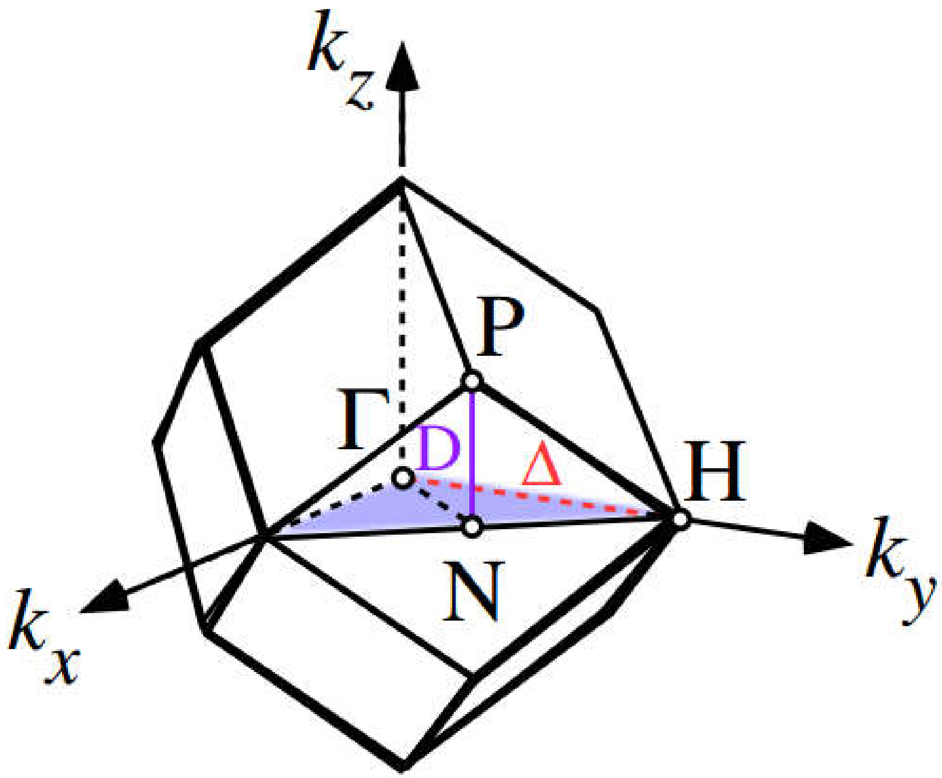
spherical shape

close to free electrons

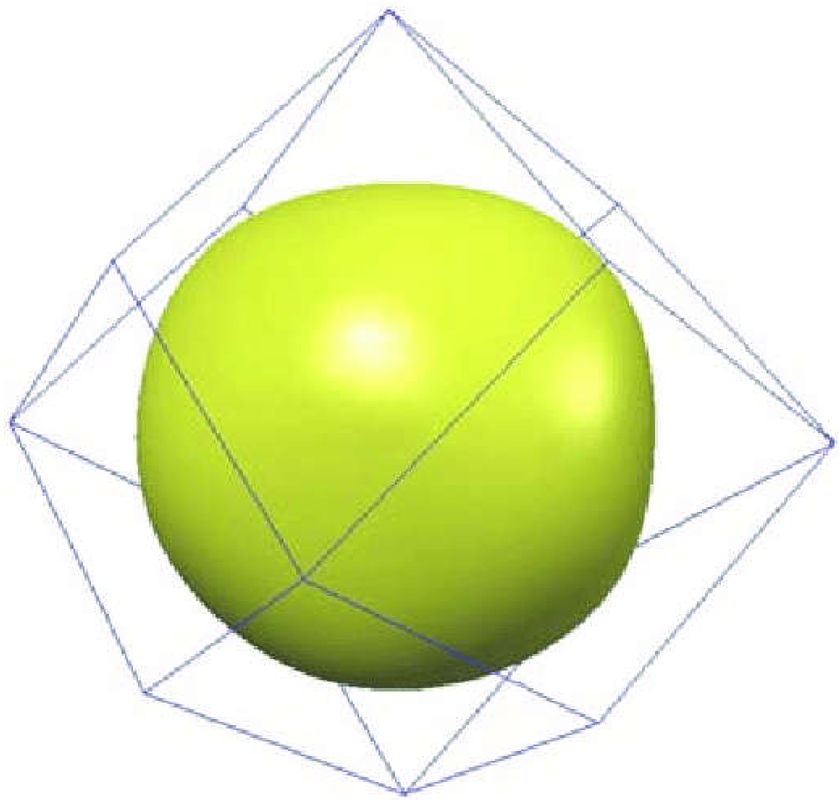
http://www.phys.ufl.edu/fermisurface/

3D case

sodium (BCC)



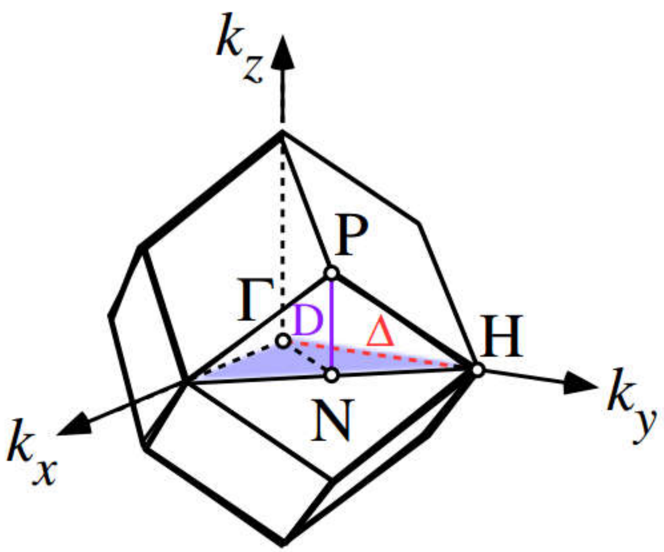
First BZ



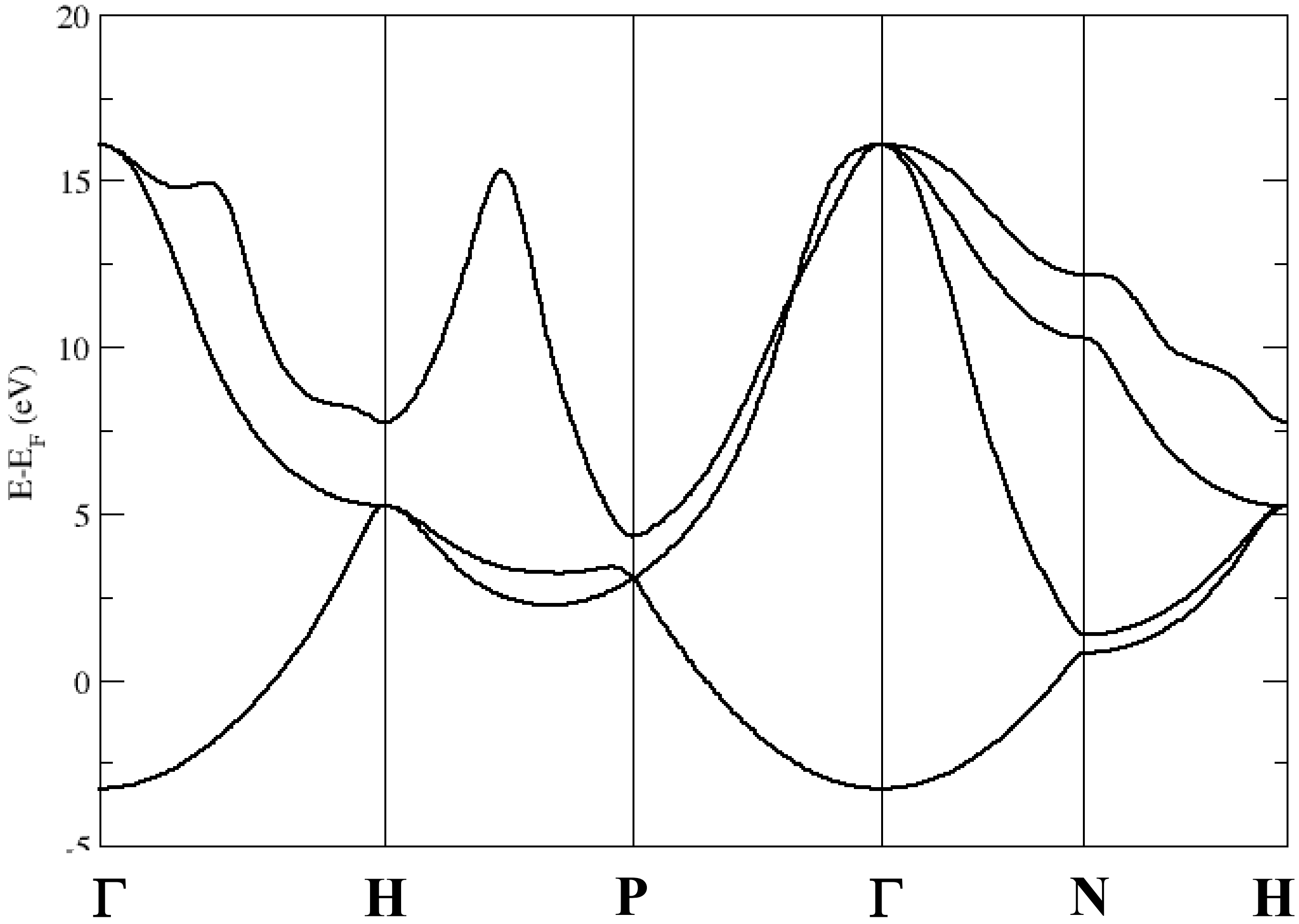
Fermi Surface

3D case

sodium (BCC): band structure



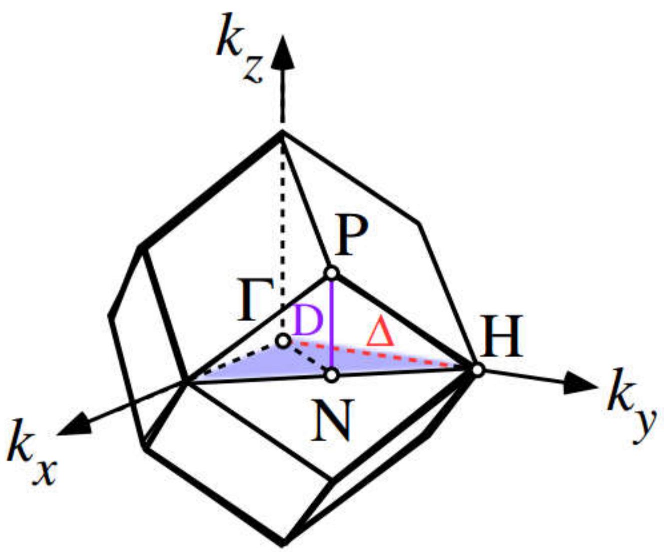
First BZ



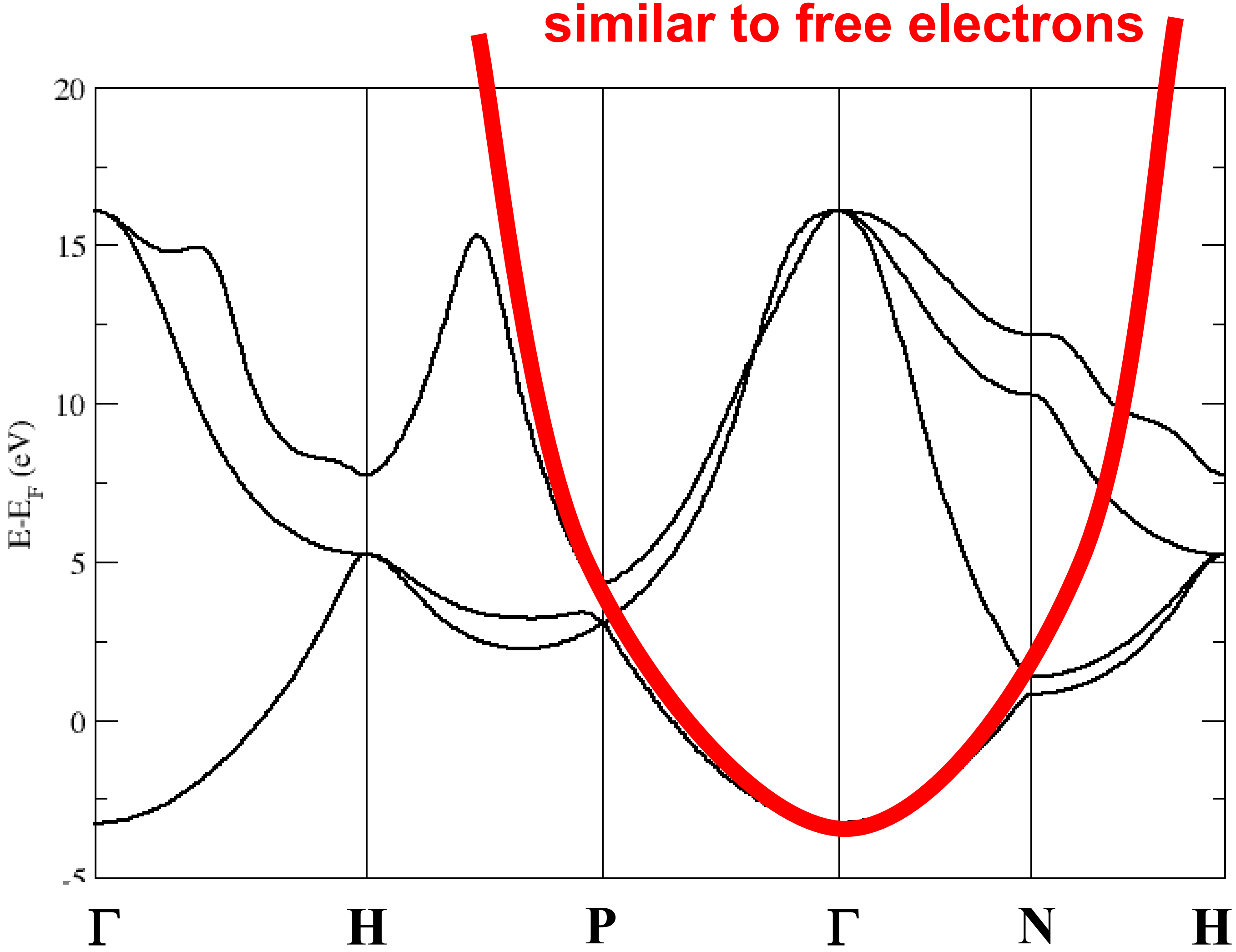
http://dipc.ehu.es/frederiksen/inelastica/index.php/Na_BCC

3D case

sodium (BCC): band structure



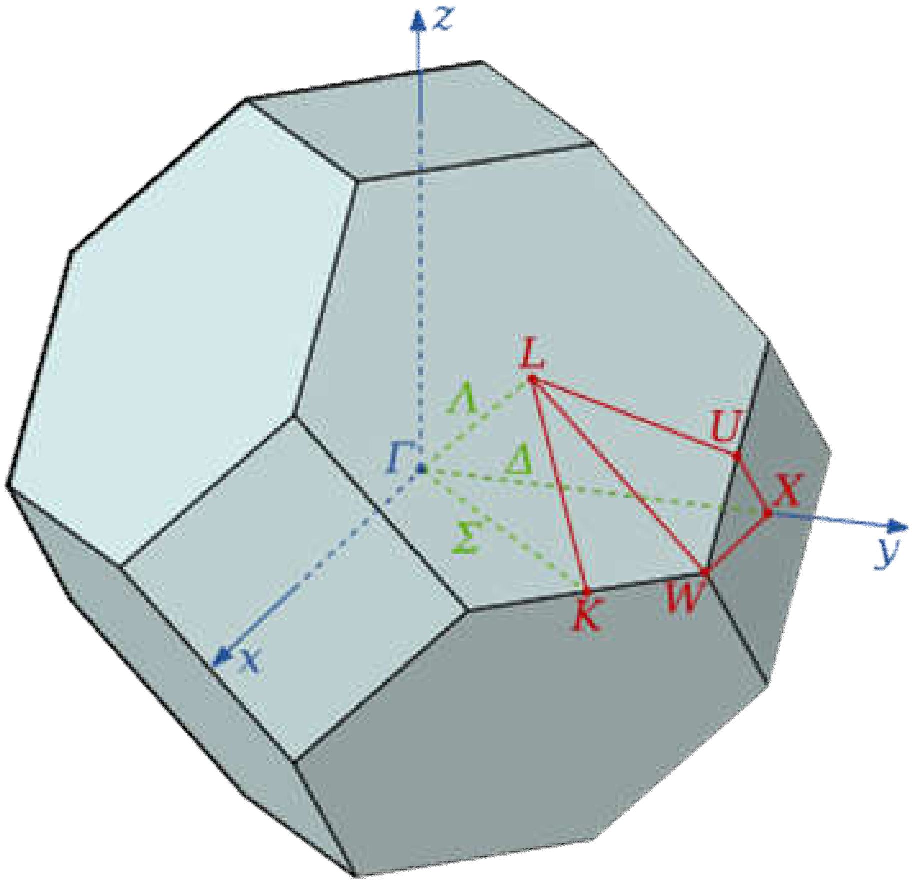
First BZ



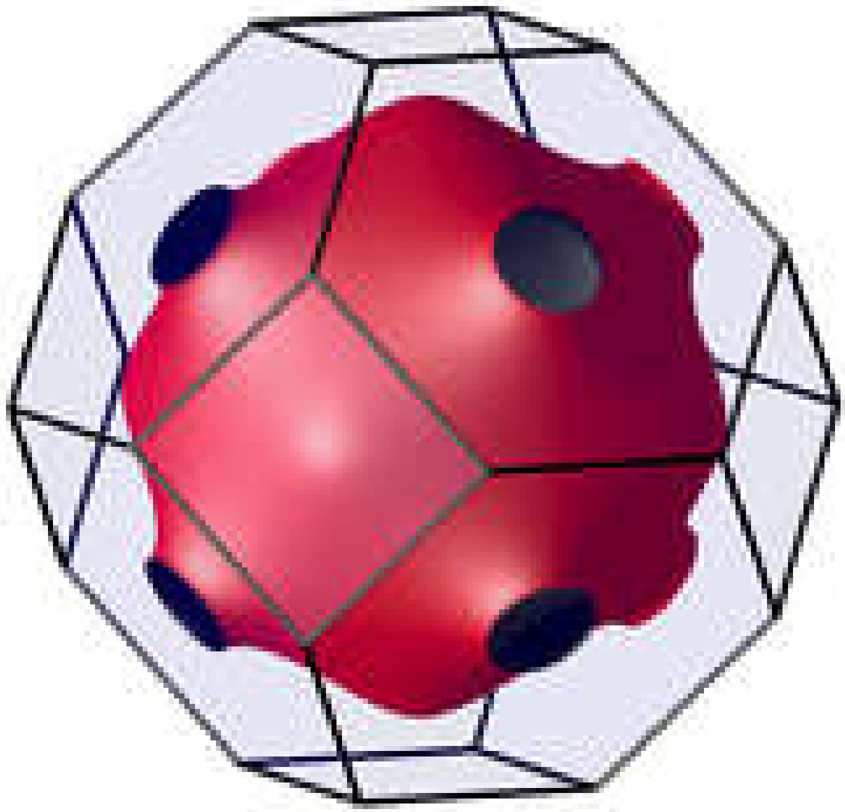
http://dipc.ehu.es/frederiksen/inelastica/index.php/Na_BCC

3D case

copper (FCC)



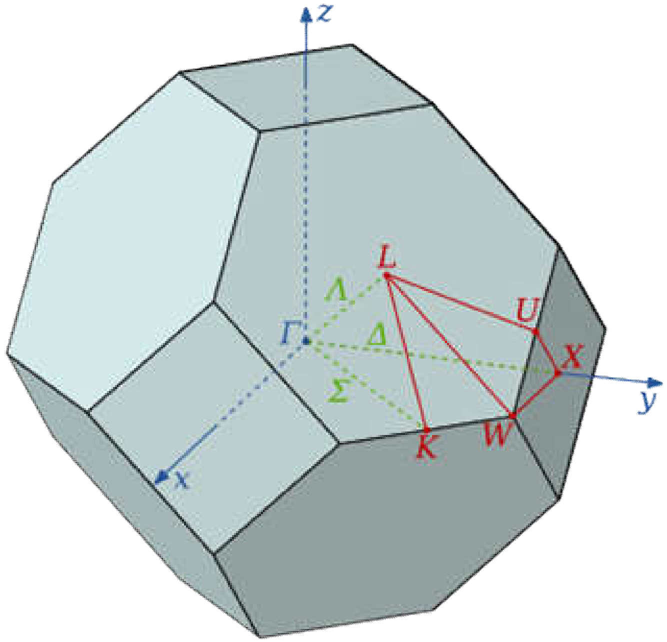
First BZ



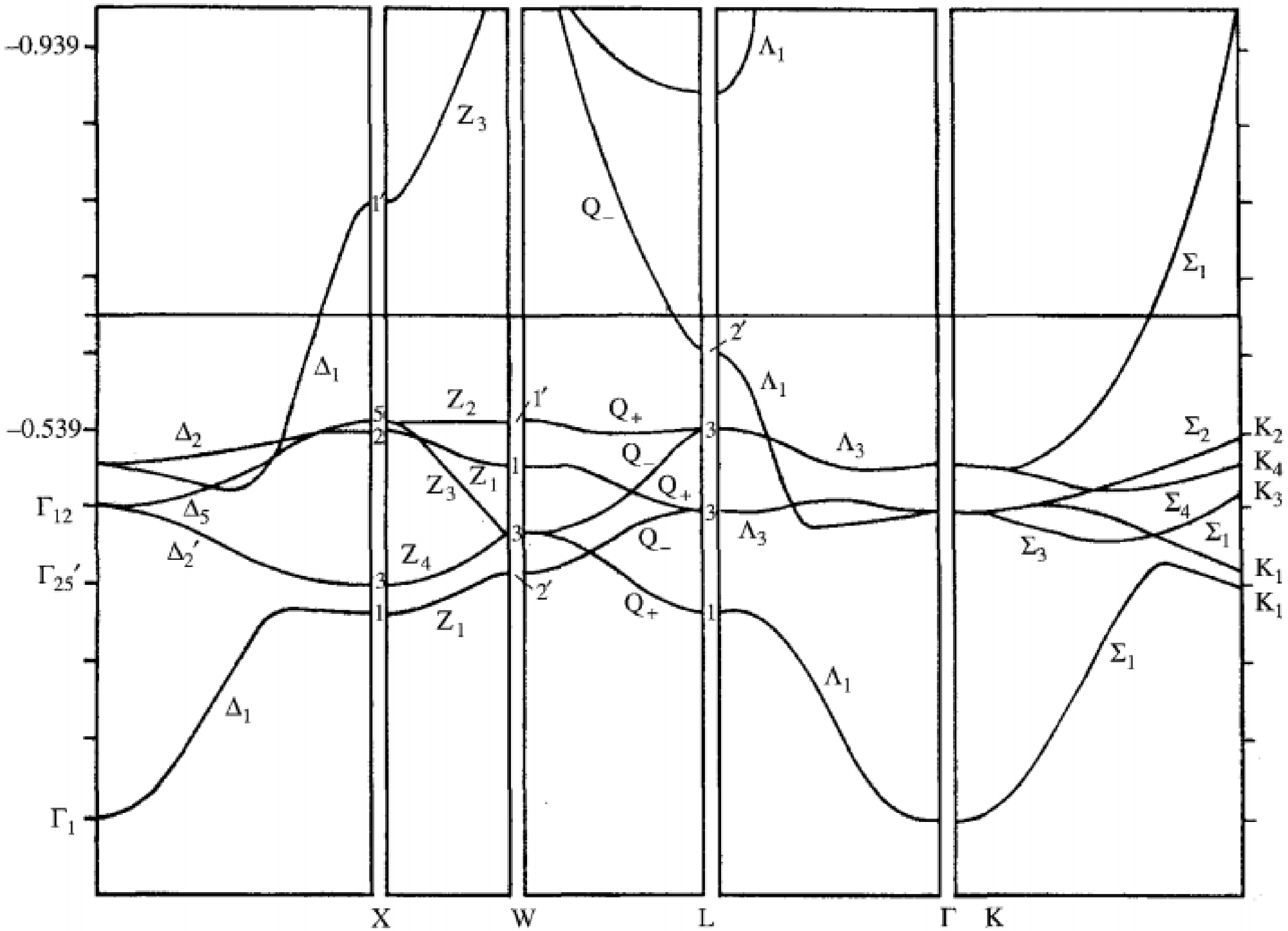
Fermi Surface

3D case

copper (FCC): band structure



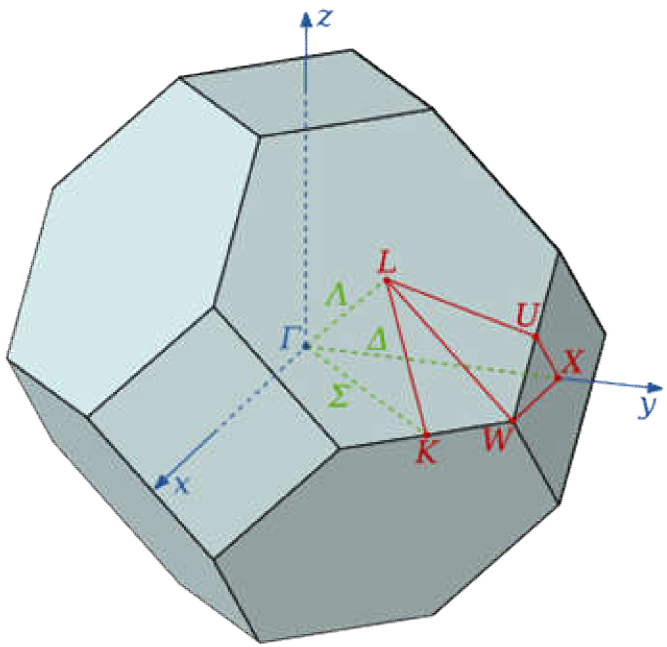
First BZ



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

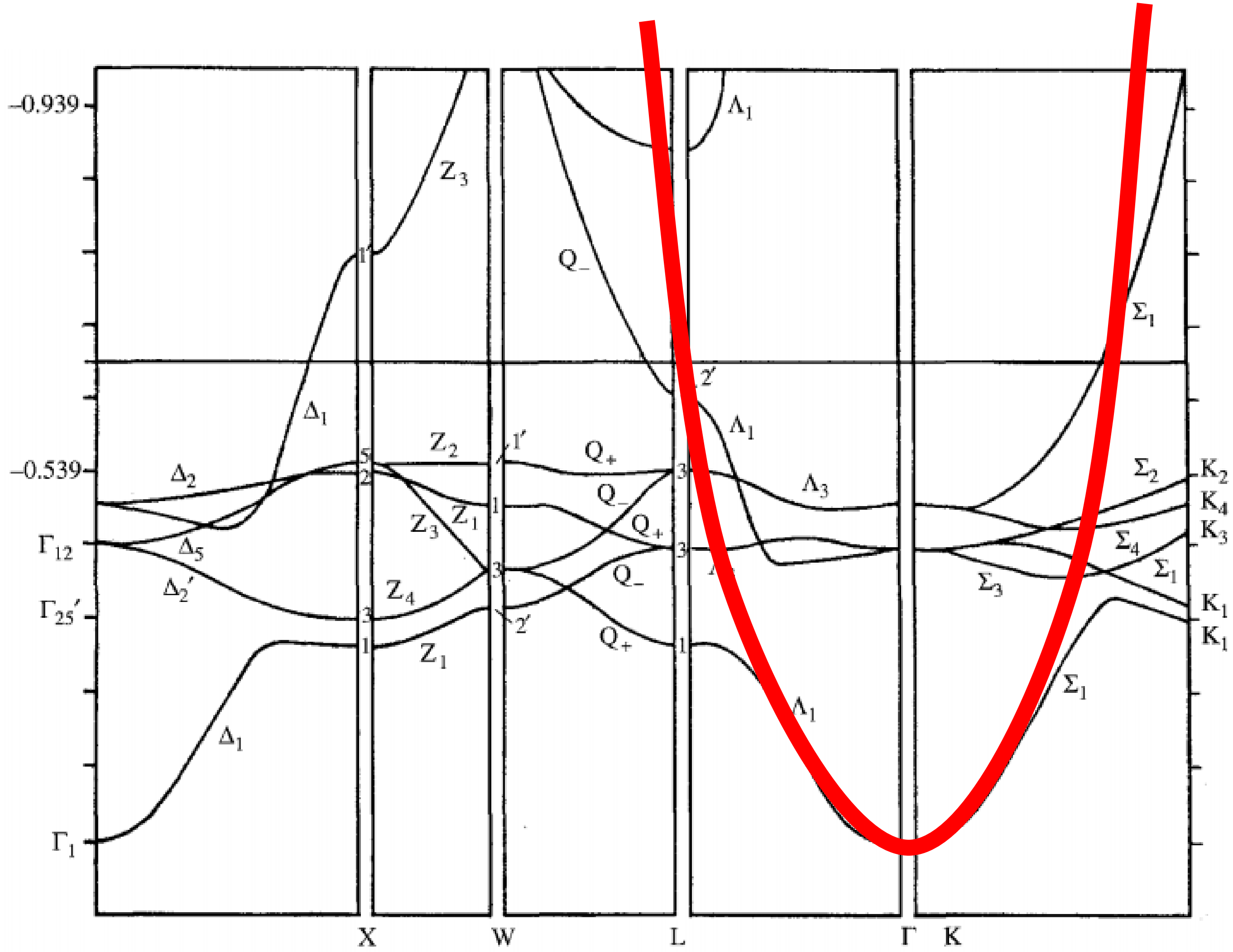
3D case

copper (FCC): band structure



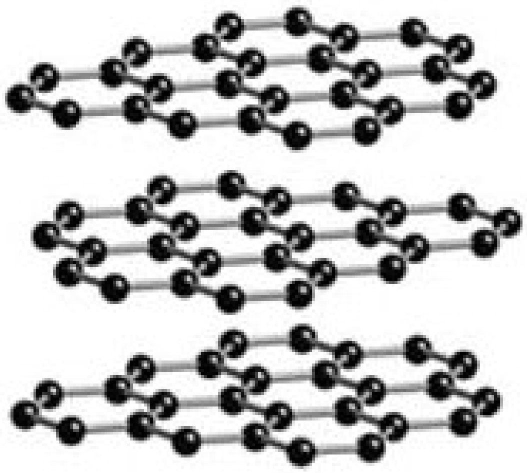
First BZ

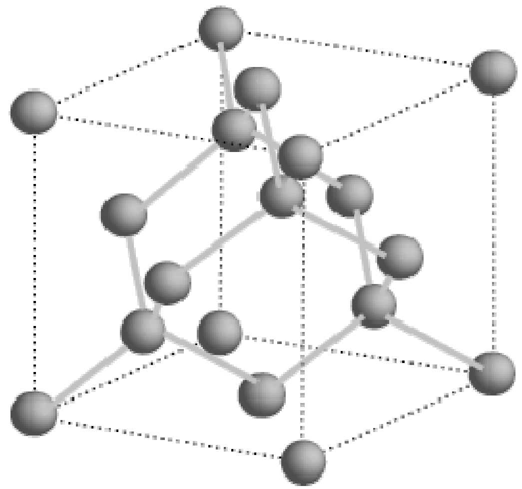
similar to free electrons



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

Example - Carbon

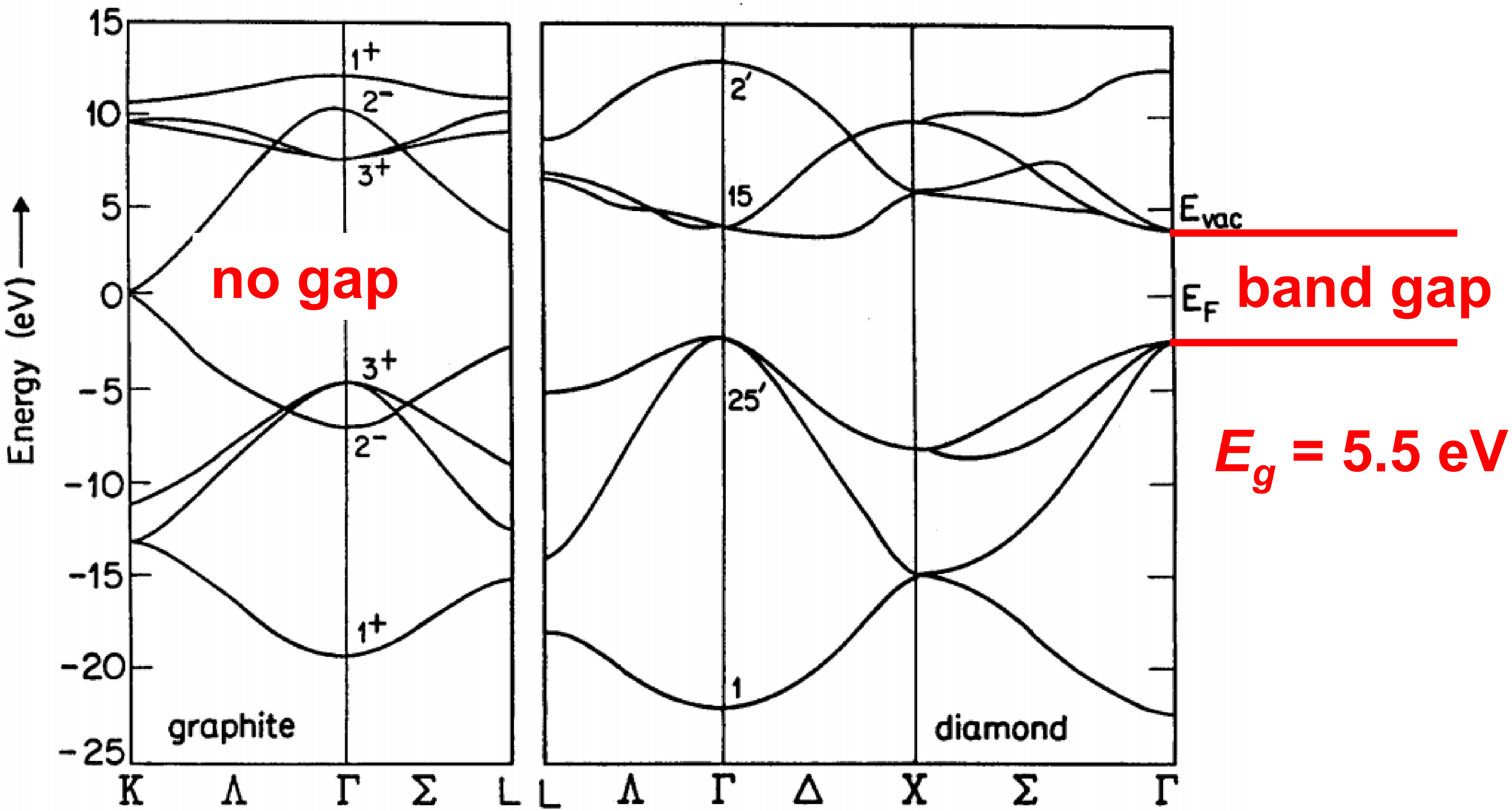




graphite
$\sigma \sim 10^{5}$ S/m

diamond
$\sigma \sim 10^{-13}$ S/m

Example - Carbon



graphite
conductor

diamond
insulator

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

Temperature Dependence of σ

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

$$\frac{1}{\rho} = \sigma = ne\mu = \frac{ne^2\tau}{m^*}$$

$$\tau = \frac{l}{v}$$

τ - relaxation time (s)
l - mean free path (m)

- At *T* = 0 K, perfect metals should have no collision, infinite *l and* τ ---> infinite σ

Temperature Dependence of σ

- **Resistivity originates from the collision with imperfect crystals**

Matthiessen's rule

$$\rho = \rho_i + \rho_p$$

impurity

phonon (thermal vibration)

$$\rho_i \sim 1/l_i \sim n_i = \text{constant}$$

$$\rho_p \sim 1/l_p \sim n_p \sim k_B T$$

(at high *T*)

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

Temperature Dependence of σ

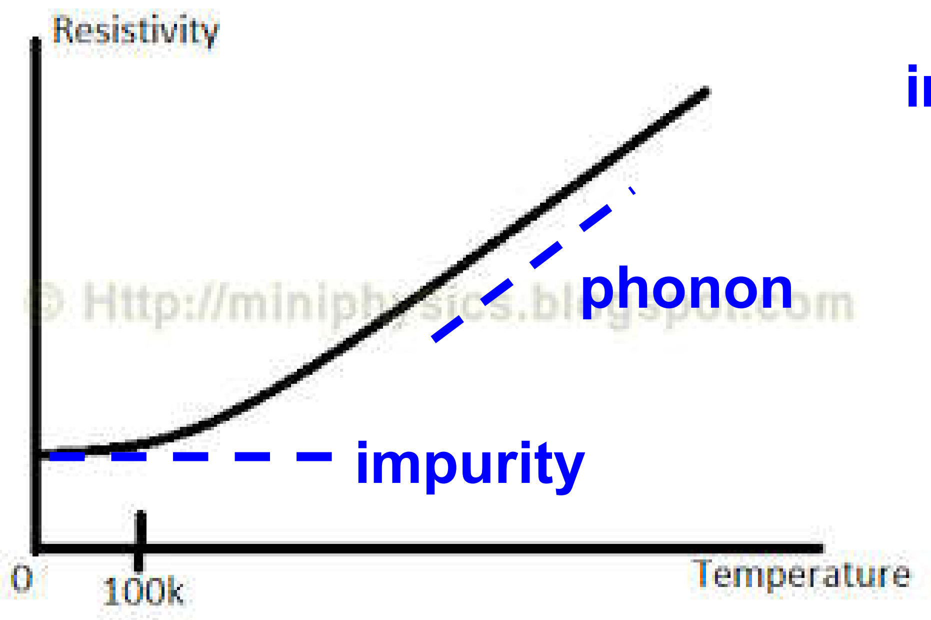
- **Resistivity originates from the collision with imperfect crystals**

Matthiessen's rule

$$\rho = \rho_i + \rho_p$$

impurity

phonon (thermal vibration)

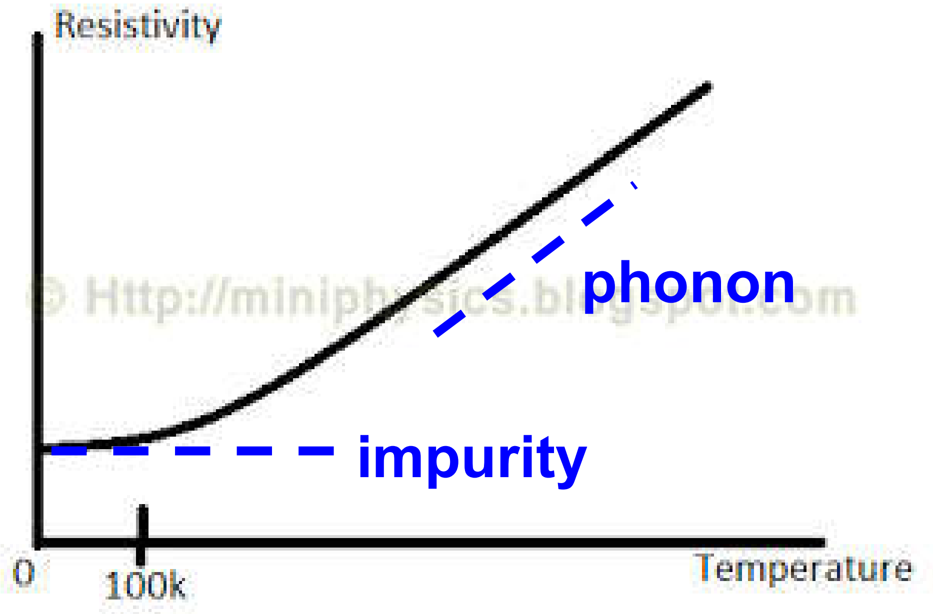


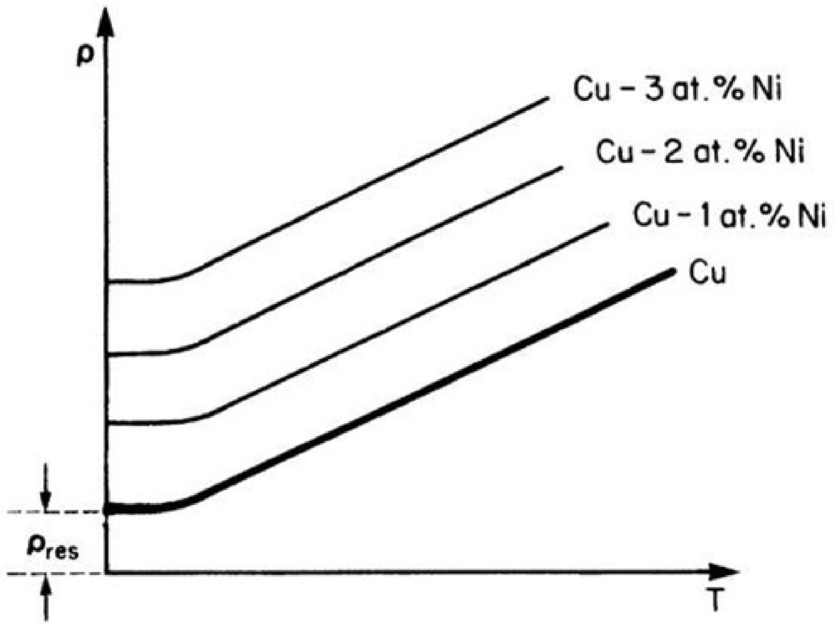
$$\rho(T) = \rho_0[1 + \alpha \Delta T]$$

Temperature Dependence of σ

- **Resistivity originates from the collision with imperfect crystals**

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



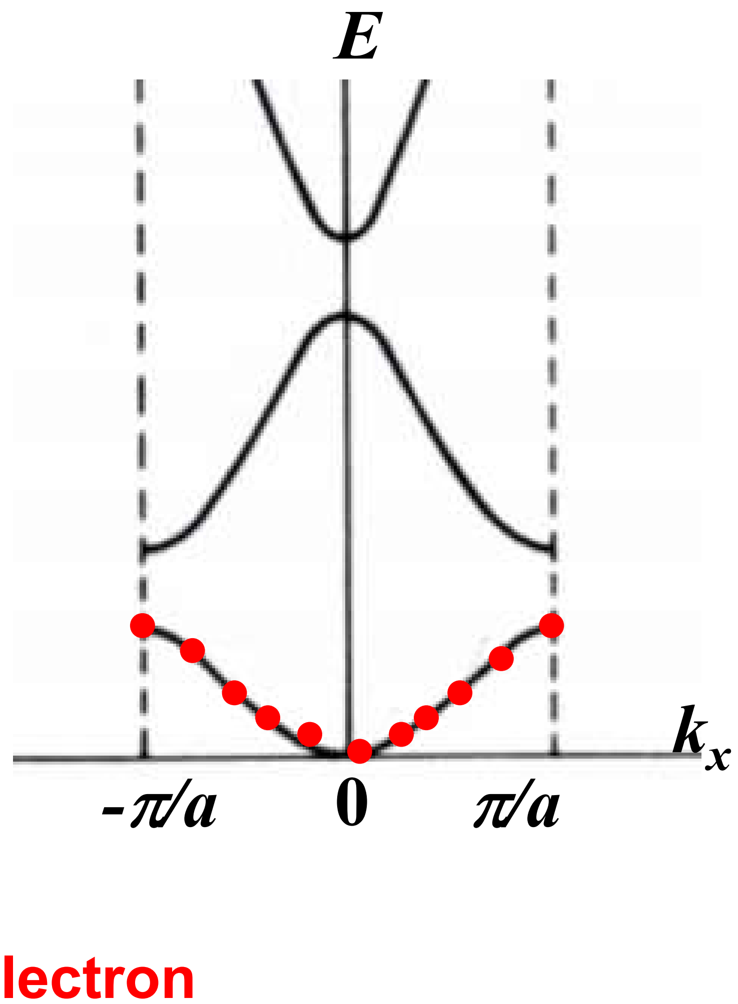


http://what-when-how.com/electronic-properties-of-materials/electrical-conduction-in-metals-and-alloys-electrical-properties-of-materials-part-2/

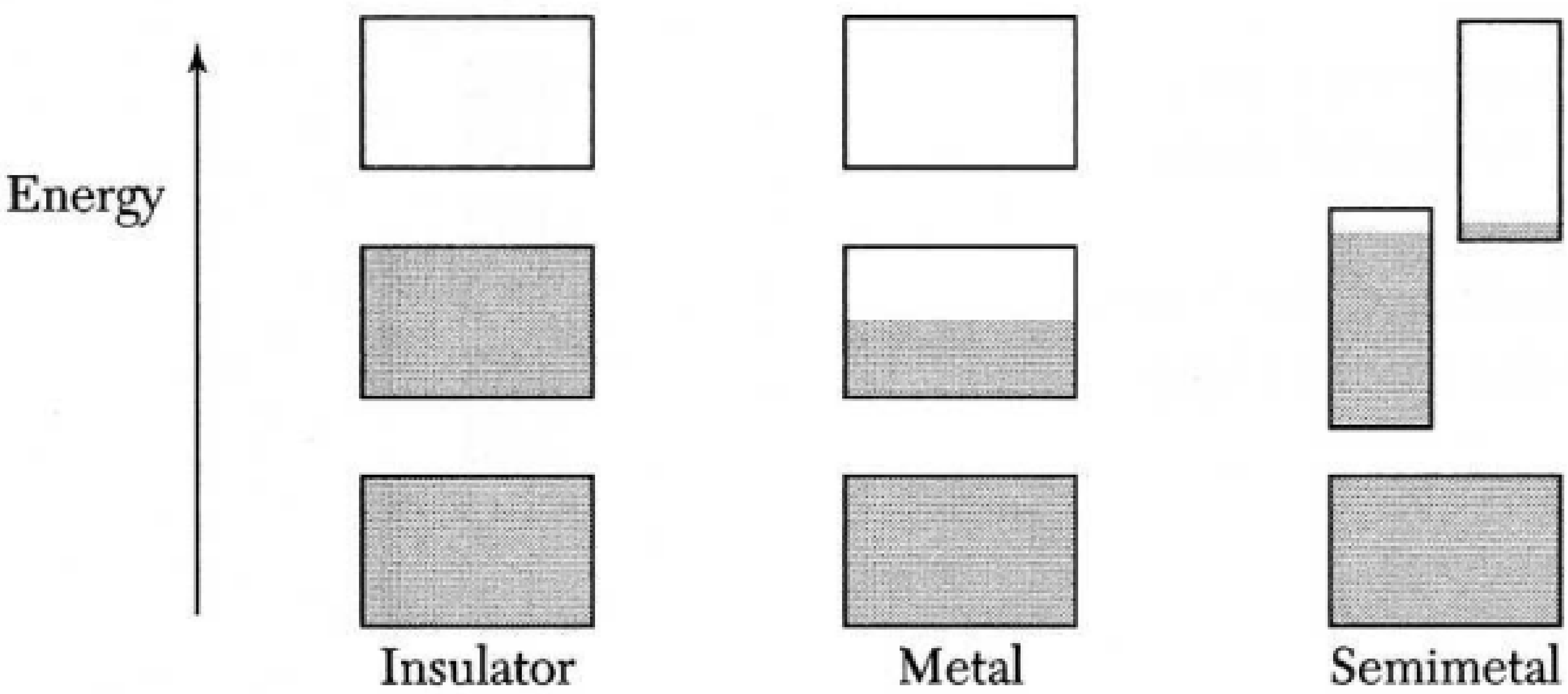
Summary

- Electronic properties of solids depend on
  - band structure
  - electron density

- also depend on
  - defects
  - temperature
  - electric field
  - ...



Summary



Thank you for your attention