

Fundamentals of Solid State Physics

Electronic Properties - Metals and Insulators

Xing Sheng 盛兴



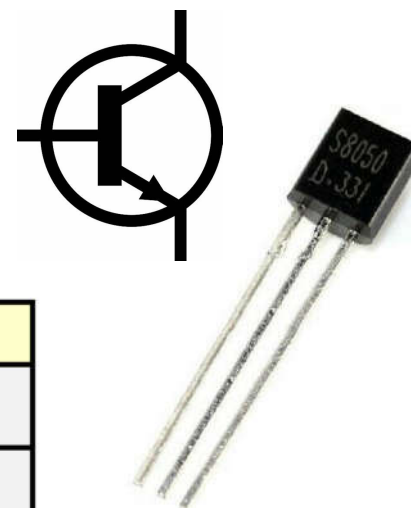
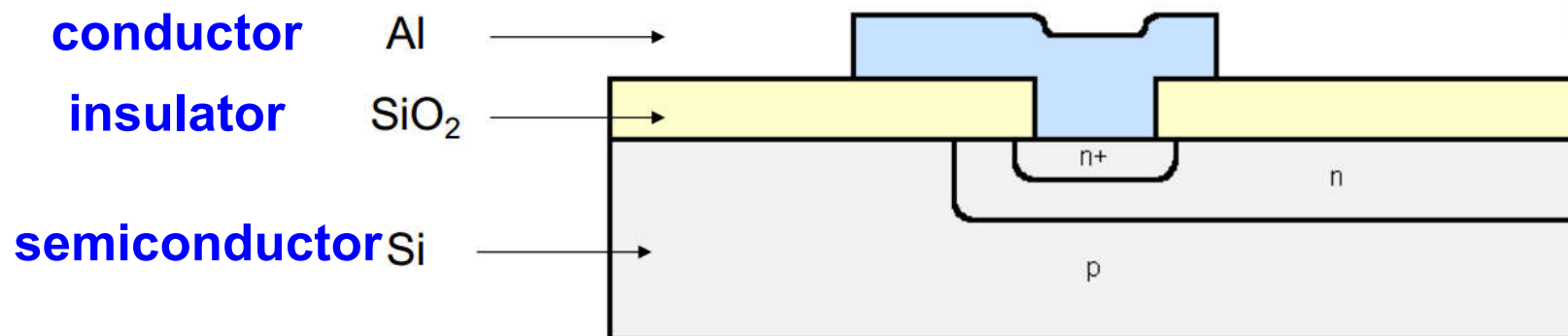
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Tsinghua University**

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Electronic Properties of Materials

CMOS transistor

- Complementary **Metal-Oxide-Semiconductor**



Metal

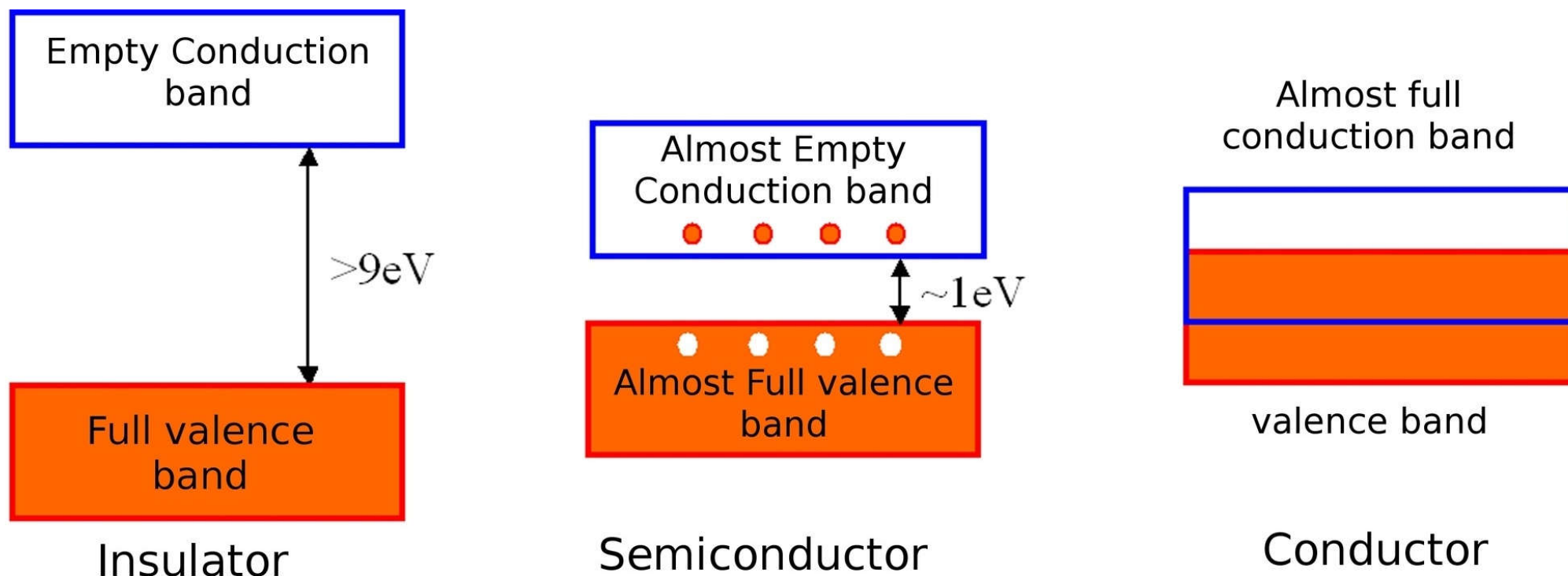


SiO_2



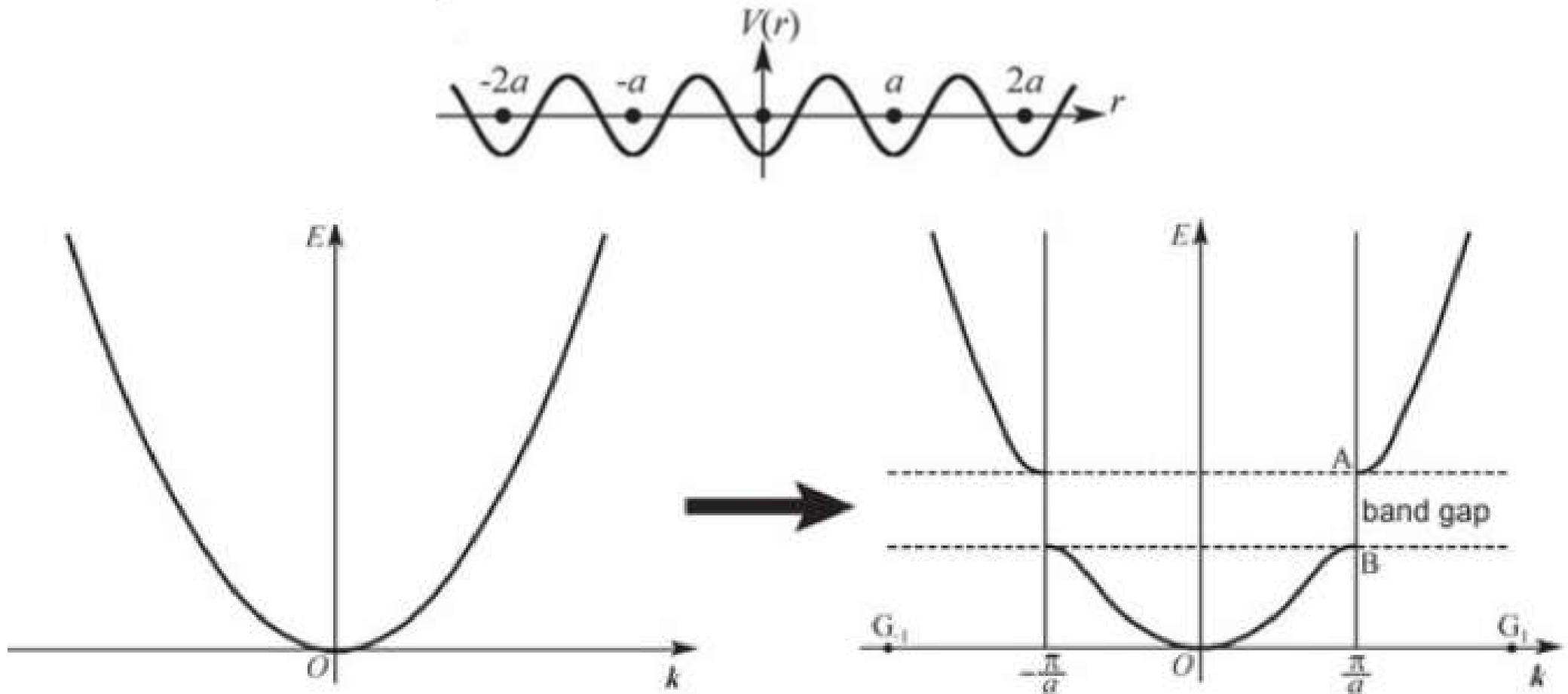
Silicon

Summary



Formation of Band Gaps

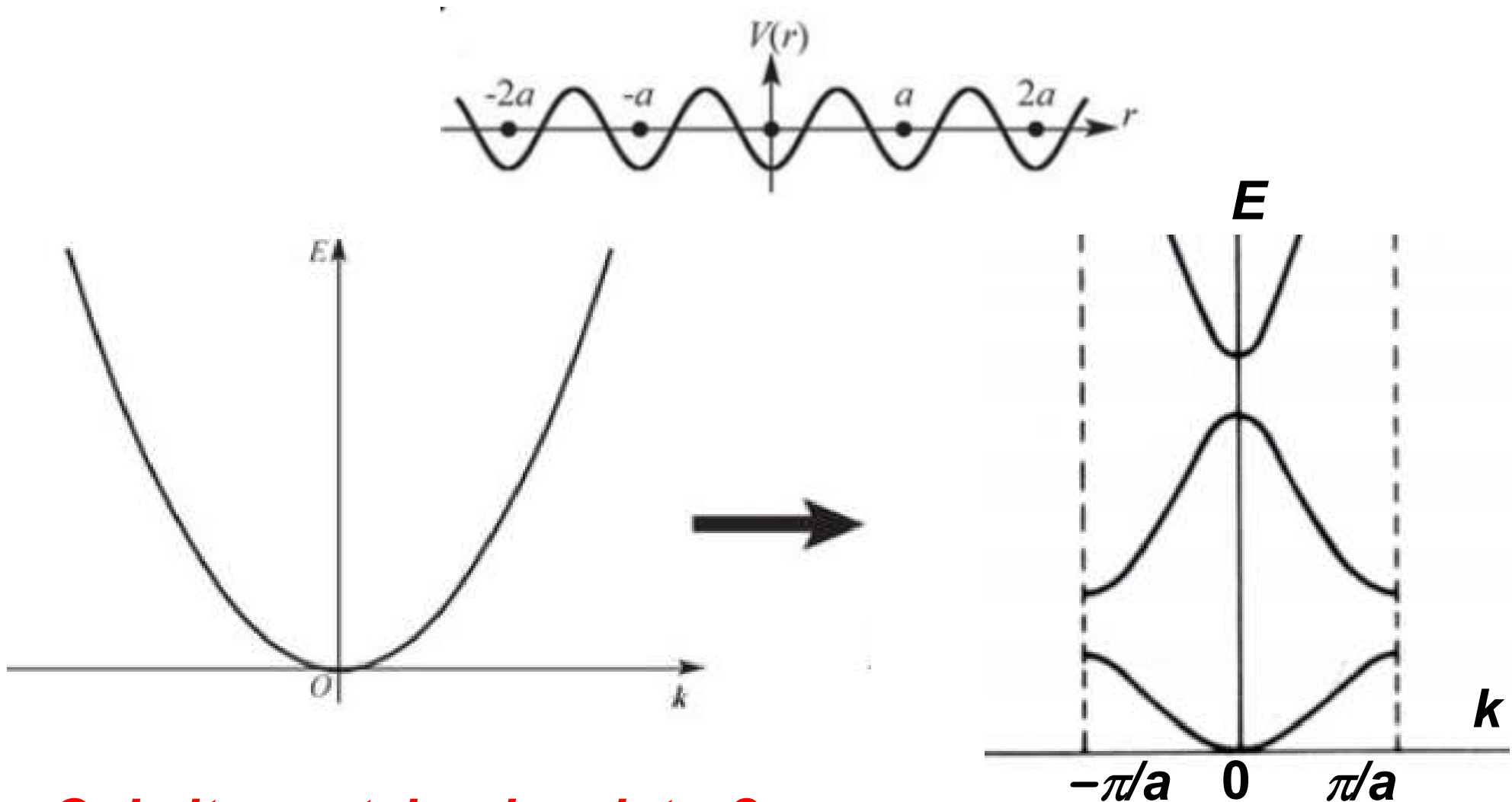
Free electrons are perturbed by a periodic potential



Q: Is it a metal or insulator?

Formation of Band Gaps

Free electrons are perturbed by a periodic potential

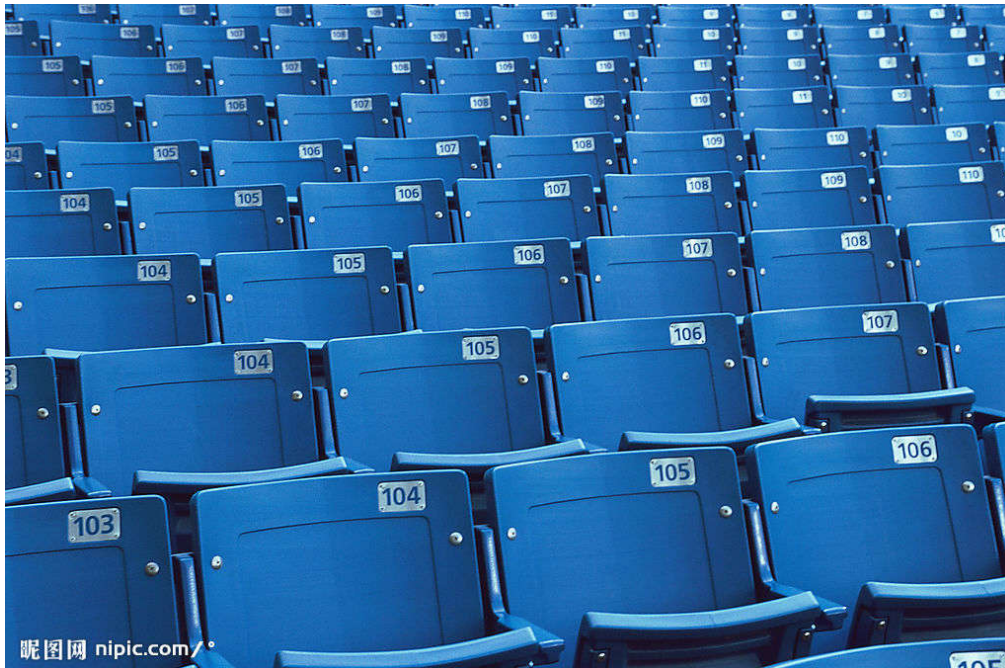


Q: Is it a metal or insulator?

State vs. Electron

energy state / level / orbital
能态 / 能级 / 轨道

electron / phonon / ...
电子 / 声子 / ...



determined by space, lattice,
environments, ...

Energy States

How many energy states in each band?

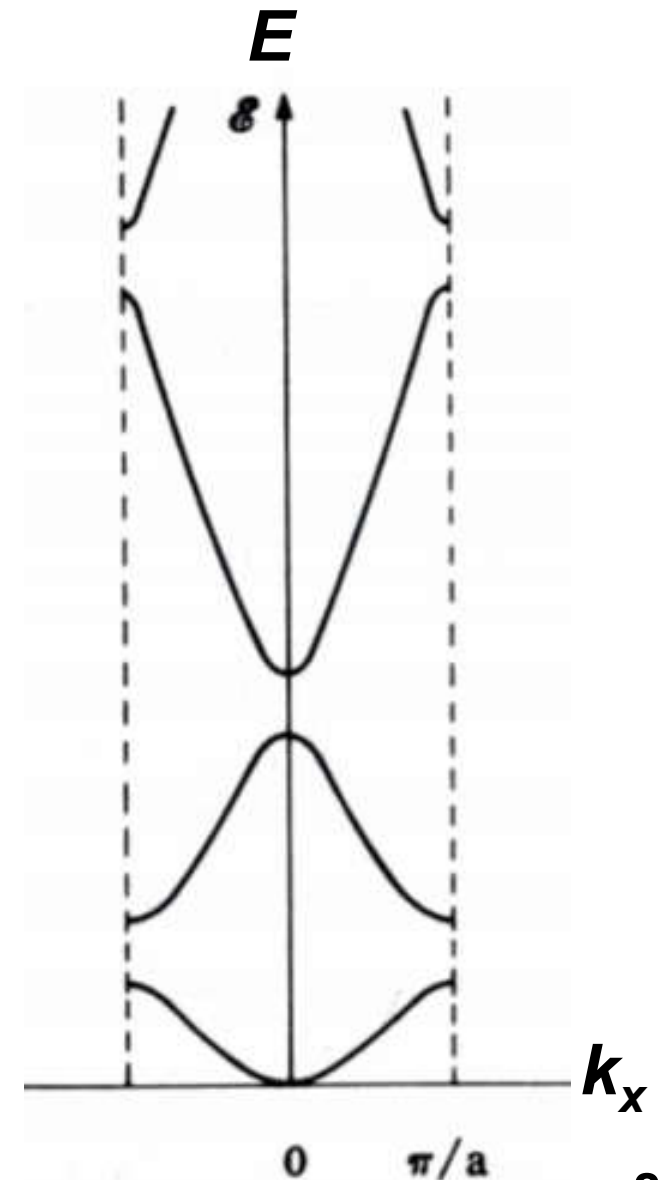
$$\begin{aligned}
 N &= 2 \cdot \frac{\text{size of FBZ}}{\text{density of } k \text{ points}} \\
 &= 2 \cdot \frac{2\pi / a}{2\pi / L_x} \\
 &= 2 \frac{L_x}{a} \\
 &= 2n
 \end{aligned}$$

FBZ - First Brillouin Zone

N - total number of states

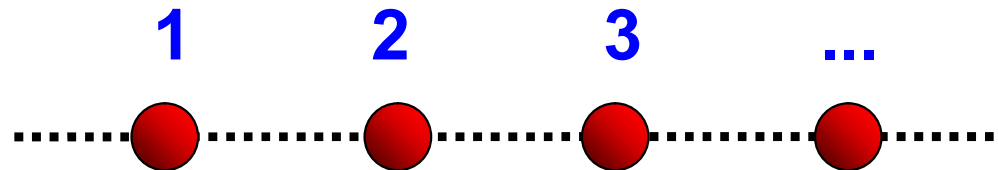
$n = L/a$ - number of primitive cells

Q: How about 2D and 3D cases?



1D Chain of *Monovalent* Atoms

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



$$N = 2n$$

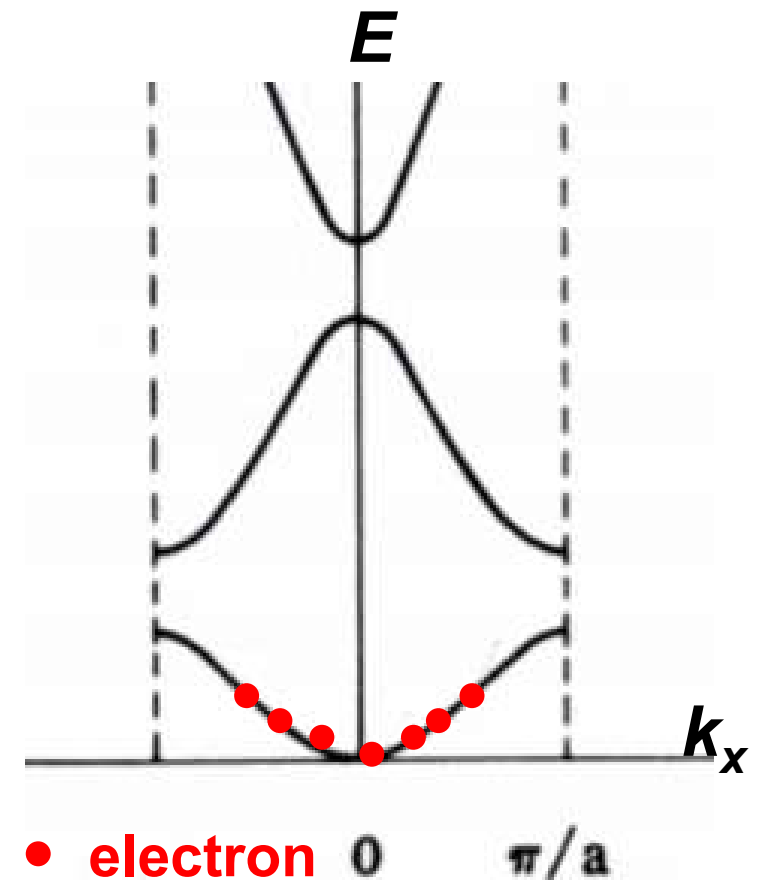
= total number of states

$$n = L/a$$

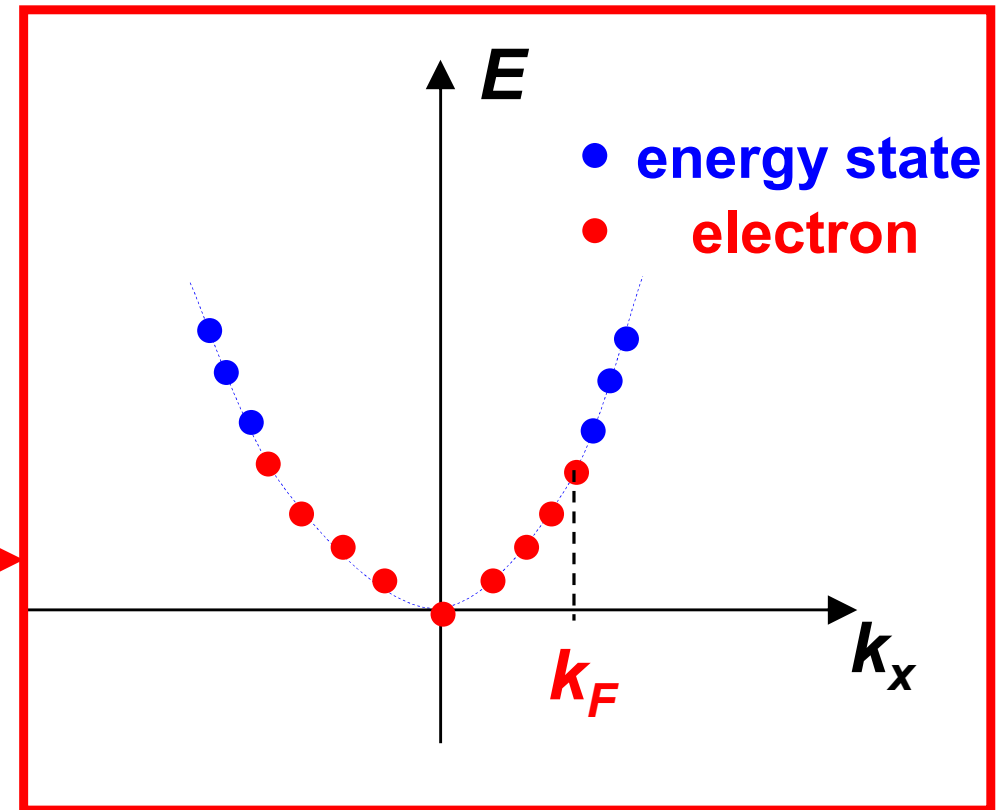
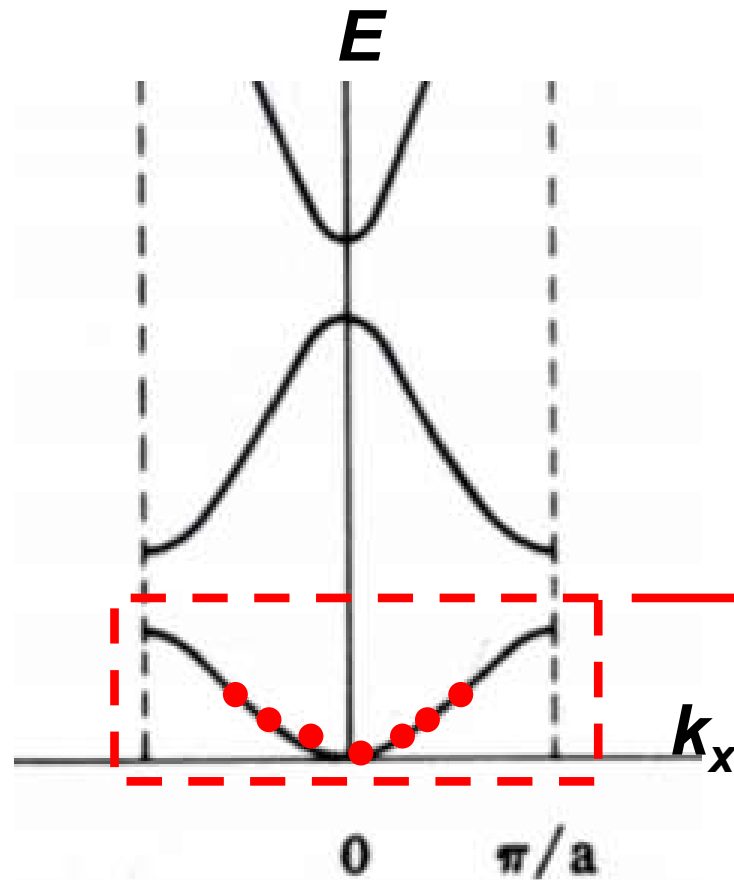
= number of primitive cells

= number of valence electrons

Electrons only fill half of the first band



1D Chain of *Monovalent* Atoms



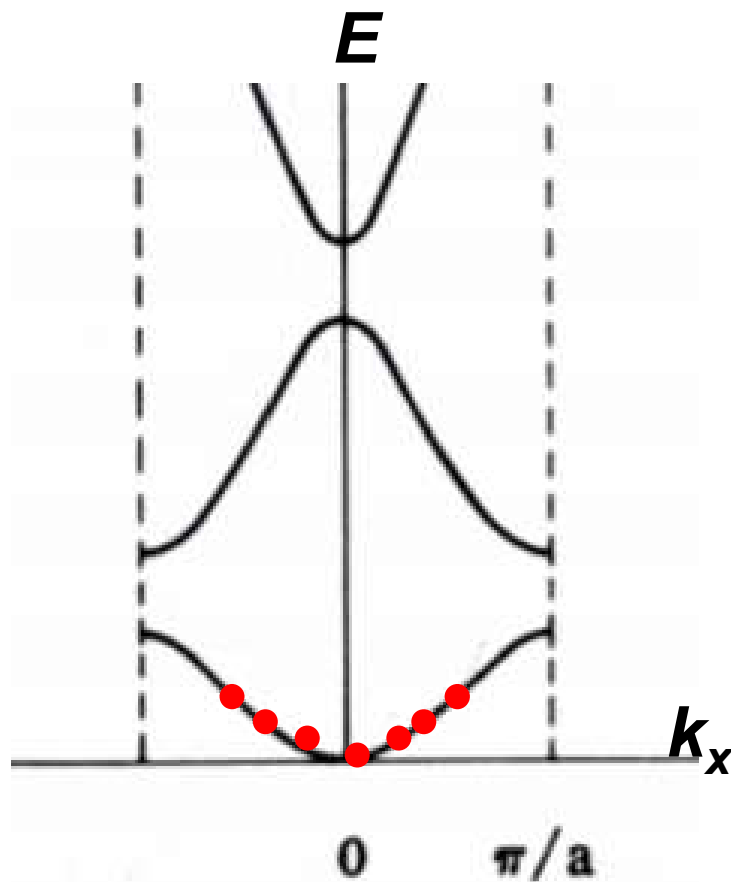
*Electrons only fill half
of the first band*

parabolic function

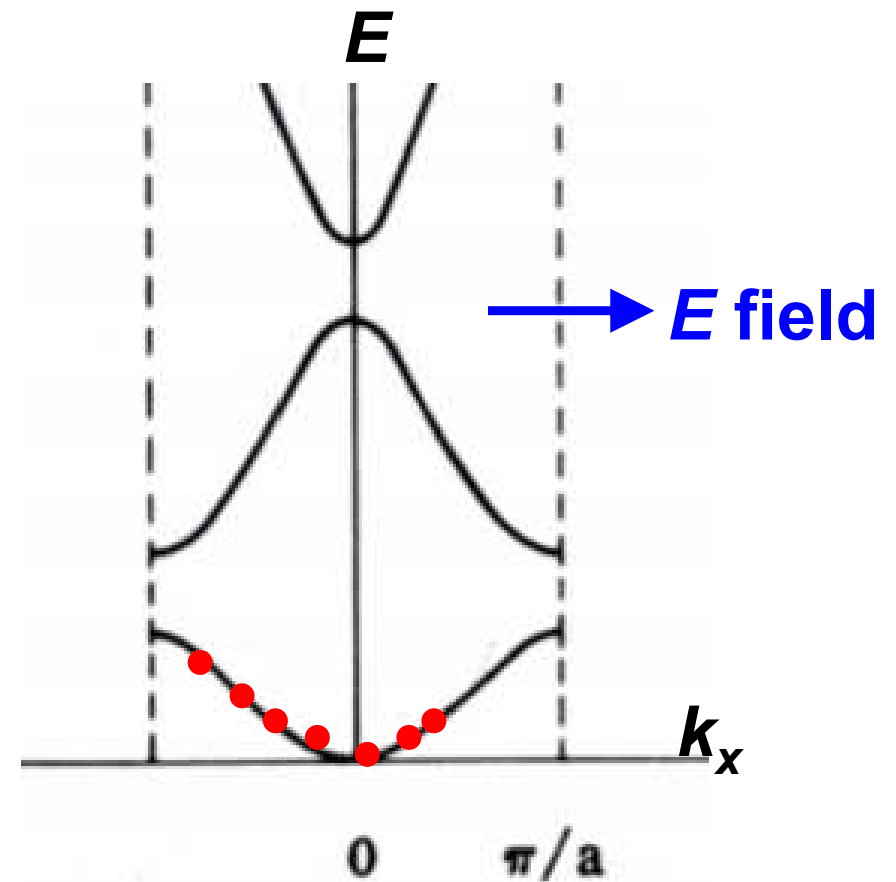
Free Electrons

Conductor

1D Chain of *Monovalent* Atoms



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

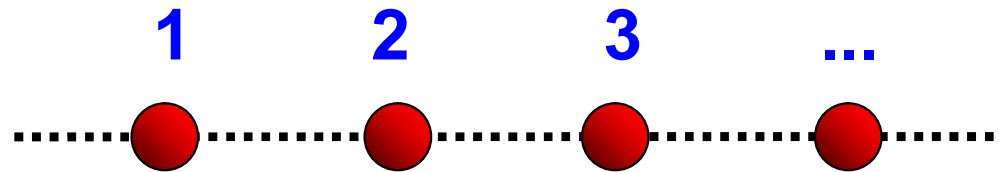


when $E \neq 0$, $v > 0$
electric current

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

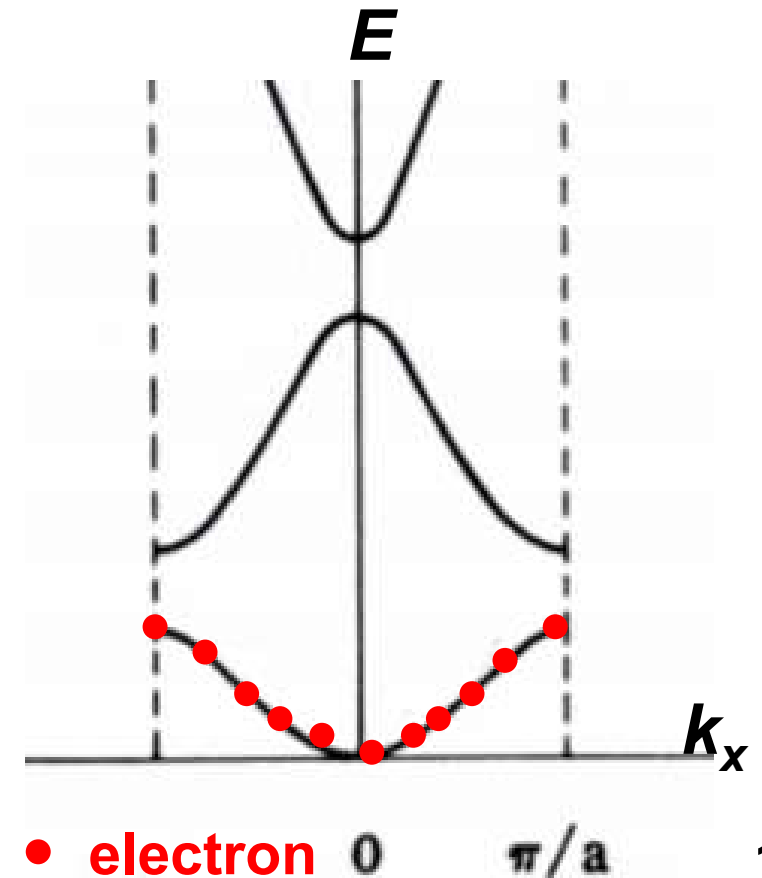
1D Chain of *Divalent* Atoms

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



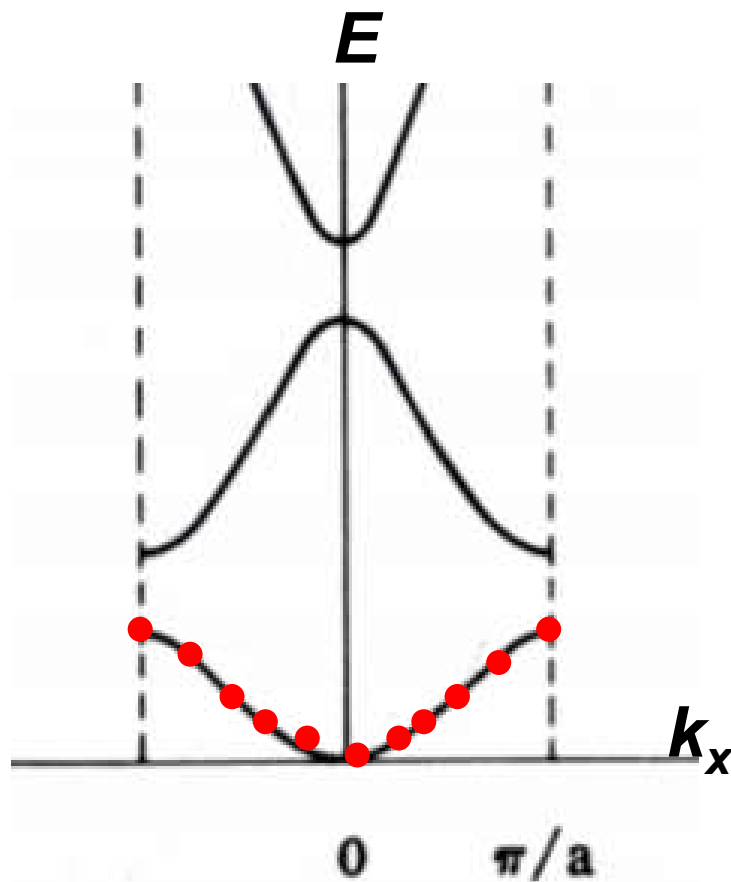
$N = 2n$
= total number of states

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

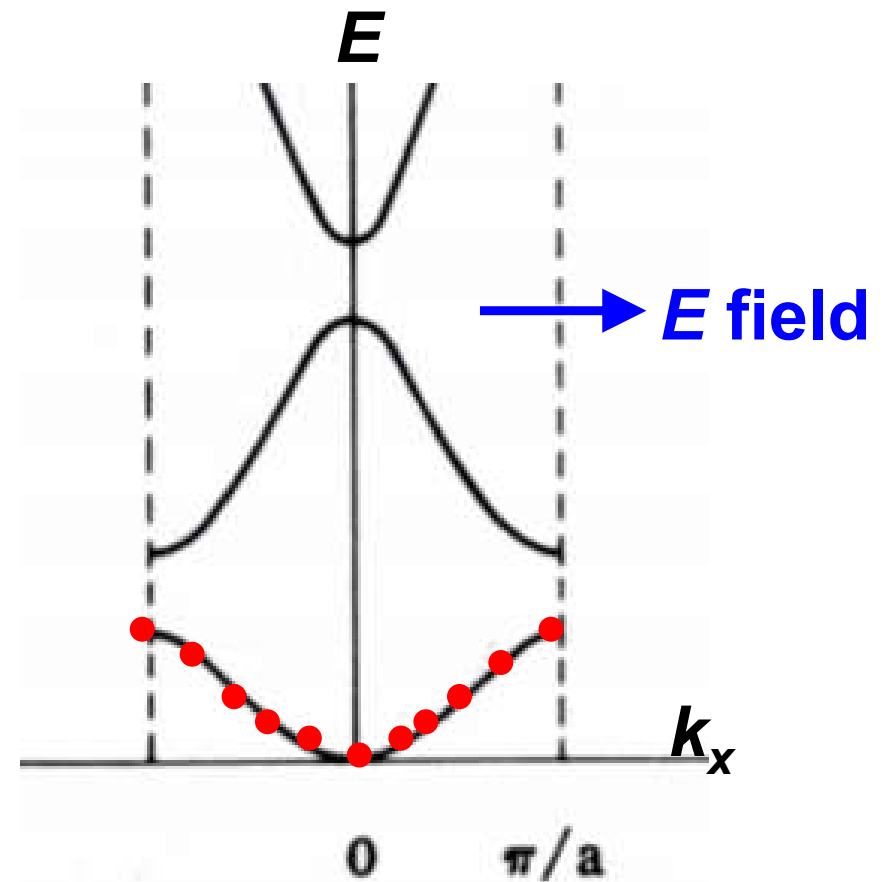


Electrons fill the entire band

1D Chain of *Divalent* Atoms



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

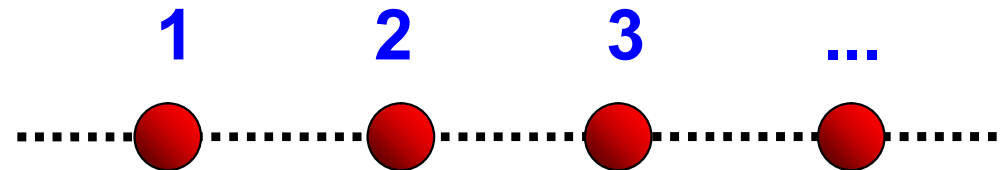


when $E \neq 0$, $v = 0$
no current

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

1D Chain of *Trivalent* Atoms

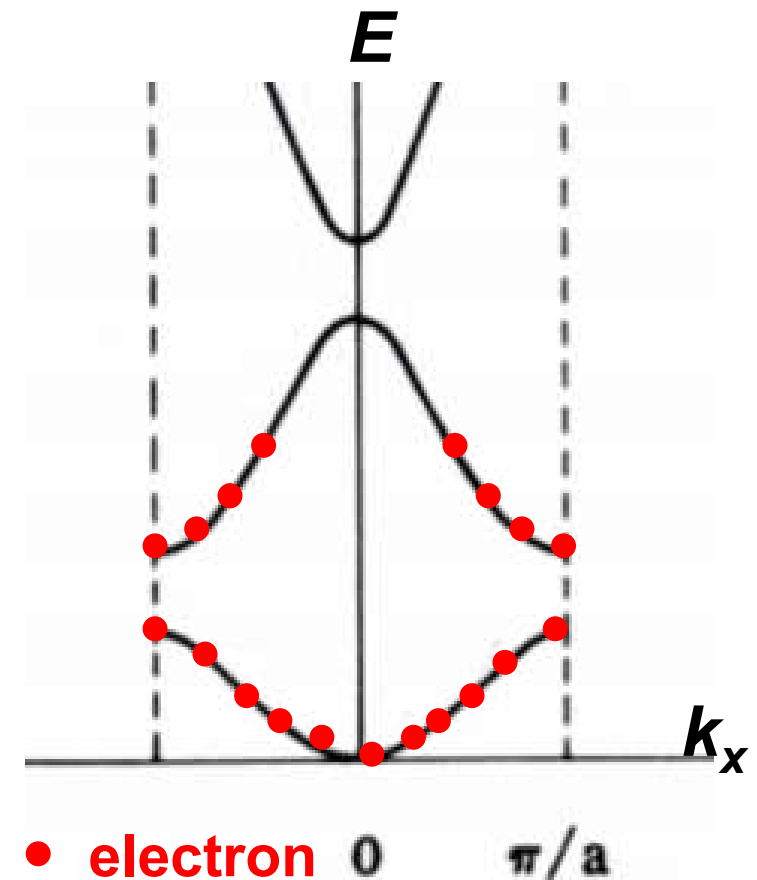
Each atom has *three* valence electrons (Al, Ga, ...)



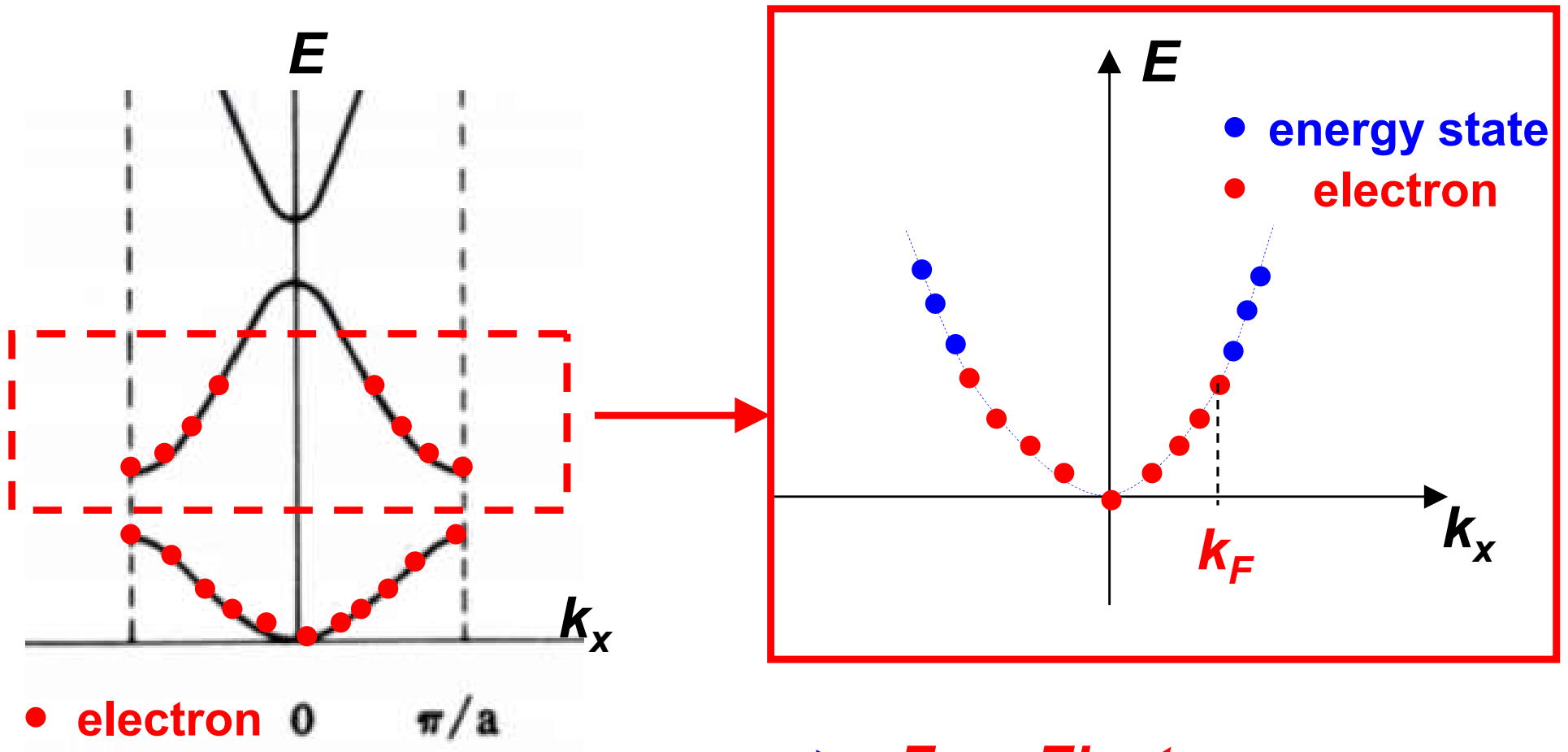
$N = 2n$
= total number of states

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

*Electrons start to fill the
second band*



1D Chain of *Trivalent* Atoms

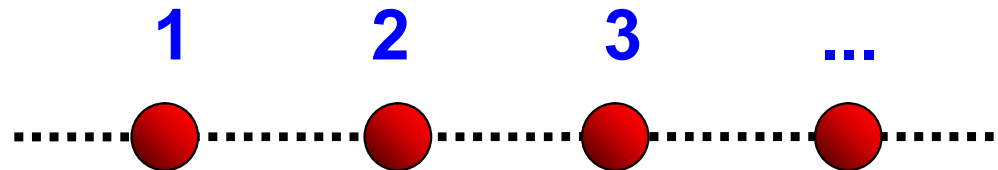


Free Electrons

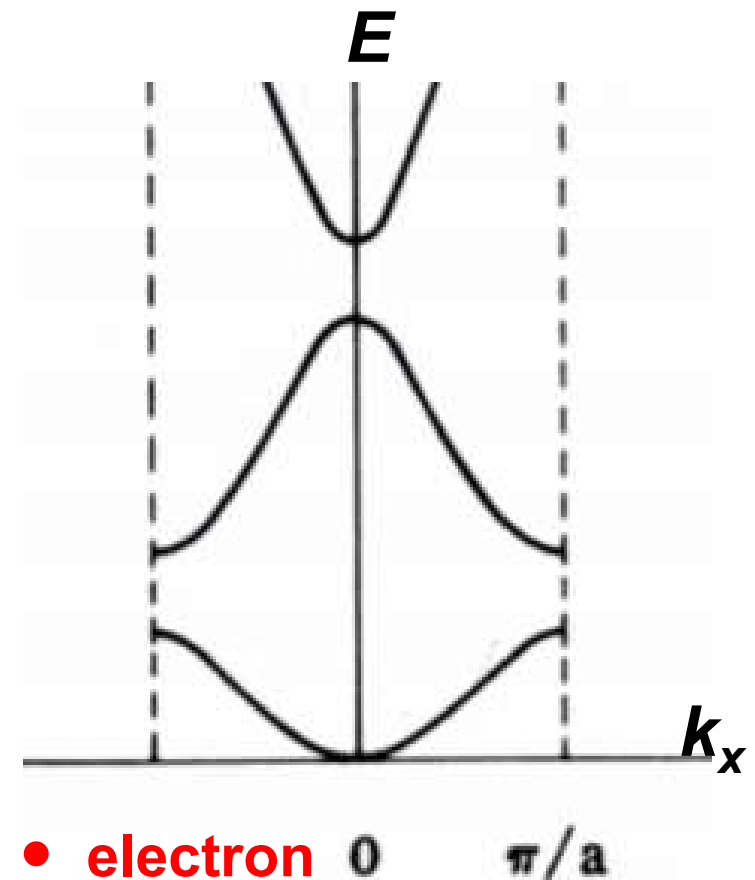
Conductor

1D Chain of *Quadrivalent* Atoms

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

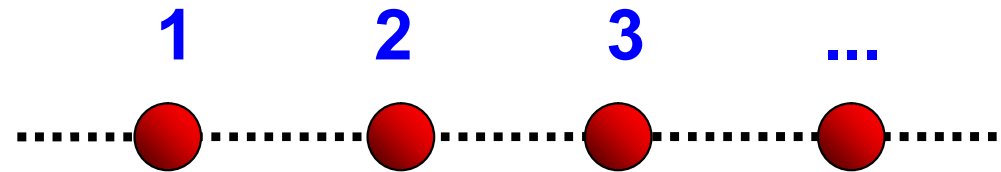


*Q: How do electrons fill the bands?
Is it a conductor, or an insulator?*



1D Chain of *Divalent* Atoms

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

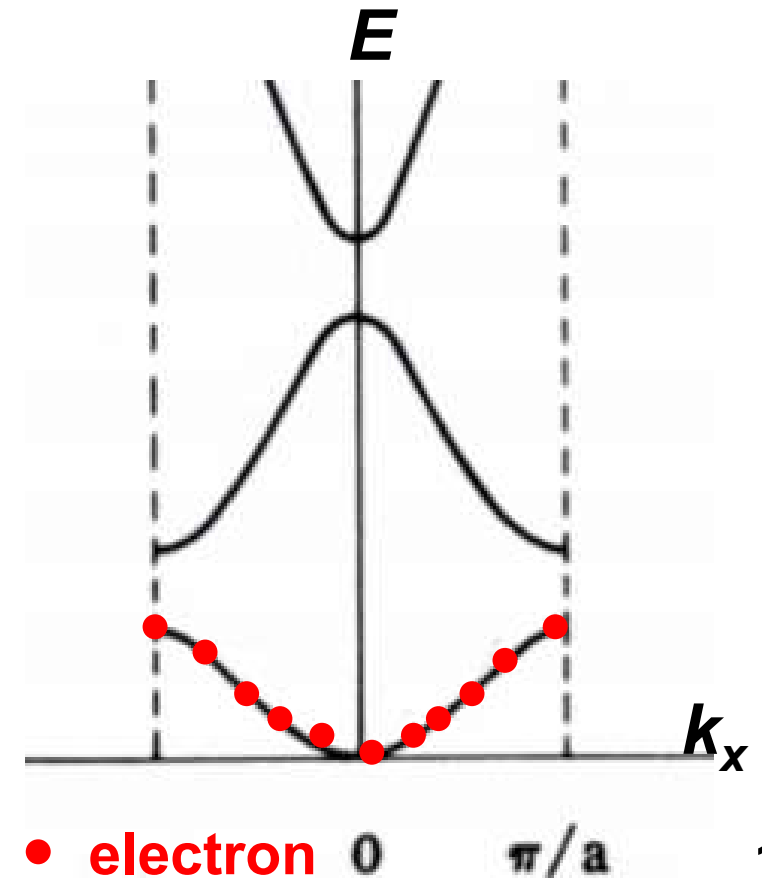


Electrons fill the entire band

--->

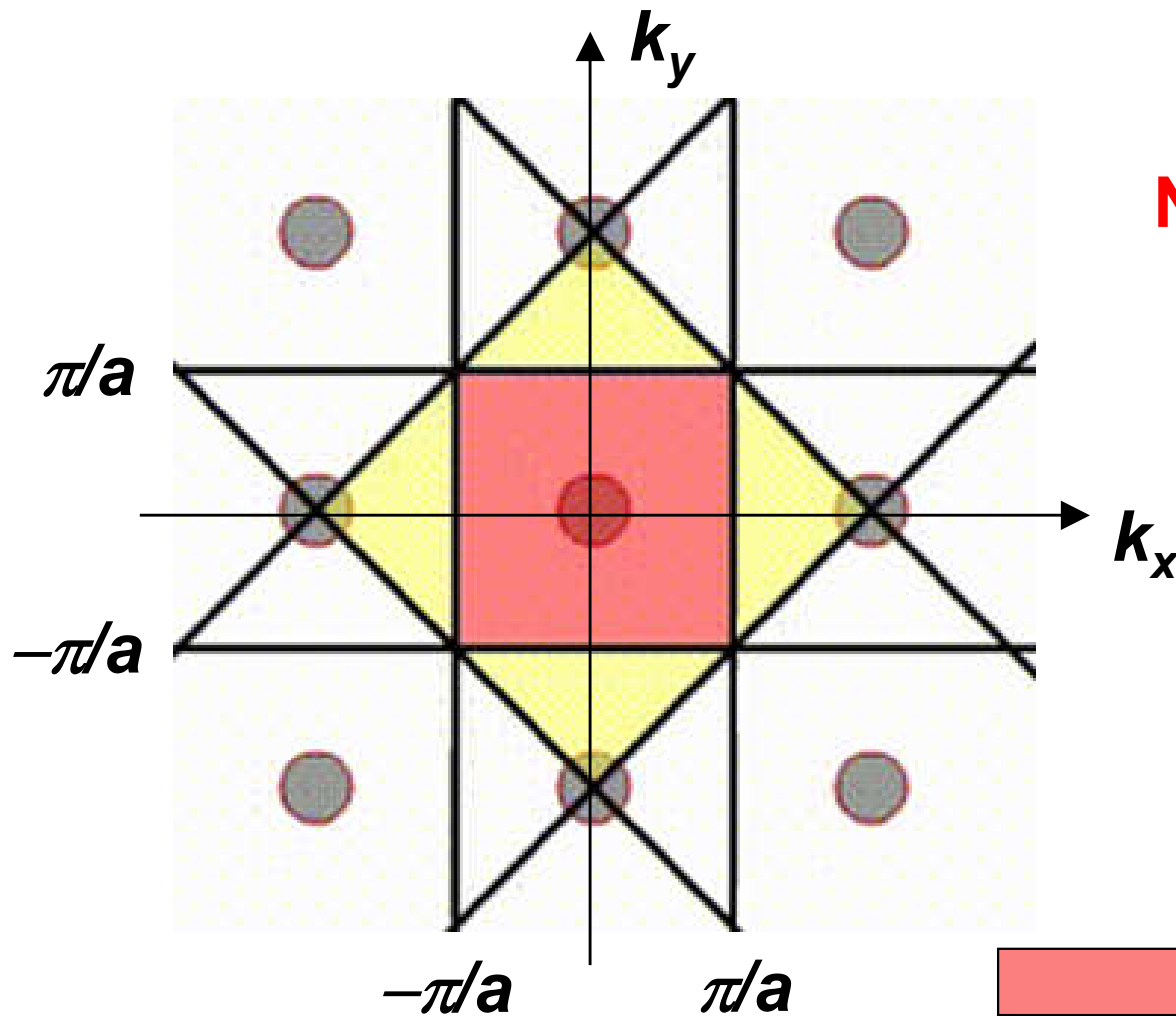
insulator

*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

$$N = 2n$$

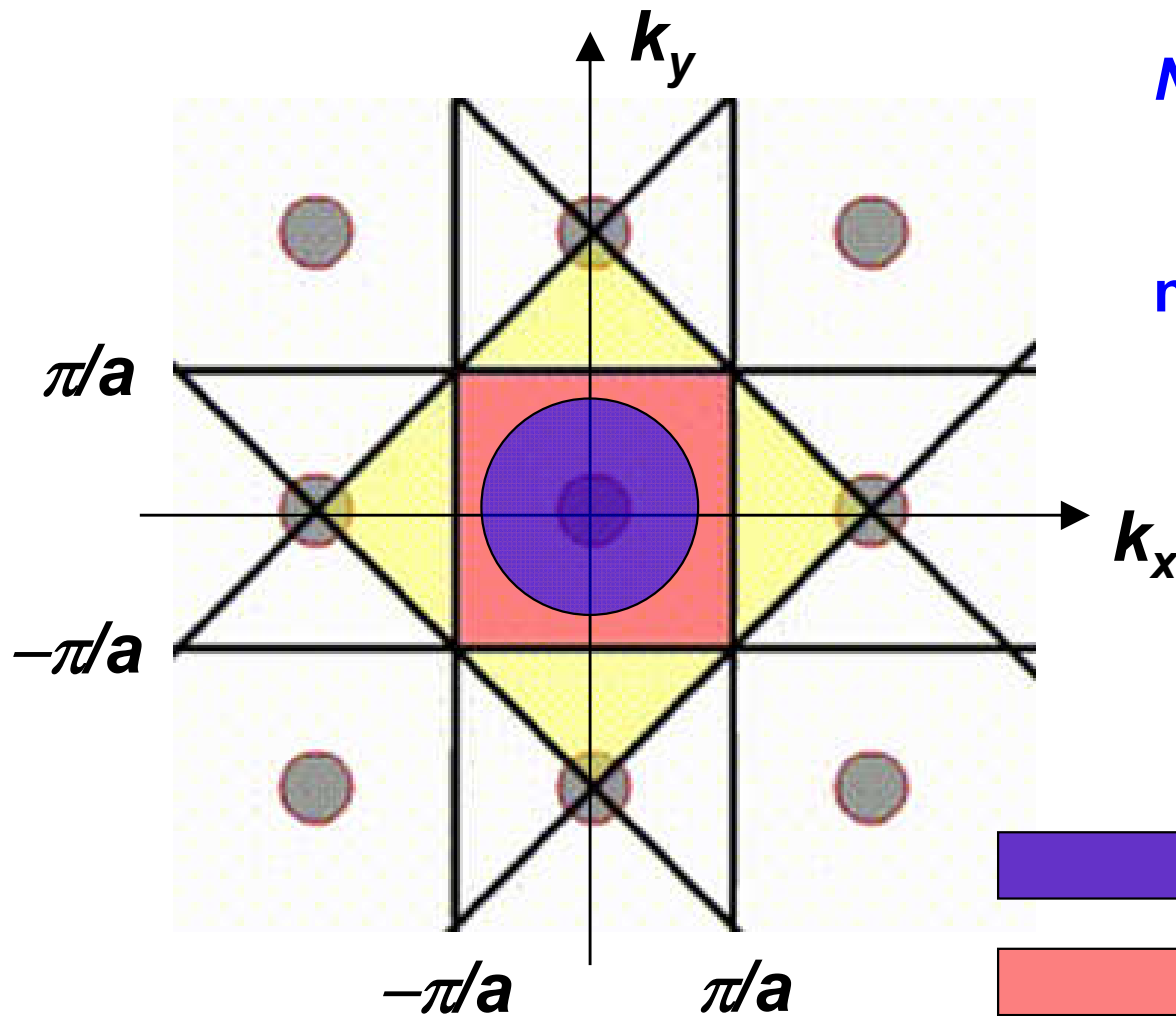
= total number of states

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

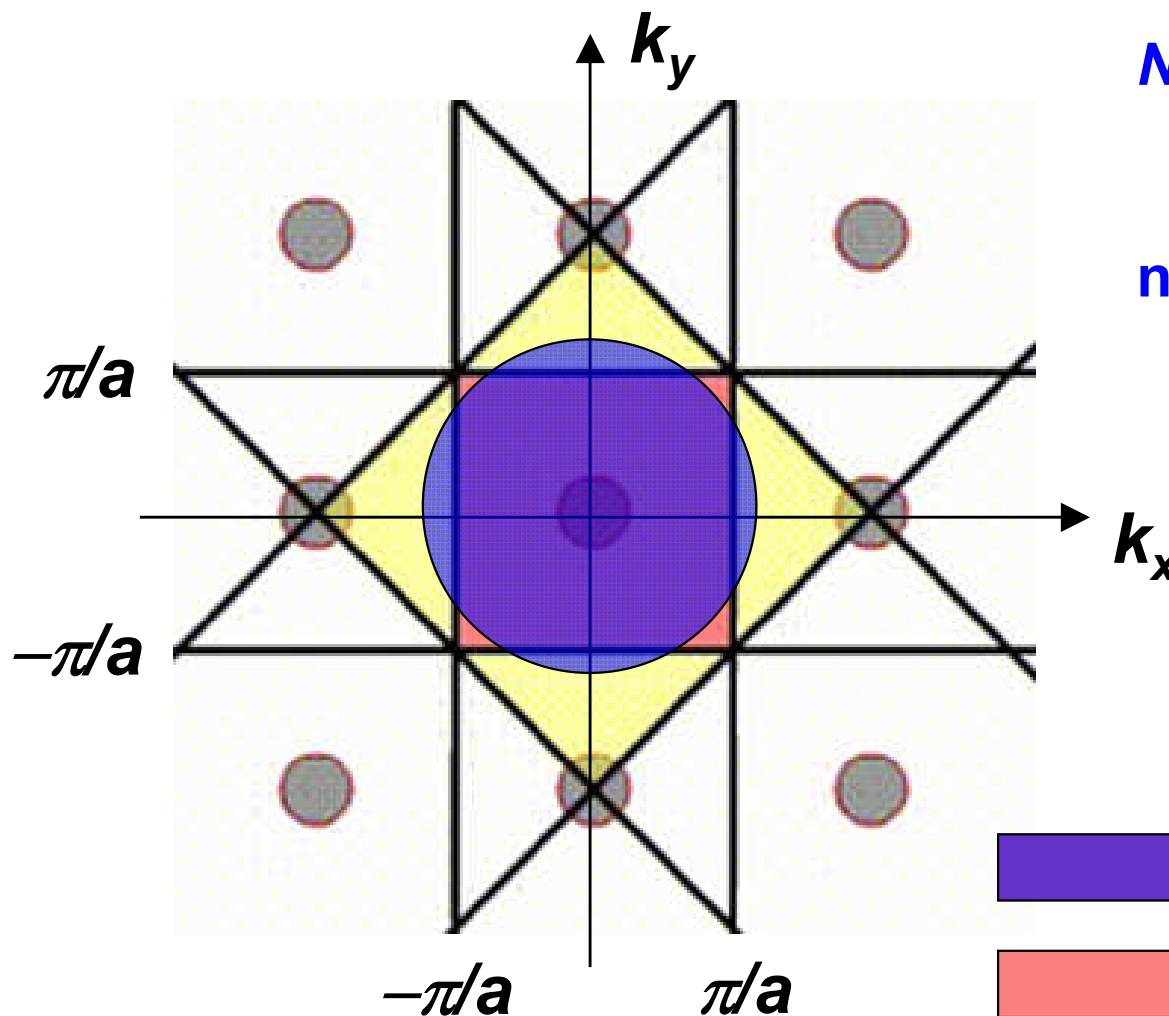
 **electrons**

 **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)

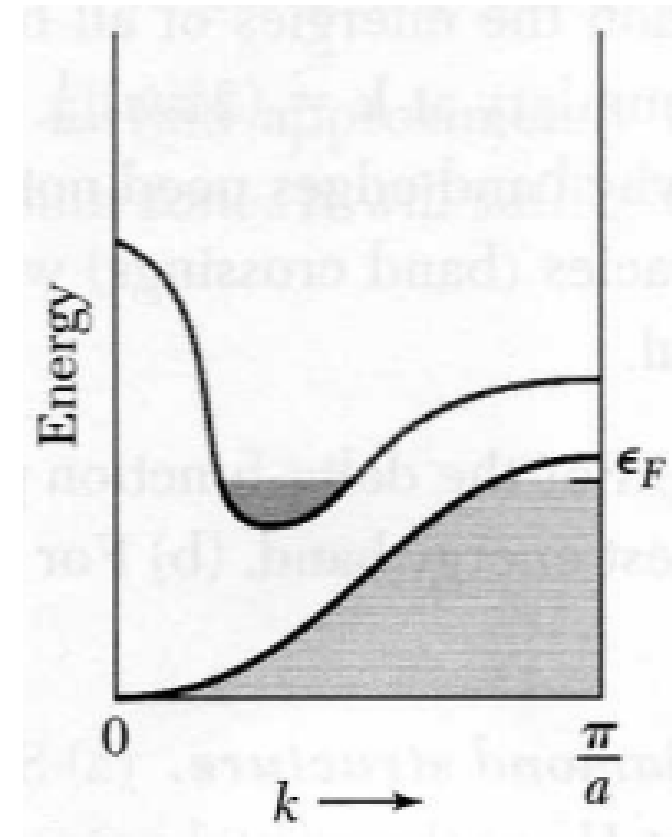
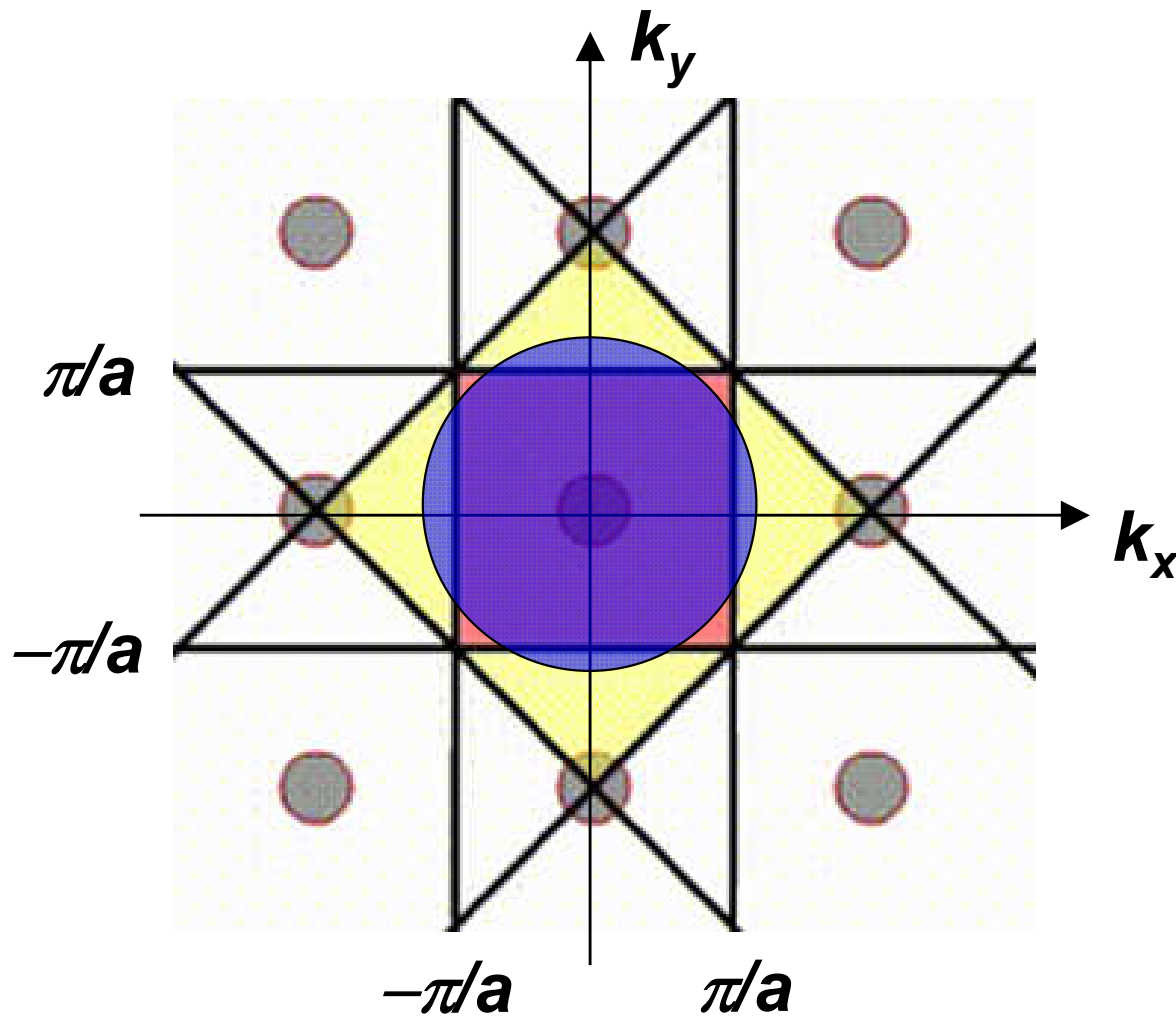
 electrons

 First BZ

 Second BZ

2D case of *Divalent* Atoms

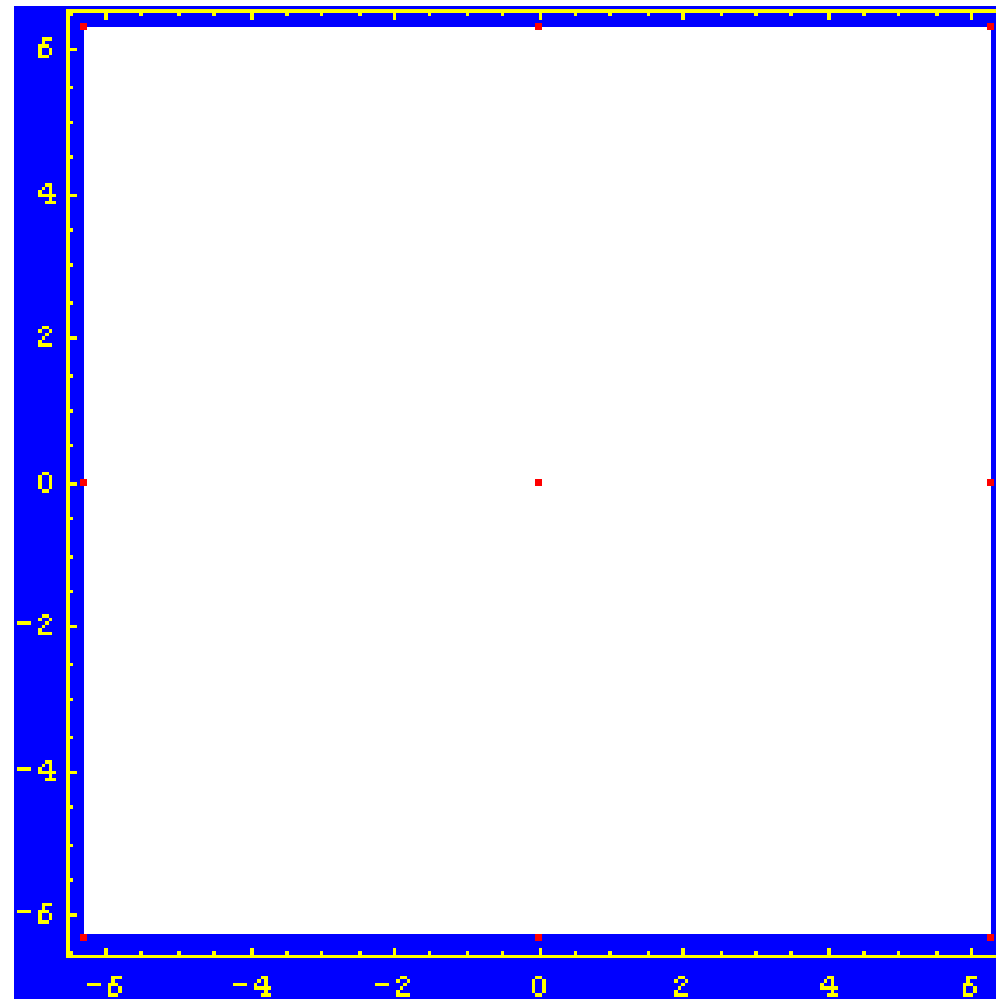
Each atom has *two* valence electrons (Mg, Ca, ...)



semimetal 半金属

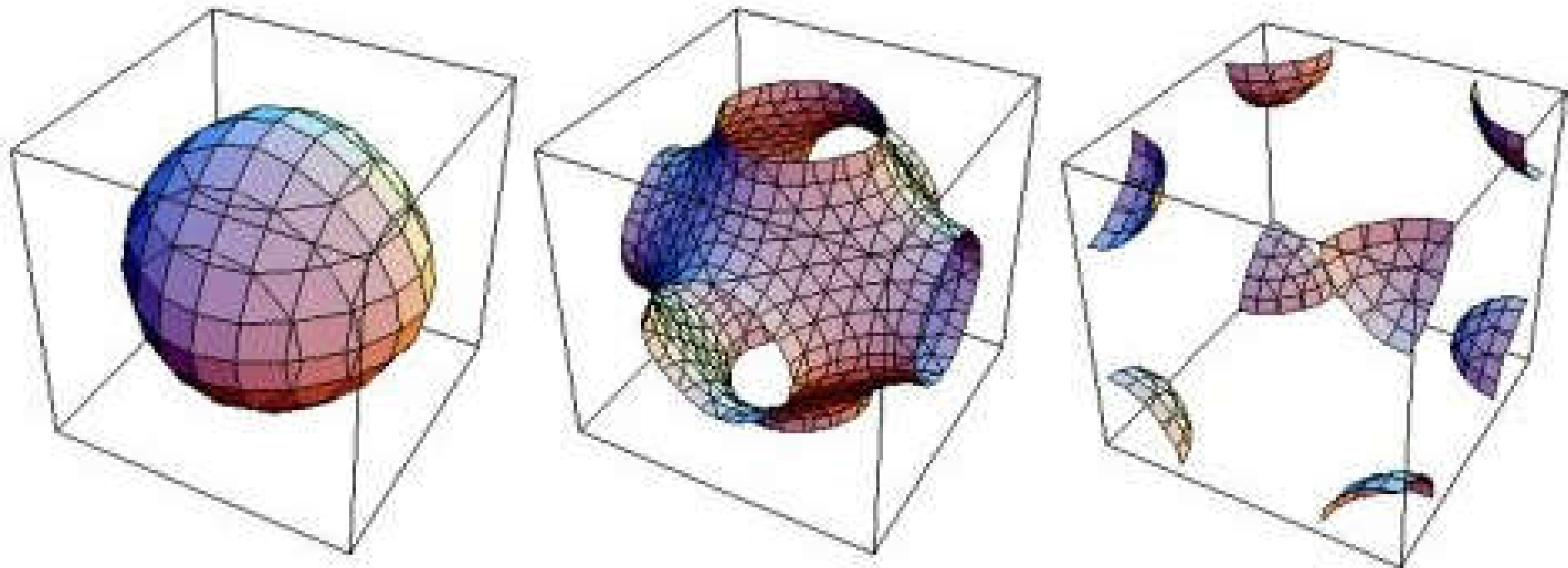
2D Fermi Surface

simple square



3D Fermi Surface

simple cubic



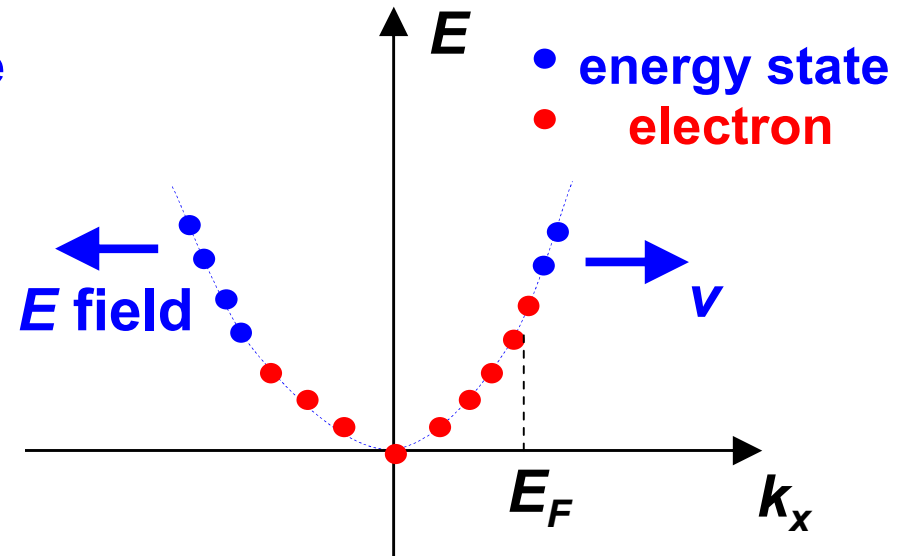
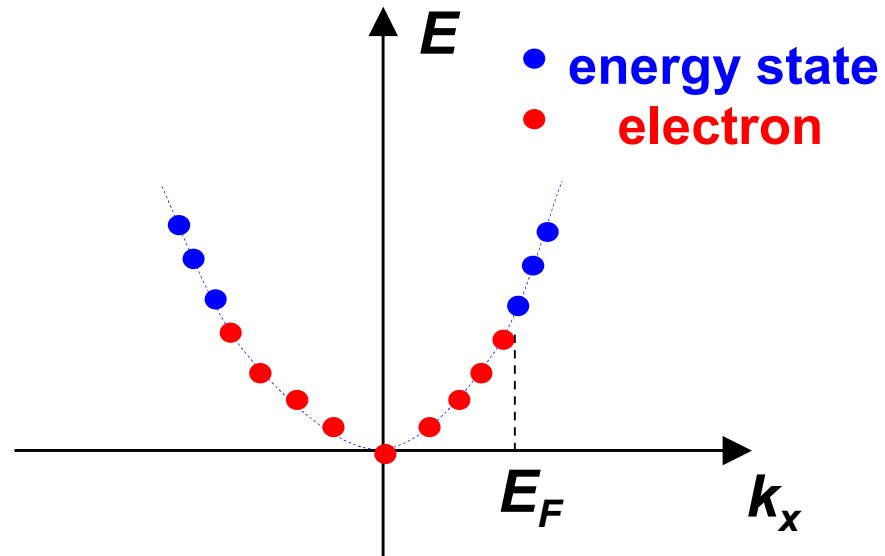
Increasing Fermi Energy \longrightarrow

generated with a tight binding model:

<http://home.cc.umanitoba.ca/~loly/fermisurf2.html>

Electrical Conductivity - Revisit

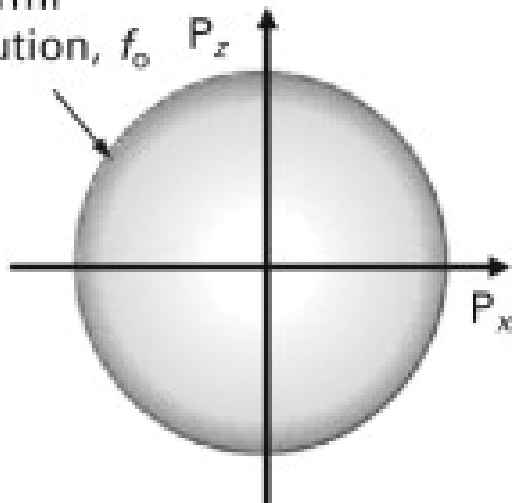
1D



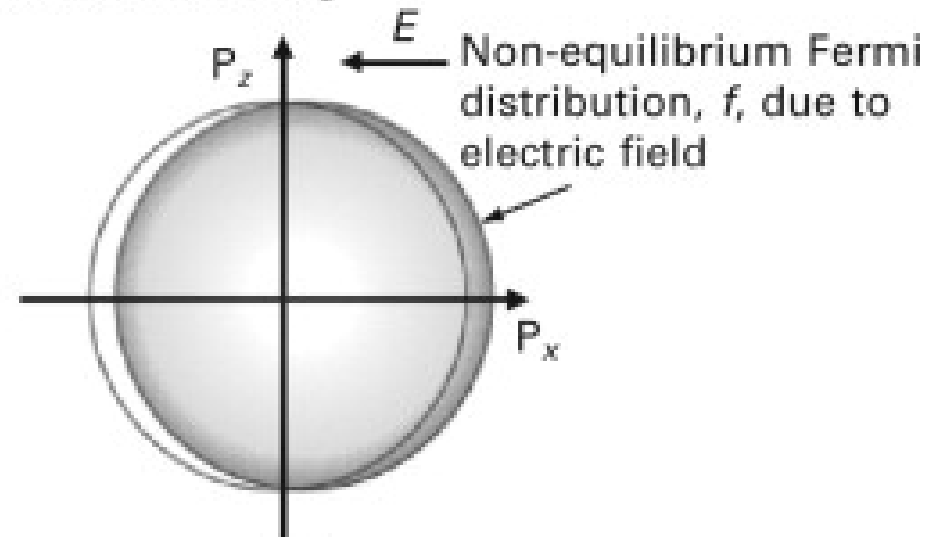
2D

Equilibrium
Fermi
distribution, f_0

3D



Diffuse scattering

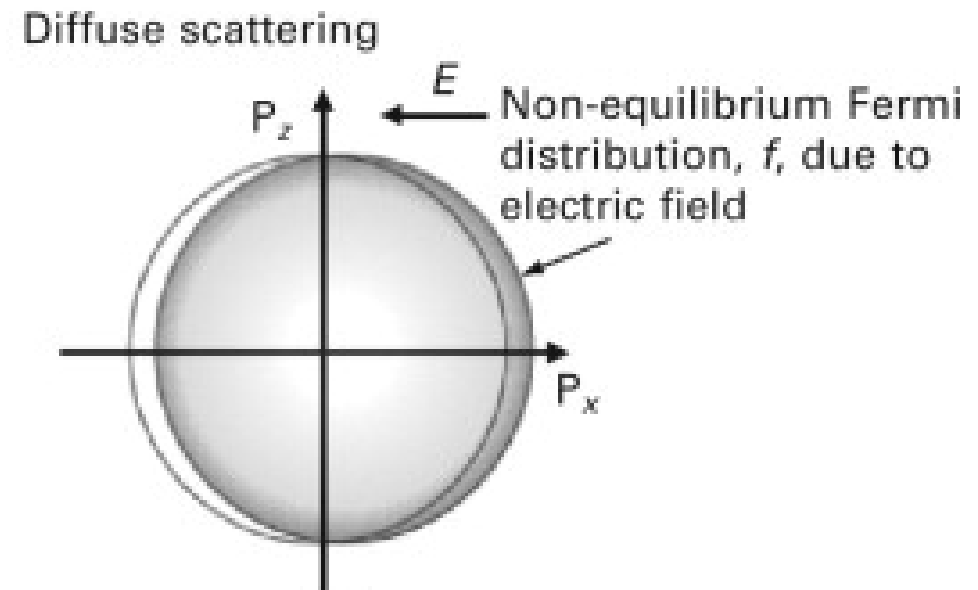
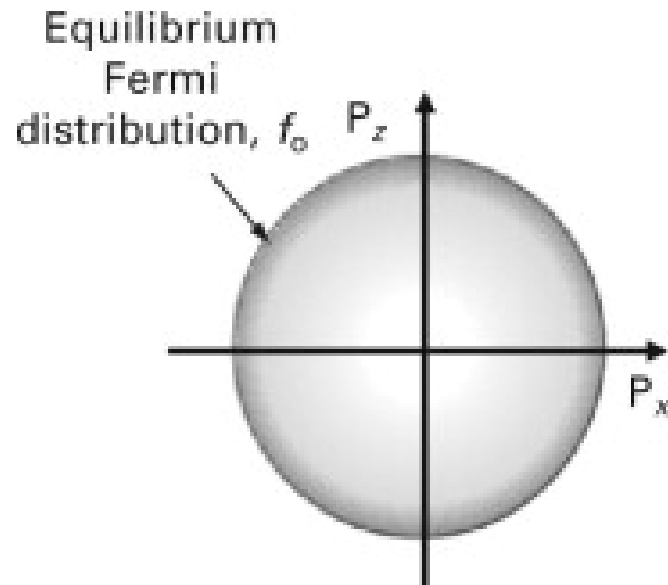


Electrical Conductivity - Revisit

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

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

Ashcroft & Mermin, Chap.13

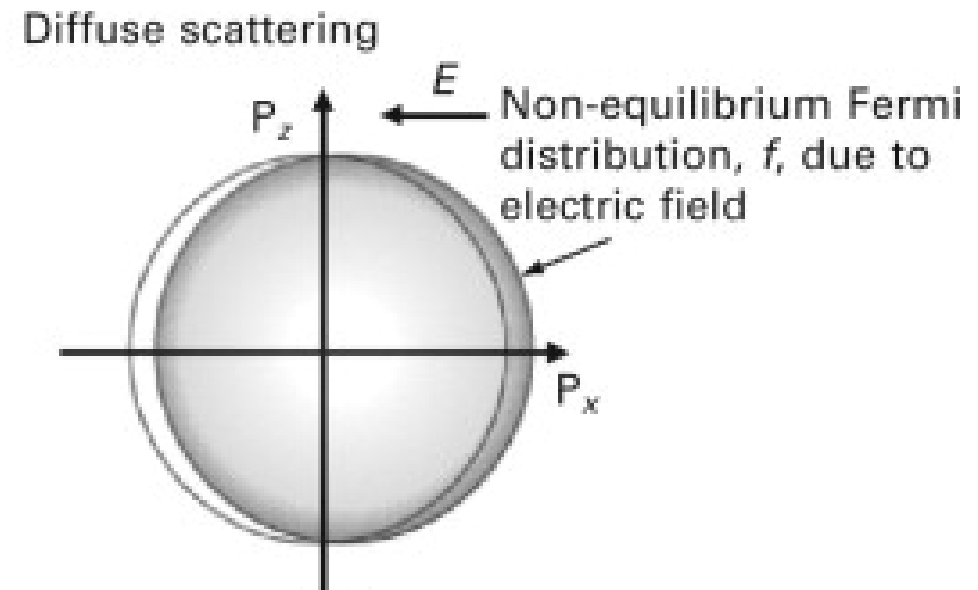
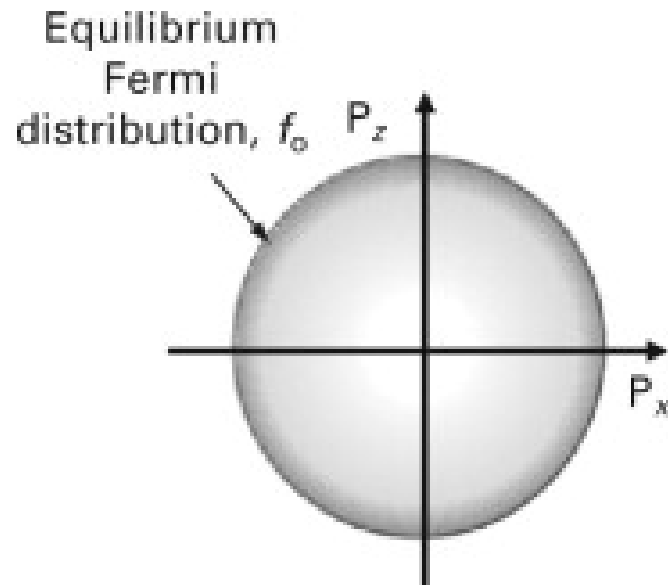


Electrical Conductivity - Revisit

- 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

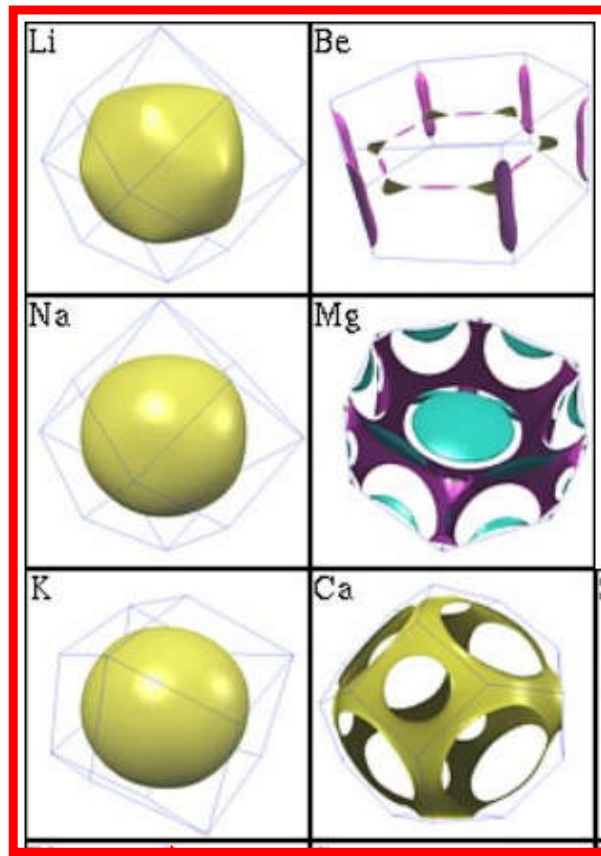
$$\sigma = ne \frac{v}{E} = ne\mu = \frac{ne^2\tau}{m^*}$$

	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

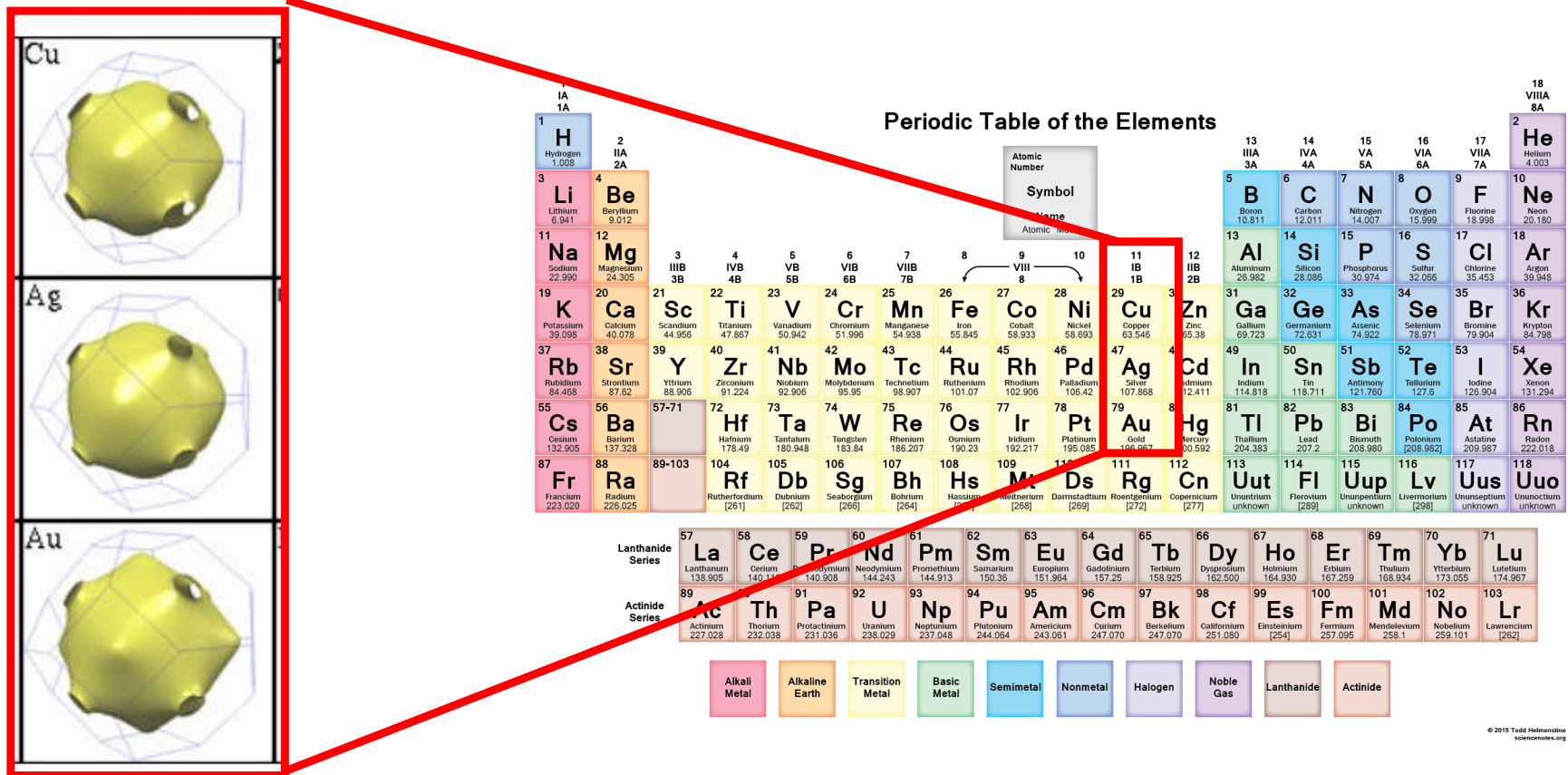
IIA



Periodic Table of the Elements																		VIII 8A																													
IA 1A																		IIA 2		He Helium 4.003																											
1 H Hydrogen 1.008																		2 He																													
3 Li Lithium 6.941		4 Be Beryllium 9.012																10 Ne Neon 20.180																													
11 Na Sodium 22.990		12 Mg Magnesium 24.305																18 Ar Argon 39.948																													
19 K Potassium 39.098		20 Ca Calcium 40.078																36 Kr Krypton 84.798																													
37 Rb Rubidium 84.468		38 Sr Strontium 87.62																54 Xe Xenon 131.29																													
55 Cs Cesium 132.905		56 Ba Barium 137.328																86 Rn Radon 222.018																													
87 Fr Francium 223.020		88 Ra Radium 226.025																118 Uuo Ununoctium unknown																													
																		13 Al Aluminum 26.982		14 Si Silicon 28.086		15 P Phosphorus 30.974		16 S Sulfur 32.065		17 Cl Chlorine 35.453		18 Ar																			
																		5 B Boron 10.811		6 C Carbon 12.011		7 N Nitrogen 14.007		8 O Oxygen 15.999		9 F Fluorine 18.998		10 Ne																			
																		13 Al Aluminum 26.982		14 Si Silicon 28.086		15 P Phosphorus 30.974		16 S Sulfur 32.065		17 Cl Chlorine 35.453		18 Ar																			
																		31 Ga Gallium 69.723		32 Ge Germanium 72.631		33 As Arsenic 74.922		34 Se Selenium 78.971		35 Br Bromine 79.904		36 Kr																			
																		49 In Indium 114.818		50 Sn Tin 118.711		51 Sb Antimony 121.760		52 Te Tellurium 127.6		53 I Iodine 126.904		54 Xe																			
																		81 Tl Thallium 204.383		82 Pb Lead 207.2		83 Bi Bismuth 208.980		84 Po Polonium [209]		85 At Astatine [210]		86 Rn																			
																		113 Uut Ununtrium unknown		114 Fl Flerovium [289]		115 Uup Ununpentium unknown		116 Lv Livermorium [293]		117 Uus Ununseptium unknown		118 Uuo																			
																		57 La Lanthanum 138.905		58 Ce Cerium 140.116		59 Pr Praseodymium 140.908		60 Nd Neodymium 144.243		61 Pm Promethium 144.913		62 Sm Samarium 150.36		63 Eu Europium 151.964		64 Gd Gadolinium 157.25		65 Tb Terbium 158.925		66 Dy Dysprosium 162.500		67 Ho Holmium 164.930		68 Er Erbium 167.259		69 Tm Thulium 168.934		70 Yb Ytterbium 173.055		71 Lu Lutetium 174.967	
																		89 Ac Actinium 227.028		90 Th Thorium 232.038		91 Pa Protactinium 231.036		92 U Uranium 238.029		93 Np Neptunium 237.048		94 Pu Plutonium 244.064		95 Am Americium 243.061		96 Cm Curium 247.070		97 Bk Berkelium 247.070		98 Cf Californium 251.080		99 Es Einsteinium [254]		100 Fm Fermium 257.095		101 Md Mendelevium 258.1		102 No Nobelium 259.101		103 Lr Lawrencium [262]	
Alkali Metal		Alkaline Earth		Transition Metal		Basic Metal		Semimetal		Nonmetal		Halogen		Noble Gas		Lanthanide		Actinide																													

3D Fermi Surface

IB

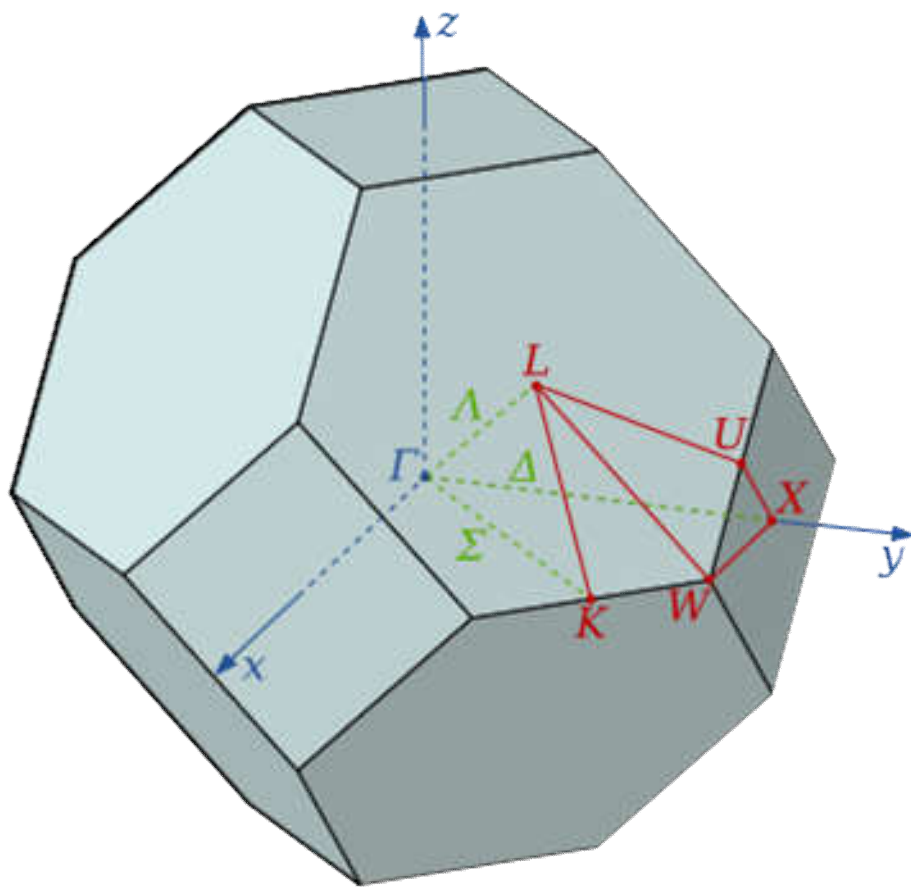


nearly free electrons

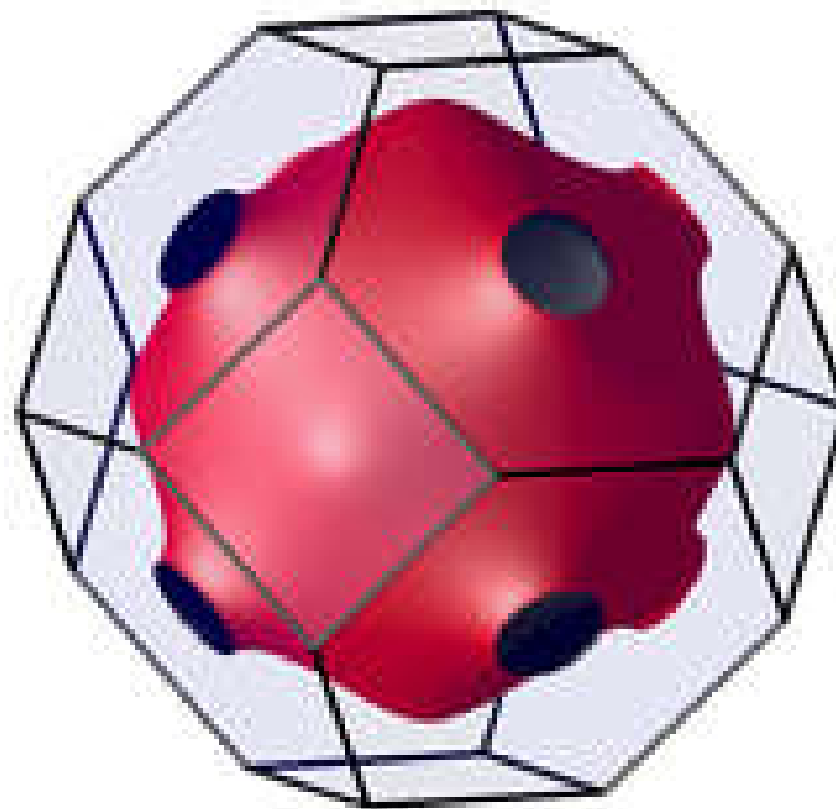
<http://www.phys.ufl.edu/fermisurface/>

3D case

copper (FCC)



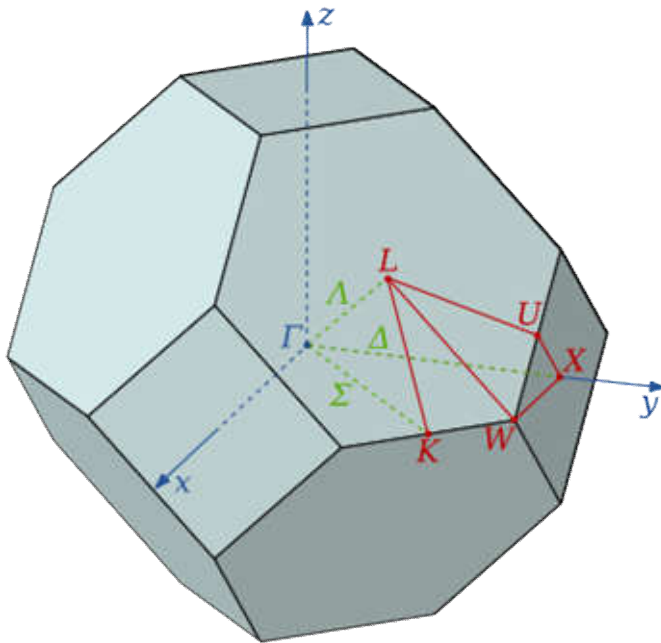
First BZ



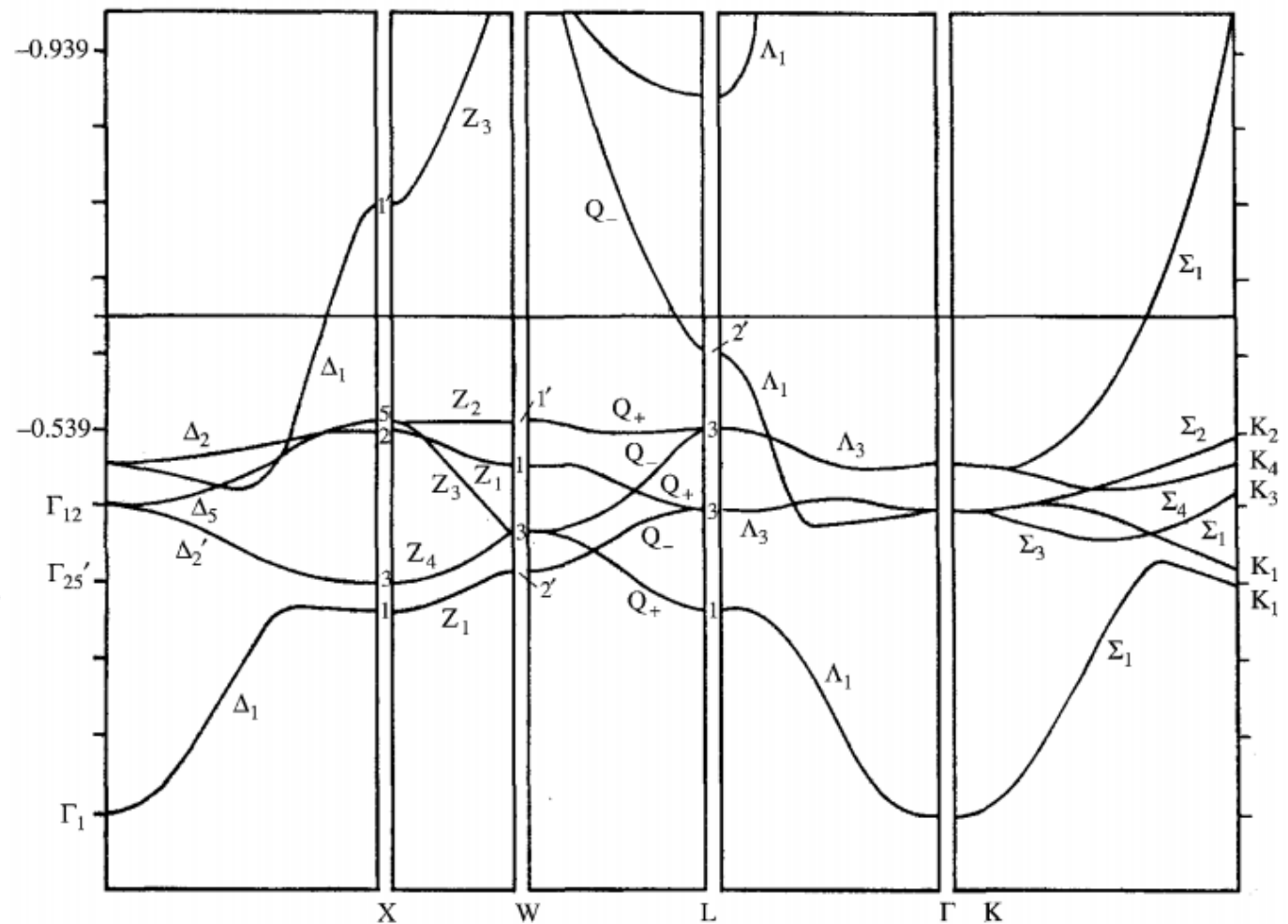
Fermi Surface

3D case

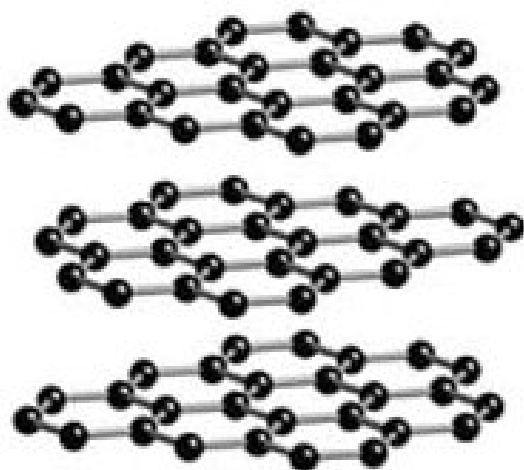
copper (FCC): band structure



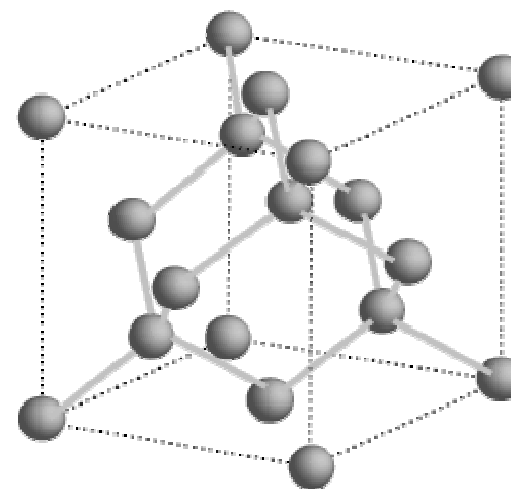
First BZ



Example - Carbon

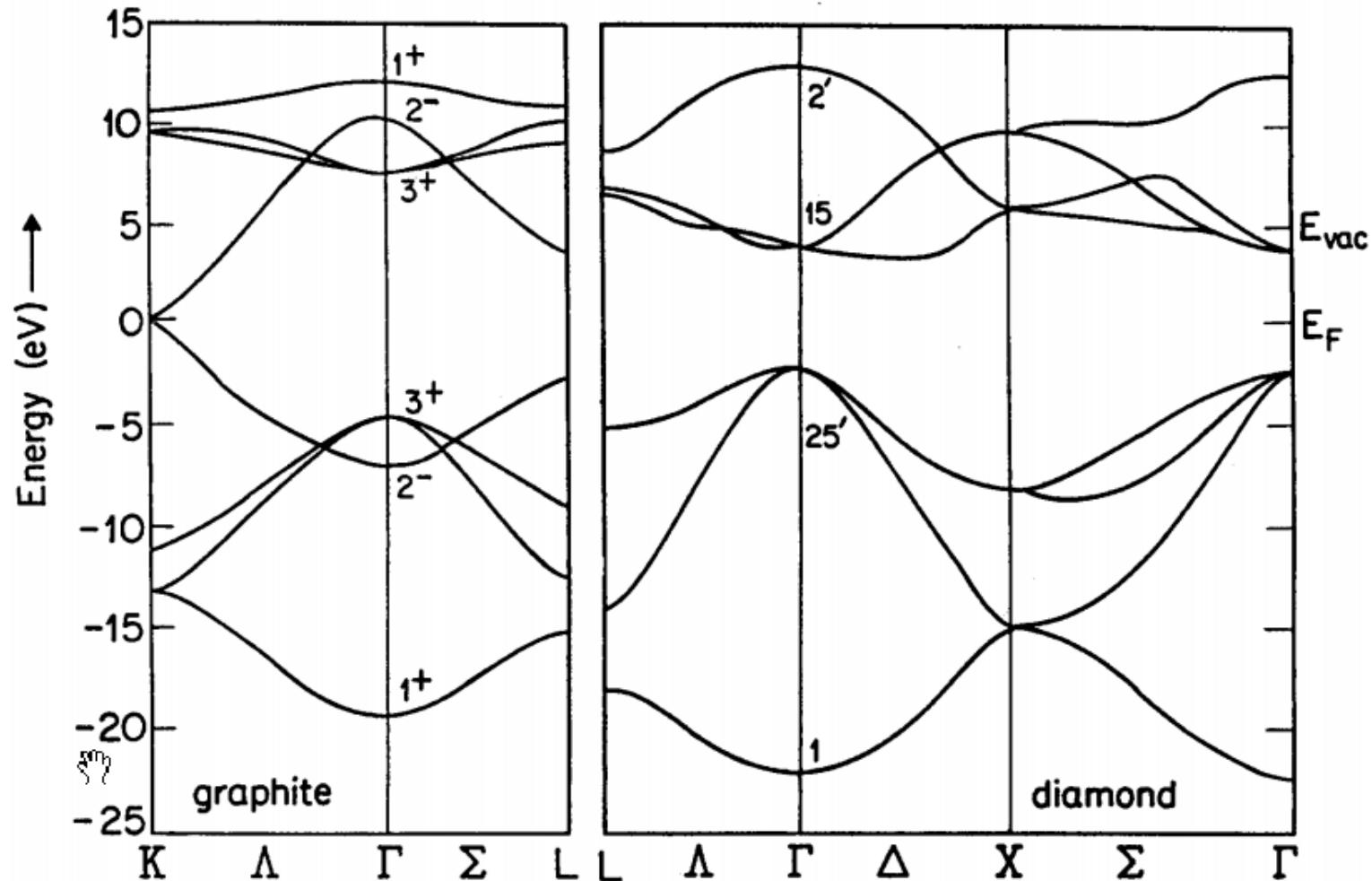


graphite
 $\sigma \sim 10^5 \text{ S/m}$



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

Example - Carbon



graphite
conductor

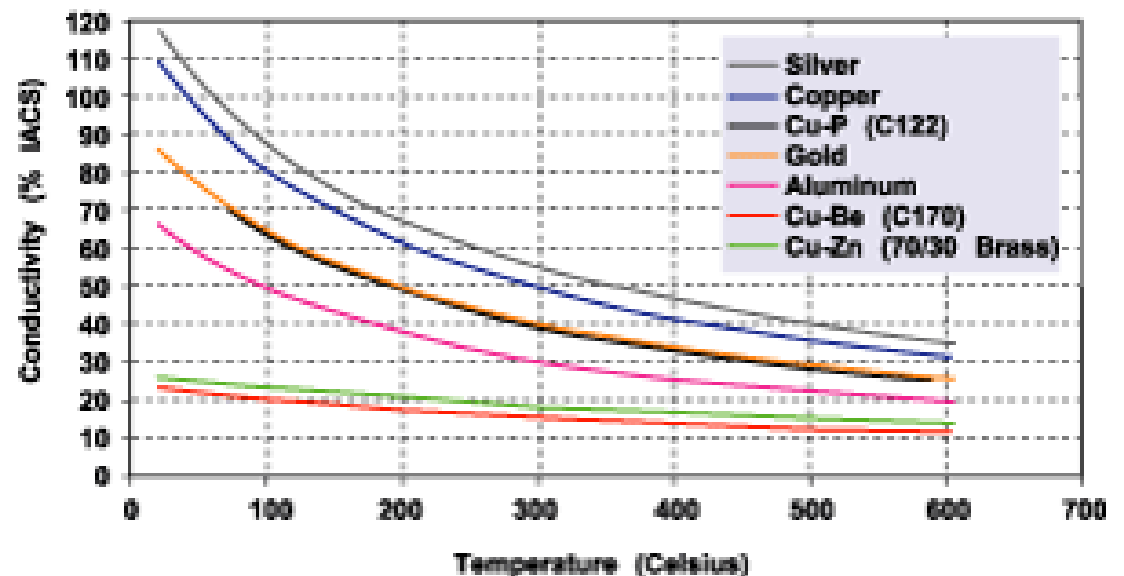
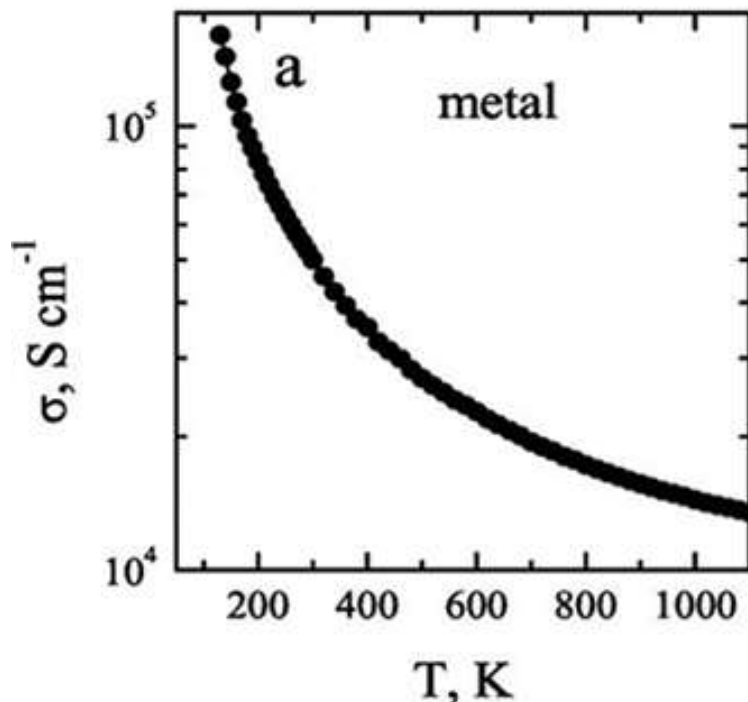
diamond
insulator ($E_g = 5.5$ eV)

Temperature Dependence of σ

■ For metals

- n and m^* have weak dependence on T
- t has a strong dependence on T
- higher T \rightarrow shorter τ \rightarrow smaller μ \rightarrow smaller σ

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

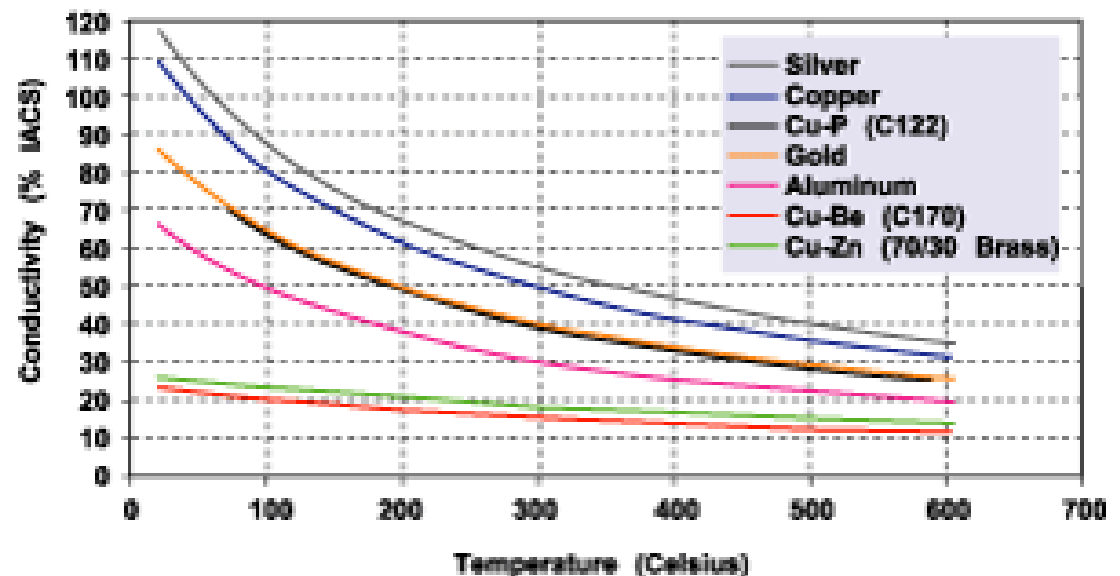
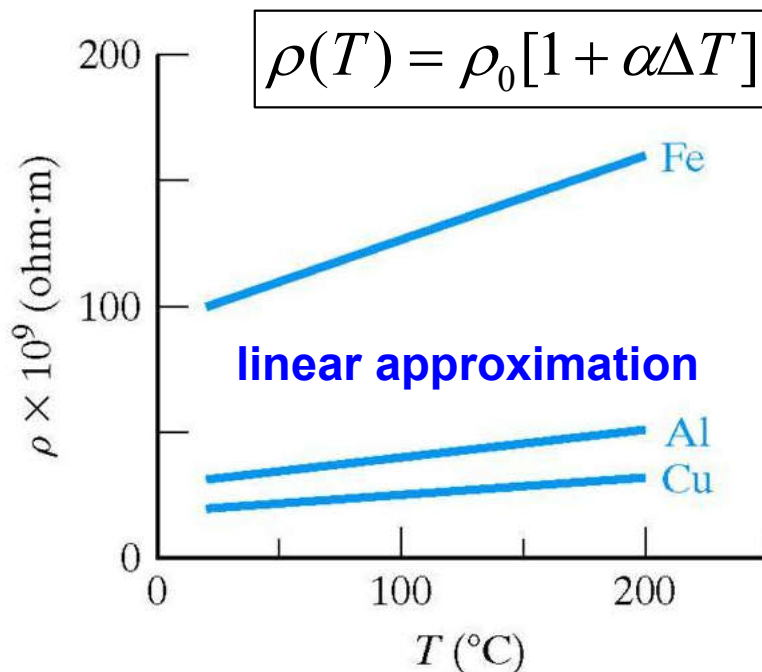


Temperature Dependence of σ

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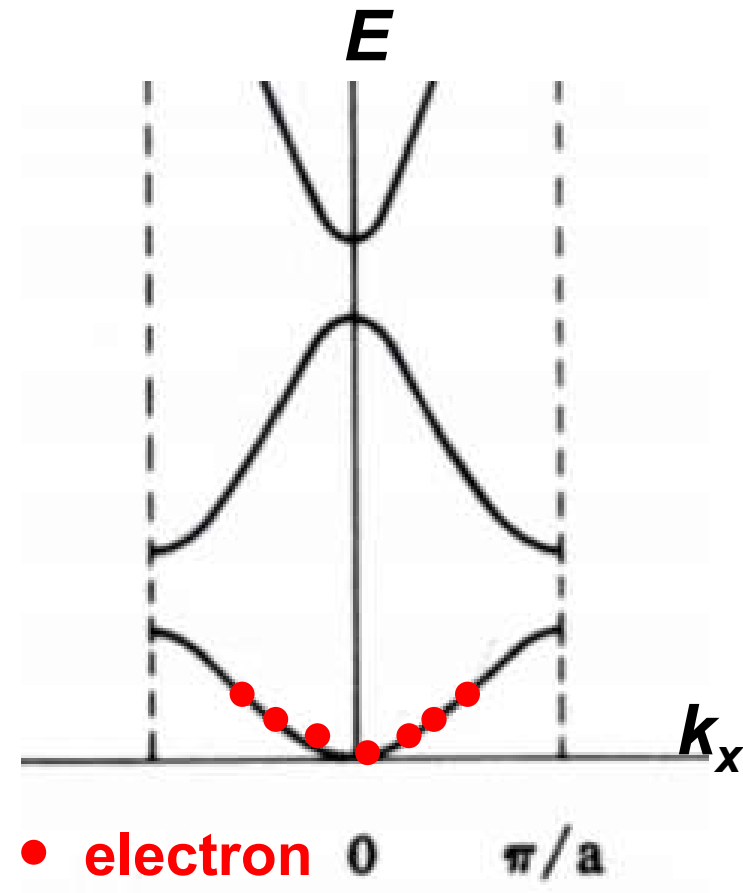
$$\sigma = ne\mu = \frac{ne^2\tau}{m^*}$$



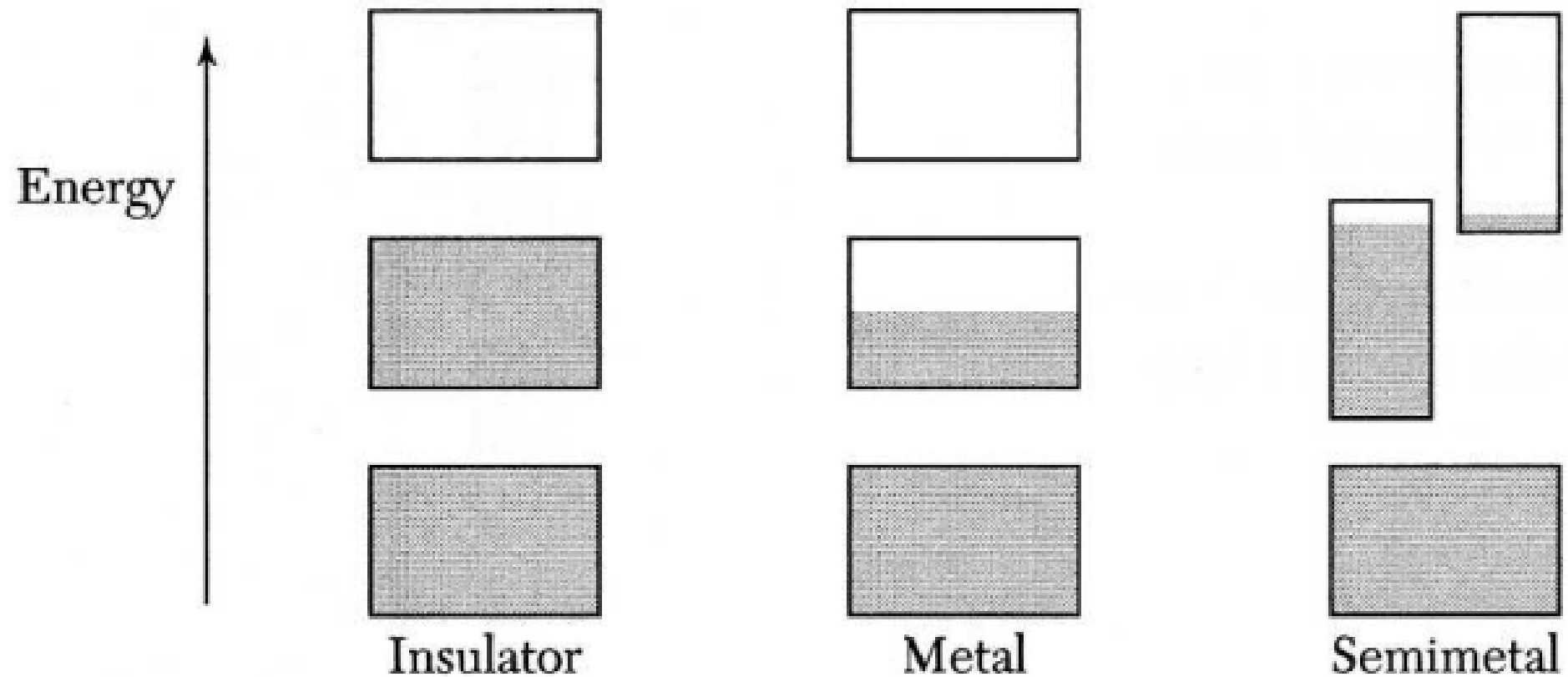
Summary

■ Electronic properties of solids depend on

- band structure
- electron density
- defects
- temperature
- electric field
- ...



Summary



Thank you for your attention