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2022.5.20

# Outline

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Semiconductor Basis

Doping

Quantum Mechanics

Quantum Theory of Solid

# Semiconductor Basis - Materials

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## The Periodic Table of the Elements

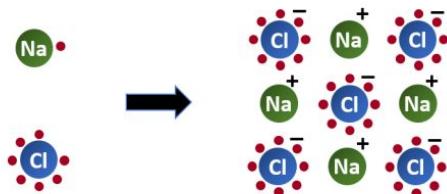
IA		IIA																VIIA																									
1 H 1.008		3 Li 6.941	4 Be 9.012															2 He 4.003																									
11 Na 22.99	12 Mg 24.31	IIIB		IVB		VB		VIB		VIIB		VIIIB						IB		IIB																							
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (96)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 116.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3								
55 Cs 132.9	56 Ba 137.3	57 La 136.9	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)	87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (269)	109 Mt (268)	110 Uun (271)	111 Uuu (272)	112 Uub (277)	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
90 Th 232.0	91 Pa (231)	92 U 238.0	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	99 Fm (257)	100 Md (258)	101 No (259)	102 Lr (262)																														

Elemental Semiconductor	Group IV Compounds	Binary III-V Compounds	Binary II-VI Compounds
Si	SiC	GaAs	ZnO
Ge	Si <sub>x</sub> Ge <sub>1-x</sub>	GaN	ZnS
		InAs	CdS
		InP	CdSe
		AlAs	

# Semiconductor Basis - Chemical Bonding

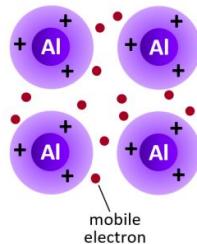
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## Ionic Bonding



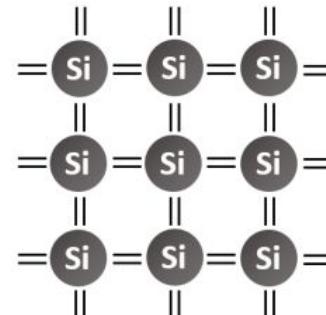
- Strong bonds, electrons tightly bound to atoms
- Good insulator

## Metallic Bonding



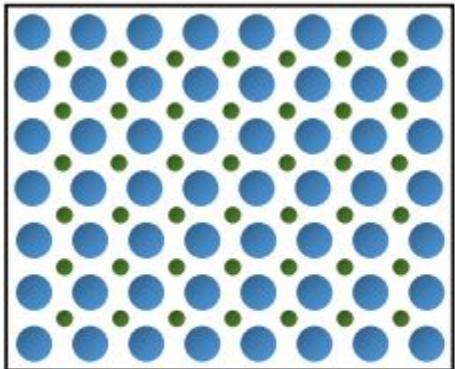
- Ions surrounded by freed mobile electrons
- Electrons can move when subject to an E-field
- Good conductor

## Covalent Bonding

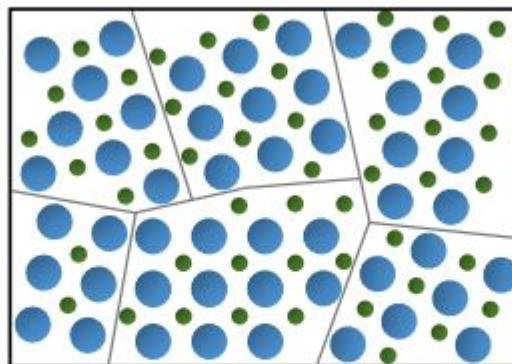


- Atoms “share” electrons with nearest neighbors
- Weaker than ionic bonds

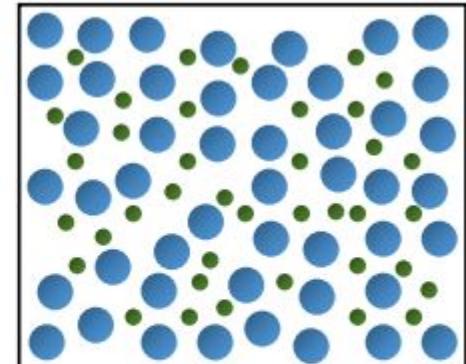
# Semiconductor Basis - Solid Types



Crystalline



Polycrystalline



Amorphous

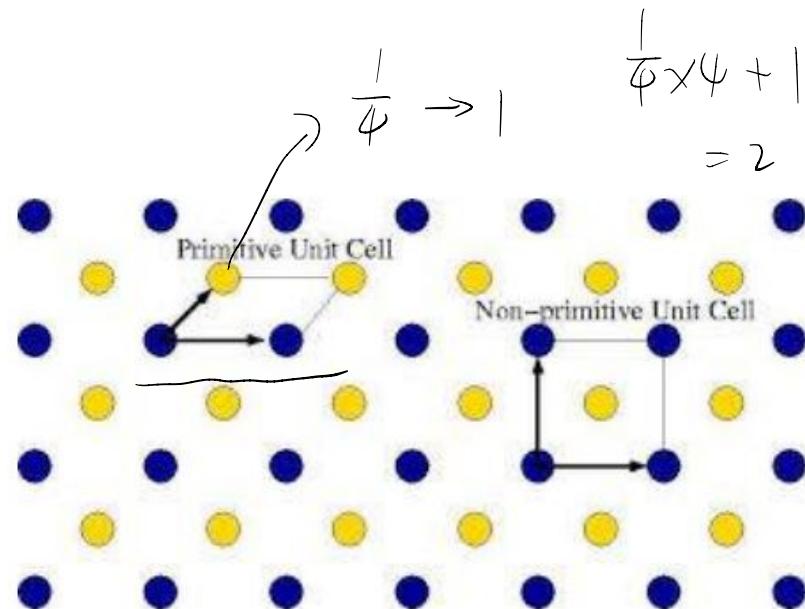
# Semiconductor Basis - Crystal Structure

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## Unit cell

Primitive cell: minimum volume unit cell and has only one lattice point in it.

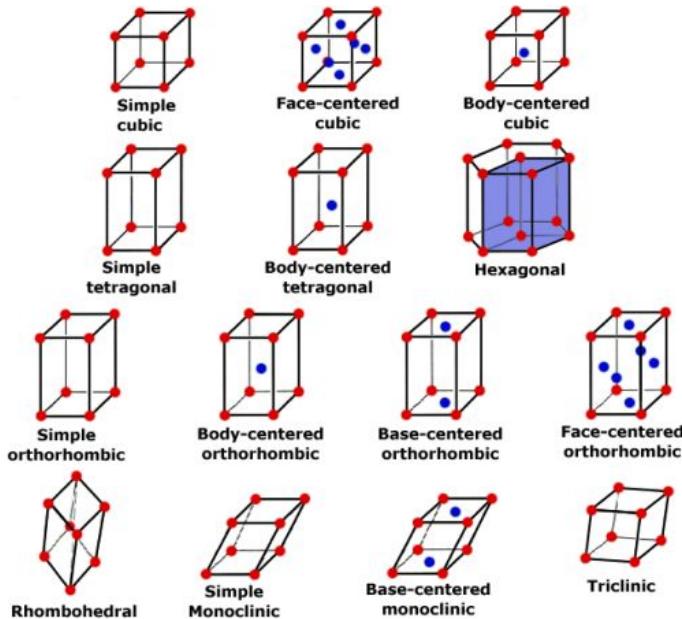
Non-primitive cell: contains more than one lattice point.



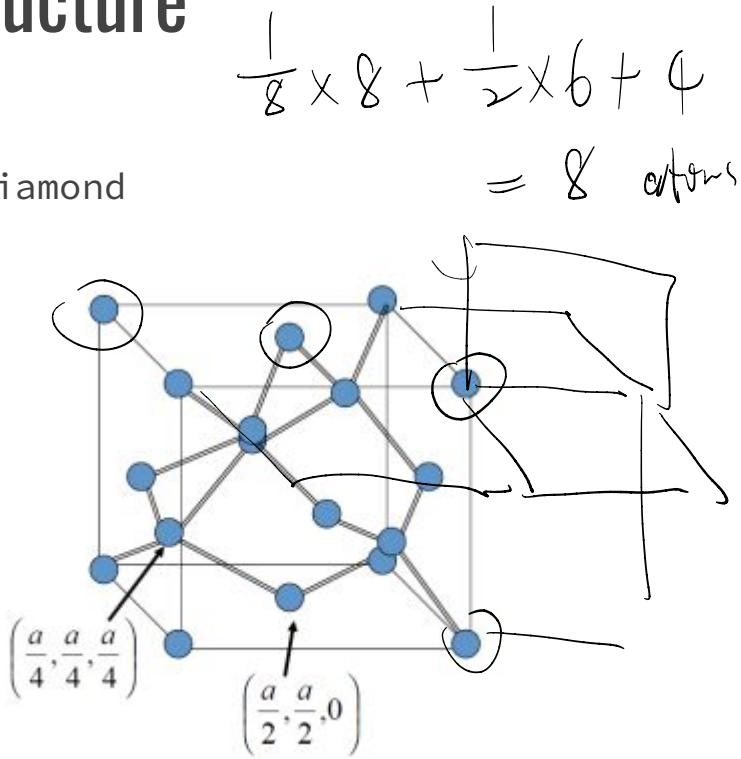
# Semiconductor Basis - Crystal Structure

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Basic Crystal Structures



Diamond



# Semiconductor Basis - Miller Index

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1. Determine intercepts ( $x$ ,  $y$ ,  $z$ )
2. Divide the values by unit cell length
3. Invert the intercept values ( $1/\text{intercept}$ )
4. Small integers  $(\infty, \infty, \infty)$

$$(\infty, \infty, \infty)$$

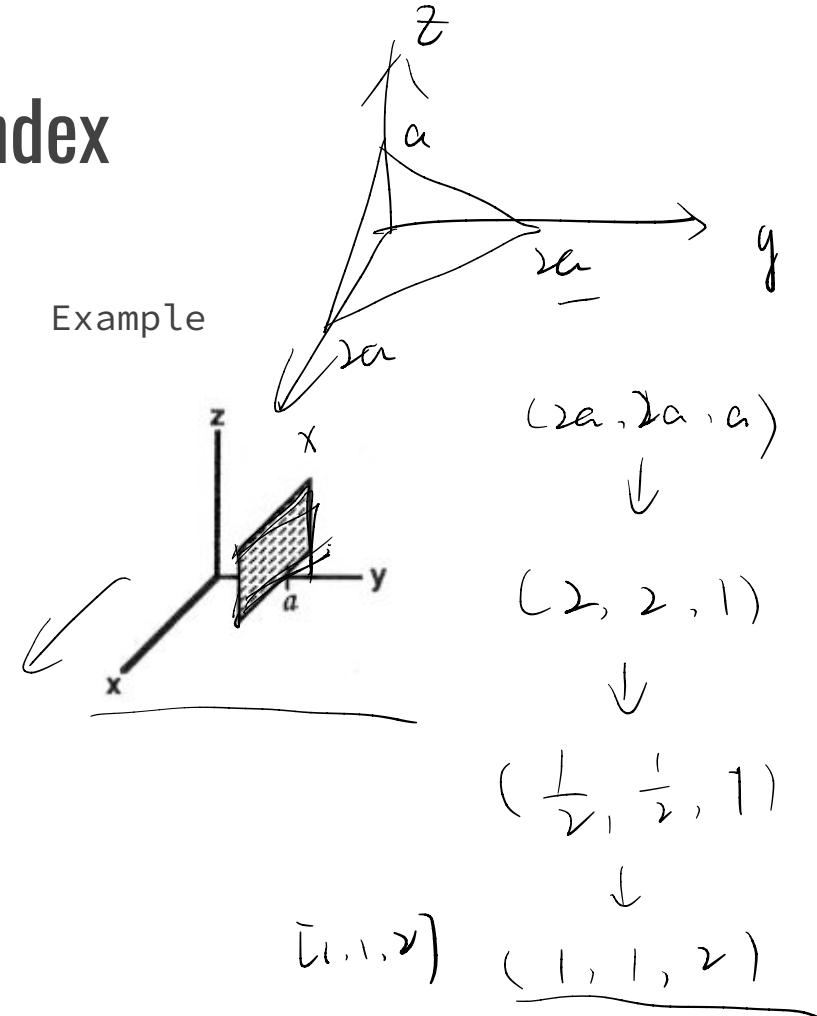


$$(\infty, 1, \infty)$$



$$(0, 1, 0)$$

Example



# Semiconductor Basis - Miller Index

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Notation Interpretation

( h k l ) Crystal plane

$$(0, 1, 0) \rightarrow \{0, 1, 0\}$$

{ h k l } Equivalent planes

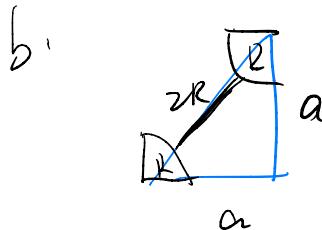
[ h k l ] Crystal direction

$$[0, 1, 0] \rightarrow <0, 1, 0>$$

< h k l > Equivalent directions

# Semiconductor Basis - Exercise

a.  $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = \underline{4 \text{ atoms}}$



$$4R = \sqrt{2}a$$

$$a = 2\sqrt{2}R$$

C.  $a^3$        $a = 2\sqrt{2}R$        $V = (2\sqrt{2}R)^3$

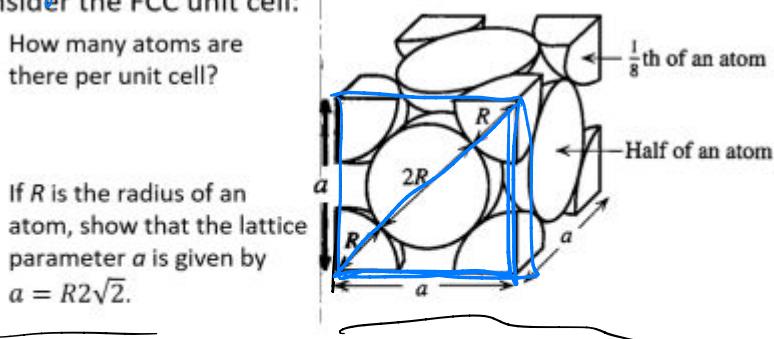
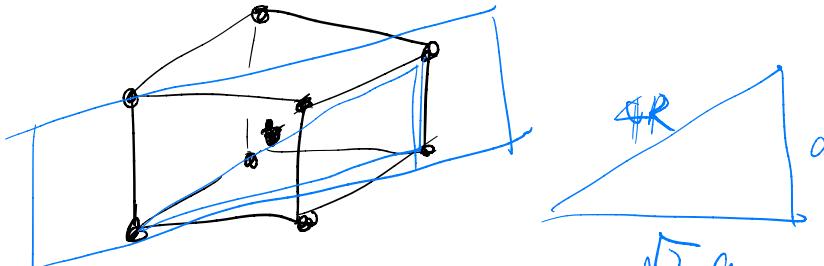
$$c = \frac{4}{V}$$

- Consider the FCC unit cell:

a. How many atoms are there per unit cell?

b. If  $R$  is the radius of an atom, show that the lattice parameter  $a$  is given by  $a = R2\sqrt{2}$ .

c. Copper has an FCC unit cell with  $R = 0.128 \text{ nm}$ . Calculate the atomic concentration (number of atoms per unit volume) in Cu.



# Semiconductor Basis - Exercise

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Consider a Ge wafer ( $a = 5.65 \text{ \AA}$ ) with a surface (110) plane.

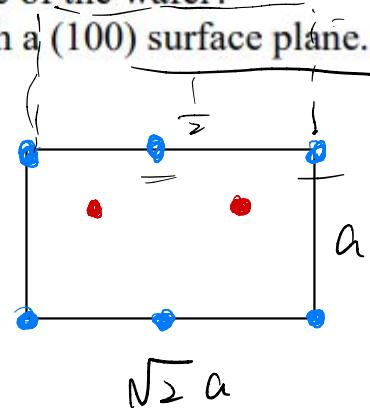
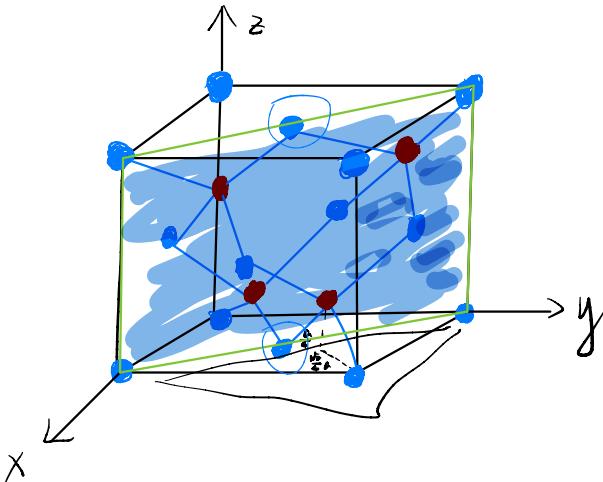
- a. Sketch the placement of Ge atoms on the surface of the wafer. Draw your diagram to scale and provide a scale bar.
- b. How many atoms per  $\text{cm}^2$  are at the surface of the wafer?
- c. Repeat parts (a) and (b) for a Ge wafer with a (100) surface plane.

# Semiconductor Basis - Exercise

( $a, a, \infty$ )

Consider a Ge wafer ( $a = 5.65 \text{ \AA}$ ) with a surface (110) plane.

- Sketch the placement of Ge atoms on the surface of the wafer. Draw your diagram to scale and provide a scale bar.
- How many atoms per  $\text{cm}^2$  are at the surface of the wafer?
- Repeat parts (a) and (b) for a Ge wafer with a (100) surface plane.



$$\frac{1}{4} \times 4 + \frac{1}{2} \times 2 + 2 = 4 \text{ atoms}$$

$$\frac{4}{a \cdot \sqrt{2}a}$$

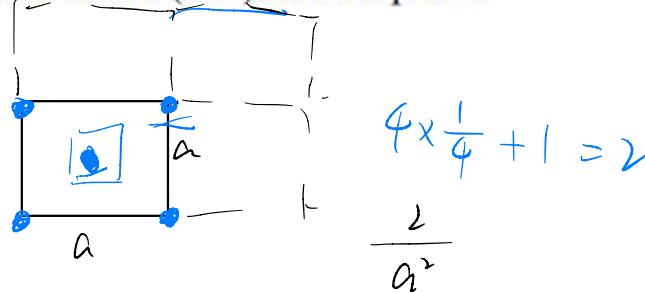
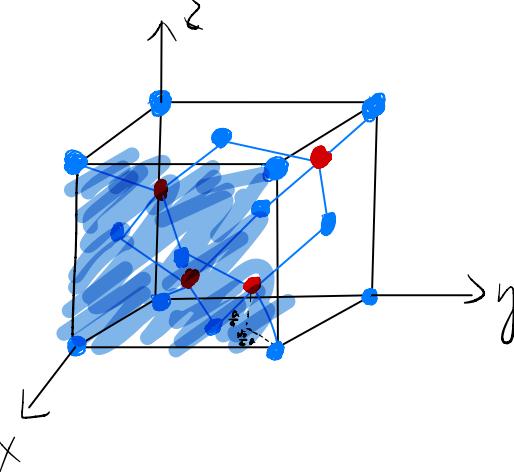
# Semiconductor Basis - Exercise

$$(1, 0, 0) \rightarrow (1, \infty, \infty)$$

$$[(a, \infty, \infty)]$$

Consider a Ge wafer ( $a = 5.65 \text{ \AA}$ ) with a surface (110) plane.

- Sketch the placement of Ge atoms on the surface of the wafer. Draw your diagram to scale and provide a scale bar.
- How many atoms per  $\text{cm}^2$  are at the surface of the wafer?
- Repeat parts (a) and (b) for a Ge wafer with a (100) surface plane.



# Doping - Occupancy of Energy Bands

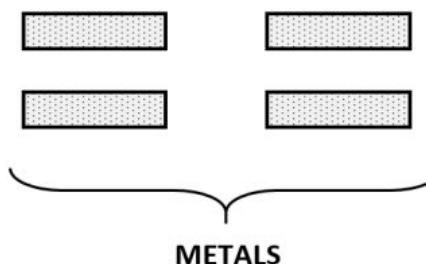
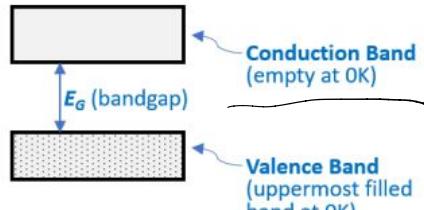
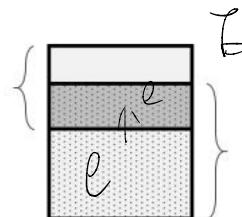
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$T \rightarrow 0 K:$

Partially filled upper band



Overlapping bands



SEMICONDUCTORS  
and  
INSULATORS

Semiconductors:

$EG \lesssim 6 \text{ eV}$

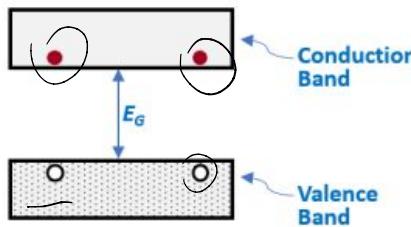
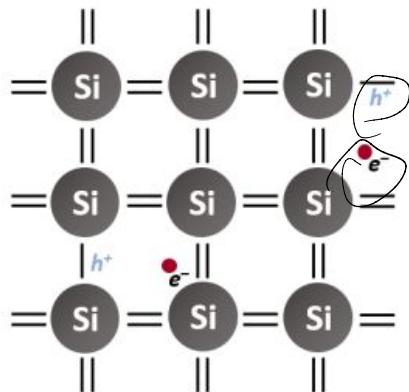
Insulators:

$EG \gtrsim 6 \text{ eV}$

# Doping - (Intrinsic) Semiconductors

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$T \cong 300\text{ K}$ :



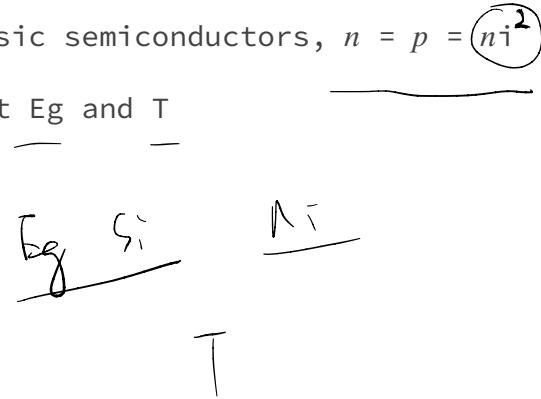
Generation of electron-hole pairs (EHPs)

$n \equiv$  concentration of conduction electrons

$p \equiv$  concentration of holes

For intrinsic semiconductors,  $n = p = n_i^2$

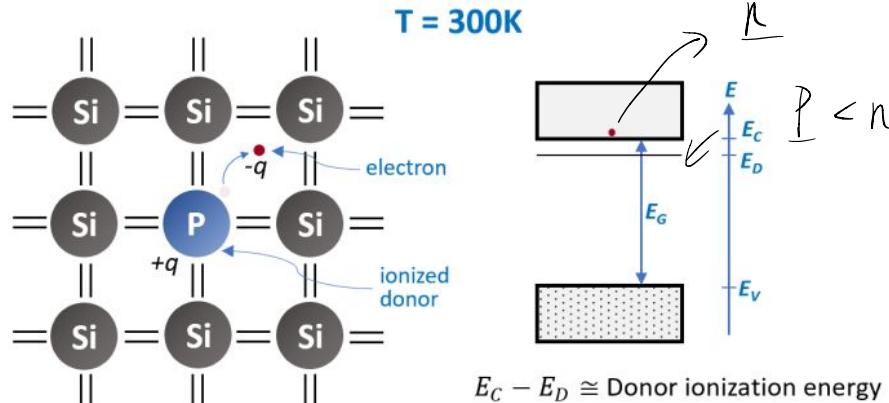
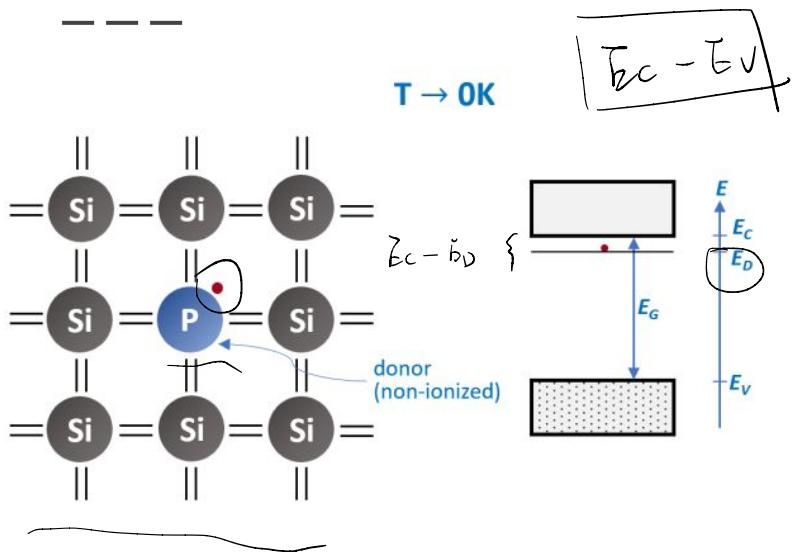
$n_i$  is about  $E_g$  and  $T$



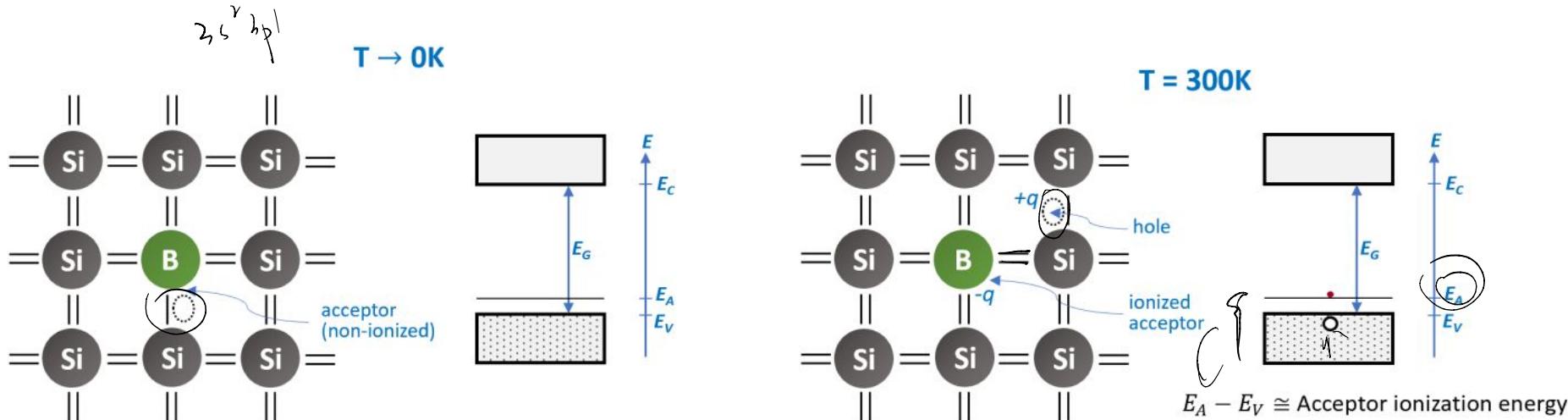
# Doping - Extrinsic Semiconductor: n-type doping

→ negative

$$n_p = \frac{n_i^2}{\mu}$$



# Doping - Extrinsic Semiconductor: p-type doping



$$\underline{P} > h$$

# Quantum Mechanics - Basic: Wave-particle duality

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Matter particle

$$p = m\omega, E = \frac{1}{2}mv^2, p = \frac{h}{\lambda}$$

Wave particle  
photon

$$p = \frac{h}{\lambda} = \hbar k, E = h\omega, \omega = \frac{\lambda}{c} \quad \text{Light: } E = mc^2 = \frac{E}{c}$$

Both  $\hbar = \frac{h}{2\pi}$  wave number  $k = \frac{2\pi}{\lambda}$

Solution to Differential Equation

$$\frac{\partial^2 y}{\partial x^2} = k^2 y \quad y = A e^{kx} + B e^{-kx}$$

$$\frac{\partial^2 y}{\partial x^2} = -k^2 y \quad y = A e^{jkx} + B e^{-jkx}$$

# Quantum Mechanics - Schrodinger Equation

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Infinite quantum well

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = E\Psi, \quad \begin{cases} \frac{V(x)}{V(x)} = +\infty, & x \leq 0 \text{ or } x \geq a \\ \frac{V(x)}{V(x)} = 0, & 0 < x < a \end{cases}$$

General solution:

$$\Psi(x) = Ae^{-ikx} + Be^{ikx}$$

Boundary condition:

$$\Psi(x)|_{x=a,0} = 0$$

$$\int_0^a \Psi(x)\Psi^*(x) dx = 1$$

Conclusion:

$$k = \frac{n\pi}{a}, n = 0, \pm 1, \pm 2, \dots$$

$$E = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Finite quantum well

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = E\Psi, \quad \begin{cases} \frac{V(x)}{V(x)} = V_0, & x \leq 0 \text{ or } x \geq a \\ \frac{V(x)}{V(x)} = 0, & 0 < x < a \end{cases}$$

General solution:

$$\Psi(x) = \begin{cases} Ae^{-ik_1 x} + Be^{ik_1 x}, & k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, \quad x \leq 0 \text{ or } x \geq a \\ Ce^{-ik_2 x} + De^{ik_2 x}, & k_2 = \sqrt{\frac{2mE}{\hbar^2}}, \quad 0 < x < a \end{cases}$$

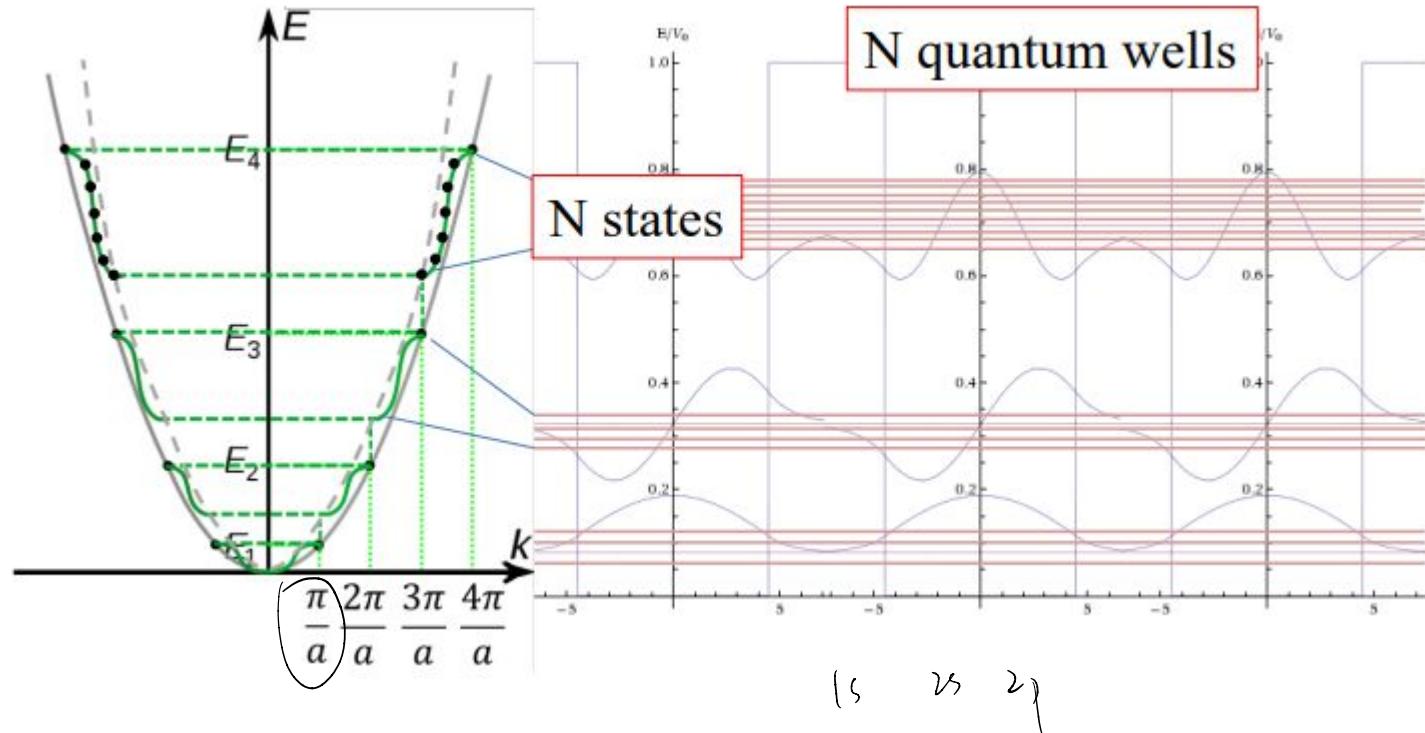
Boundary condition:

$$\Psi(x)|_{x=0} \text{ continuous}$$

$$\Psi(x)|_{x=a} \text{ continuous}$$

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x) dx = 1$$

# Quantum Theory of Solid - Simple Band Diagram



$$E = \frac{\hbar^2 k^2}{2m}$$

$$= \frac{\langle p \rangle^2}{2m}$$

a free particle

$$\frac{dE}{dk} = \frac{\hbar^2 k}{me} \Rightarrow \frac{d^2E}{dk^2} = \frac{\hbar^2}{me}$$

$$\Rightarrow me = \hbar^2 \frac{1}{\lambda^2 \frac{d^2E}{dk^2}}$$

$H$

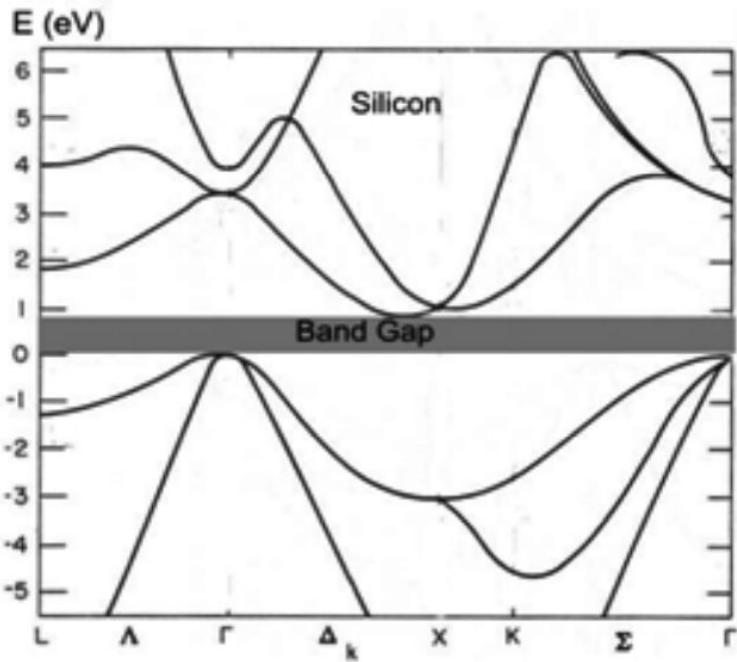
$1s^2 2s^2 2p^6 3s^2$

$1p_3$

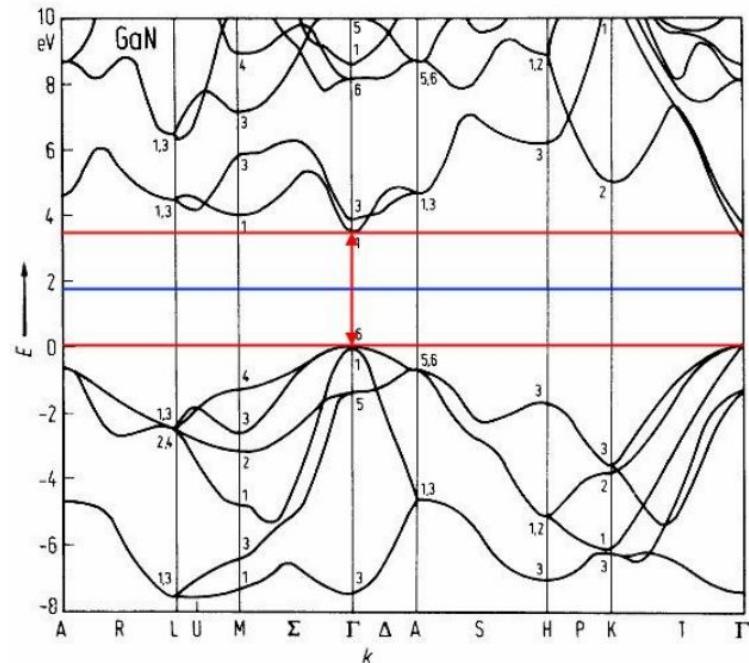
$1p_2$

$1s$

# Quantum Theory of Solid - Simple Band Diagram

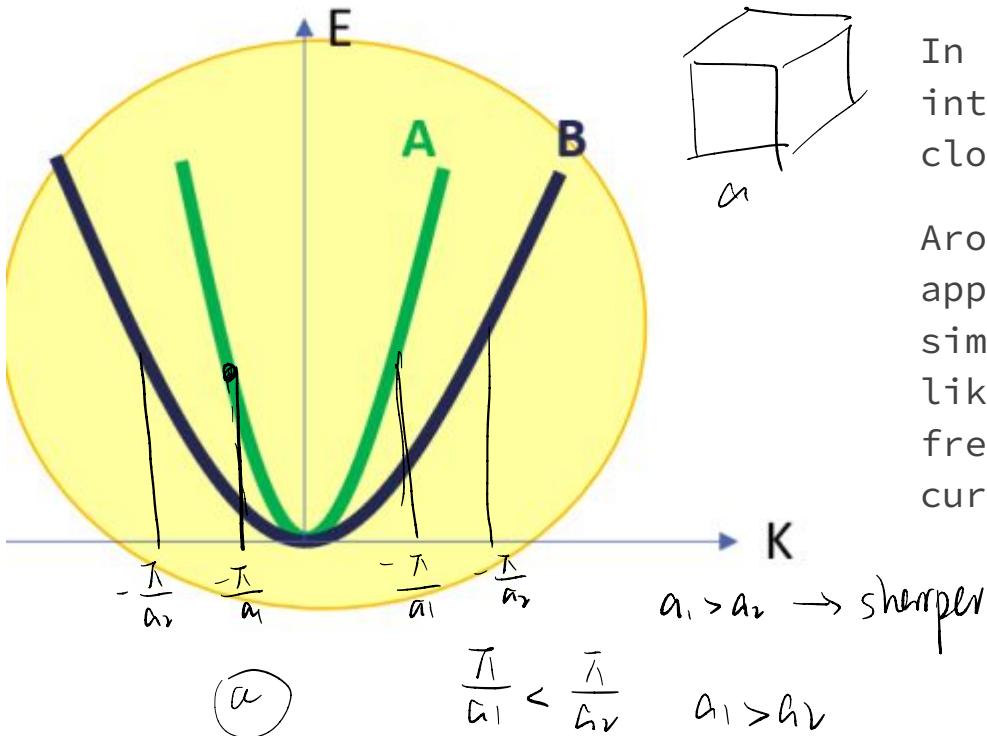


Silicon



GaN

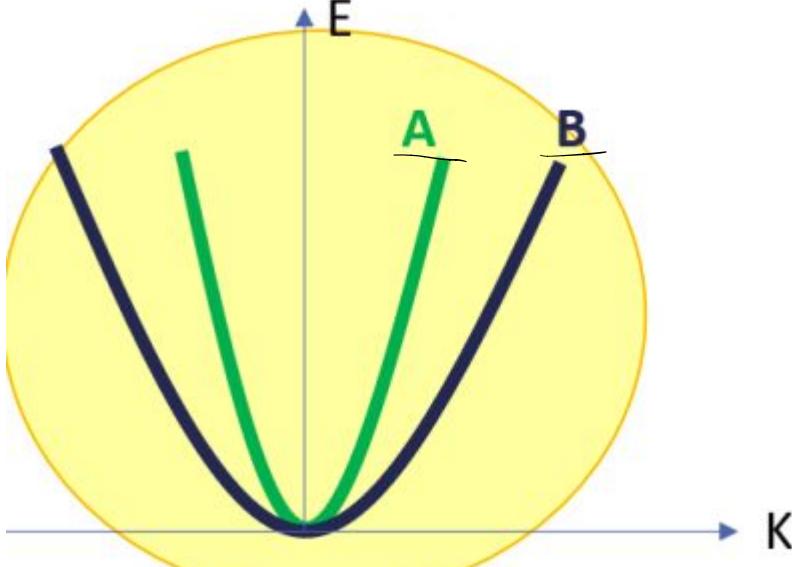
# Quantum Theory of Solid - Simple Band Diagram



In electronic devices, we are mostly interested in electrons that are close to the  $k = 0$  point.

Around this region, we can approximate the  $E$ - $k$  diagram with a simple parabolic curve, which looks like  $E$ - $K$  diagram of electron in the free space, but with a different curvature.

# Quantum Theory of Solid - Effective Mass



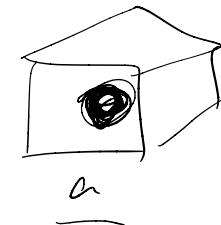
$$\left(\frac{d^2E}{dk^2}\right)_A > \left(\frac{d^2E}{dk^2}\right)_B \rightarrow m_A^* < m_B^*$$

$a_1 > a_2$

$$E = \frac{\hbar^2 k^2}{2m}$$

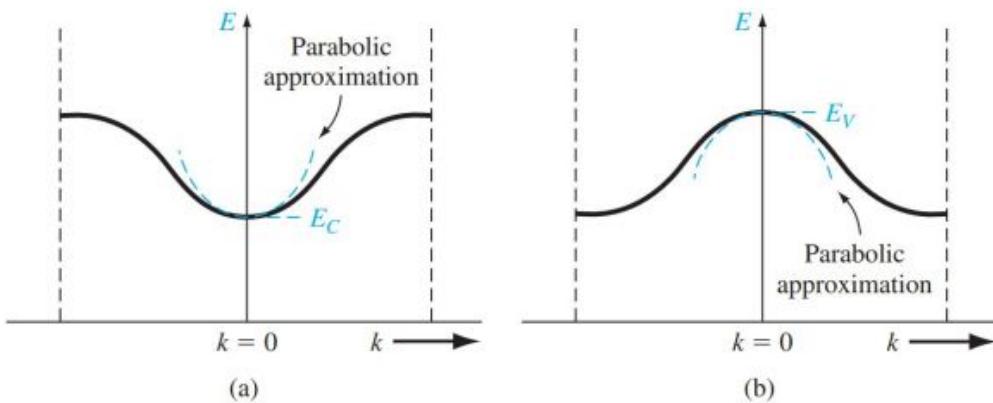
- To simplify calculations in a periodic crystal structure, we can use free-particle E-K diagram, with one difference: replacing  $m$  with  $m^*$
- $m^*$  is the effective mass of electron in the crystal structure
- Same way as when you are in a pool, you feel lighter, electrons feel lighter when they are in some crystal structures

$$\boxed{\frac{dE}{dk} = \frac{\hbar^2 k}{m_e}} \Rightarrow \frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \Rightarrow m_e = \boxed{\hbar^2 \frac{1}{d^2 E / dk^2}}$$



# Quantum Theory of Solid - Effective Mass

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$m_n^*$  effective mass, electron  
 $m_p^*$  hole

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*} (k - k_1)^2$$

$$E = E(k) = E_v - \frac{\hbar^2}{2m_p^*} (k - k_2)^2$$

# Thanks