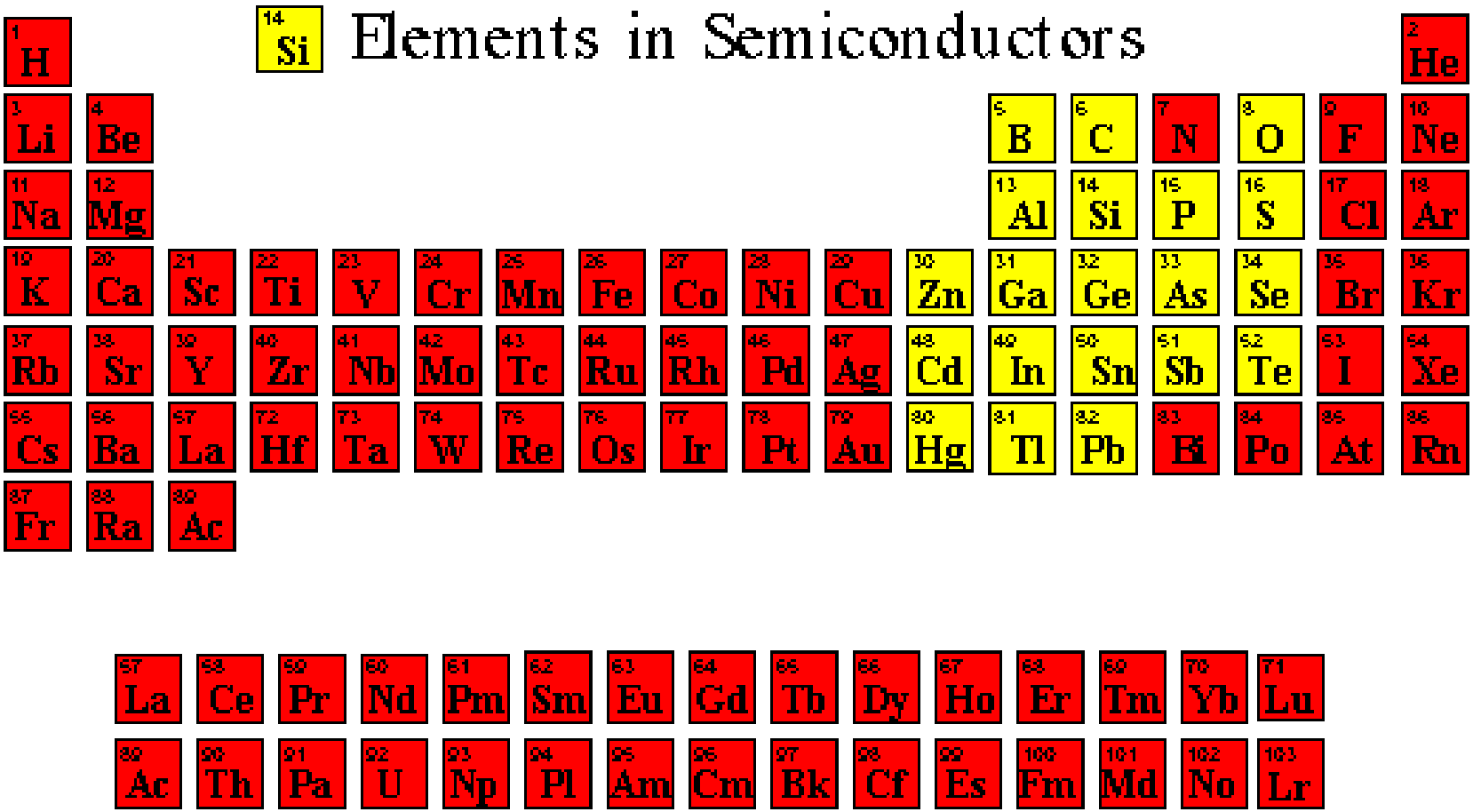
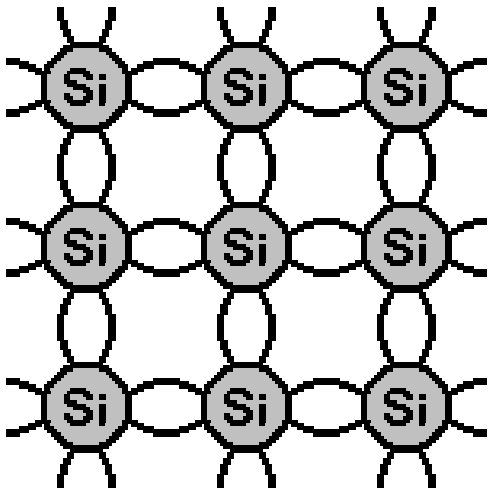
# Semiconductors

- Materials that are neither metallic nor insulator.
- Elemental Semiconductors: Si, Ge
- Si dominates IC industry: >99% is Si based devices)
- Compound Semiconductors
  - III-V semiconductors : GaAs (most widely used compound semiconductor), InSb, InP
  - II-VI semiconductors: CdS, ZnSe, ZnO
- Alloy Semiconductors: HgCdTe, $Al_xGa_{1-x}$, As, $GaAs_xP_{1-x}$

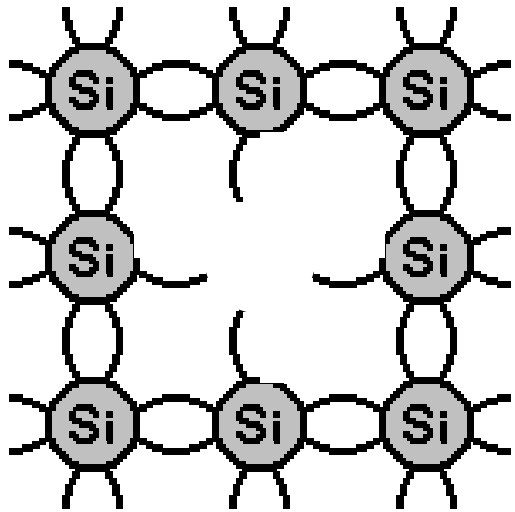
# Semiconductors



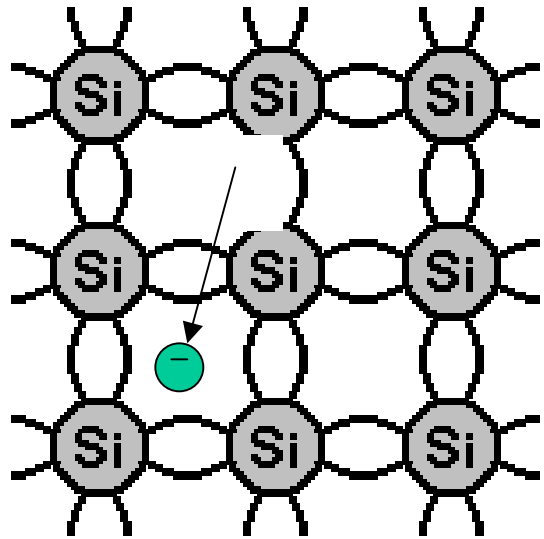
# Semiconductor Models – Bonding Model




- Lines represent shared valence electron
- Circle represent the core of Semiconductor (e.g., Si atom)



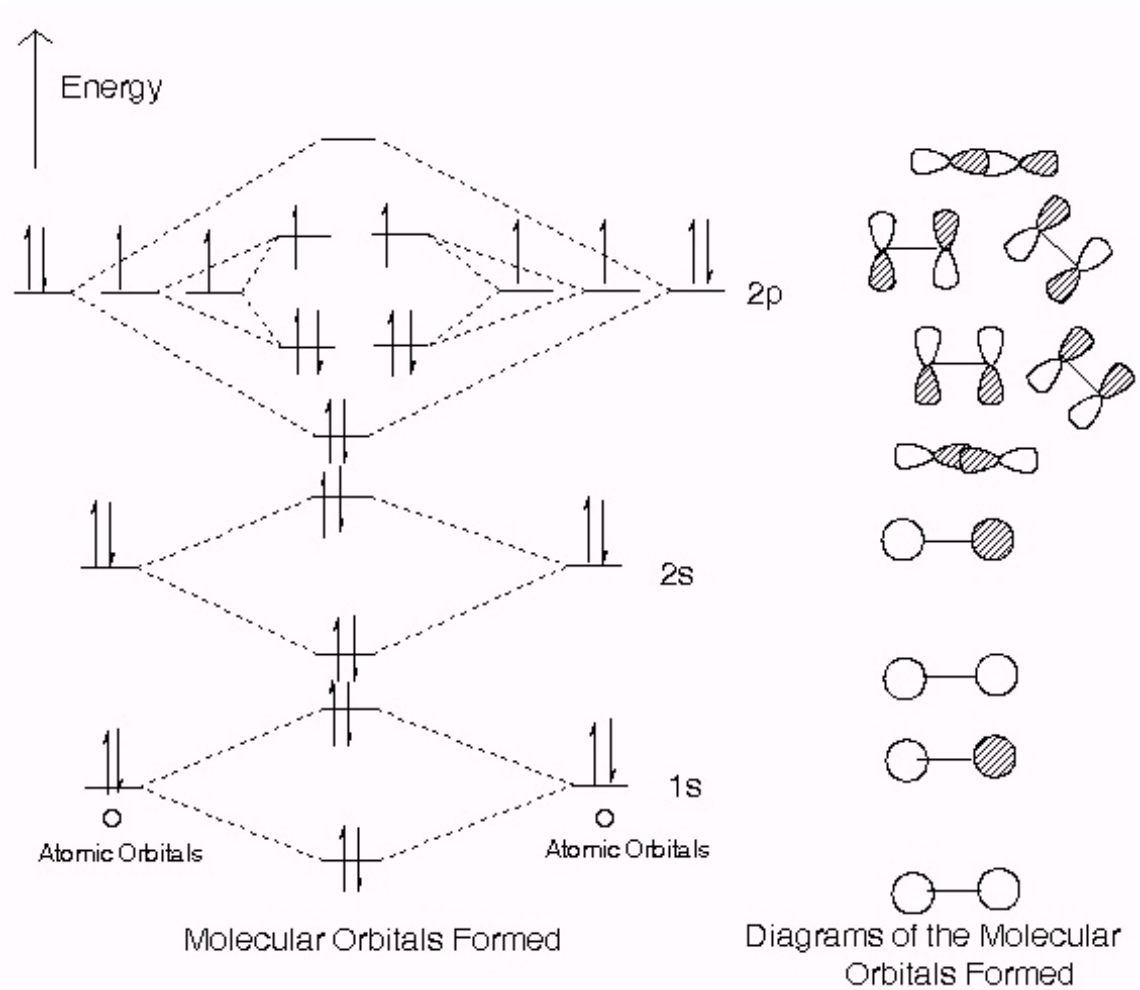

- Visualization of a vacancy point defect




- Breaking of an atom-to-atom bond and freeing of an electron

http://www.play-hookey.com/semiconductors/basicstructure.html

# Review: Molecular Orbitals by linear combination of atomic orbitals

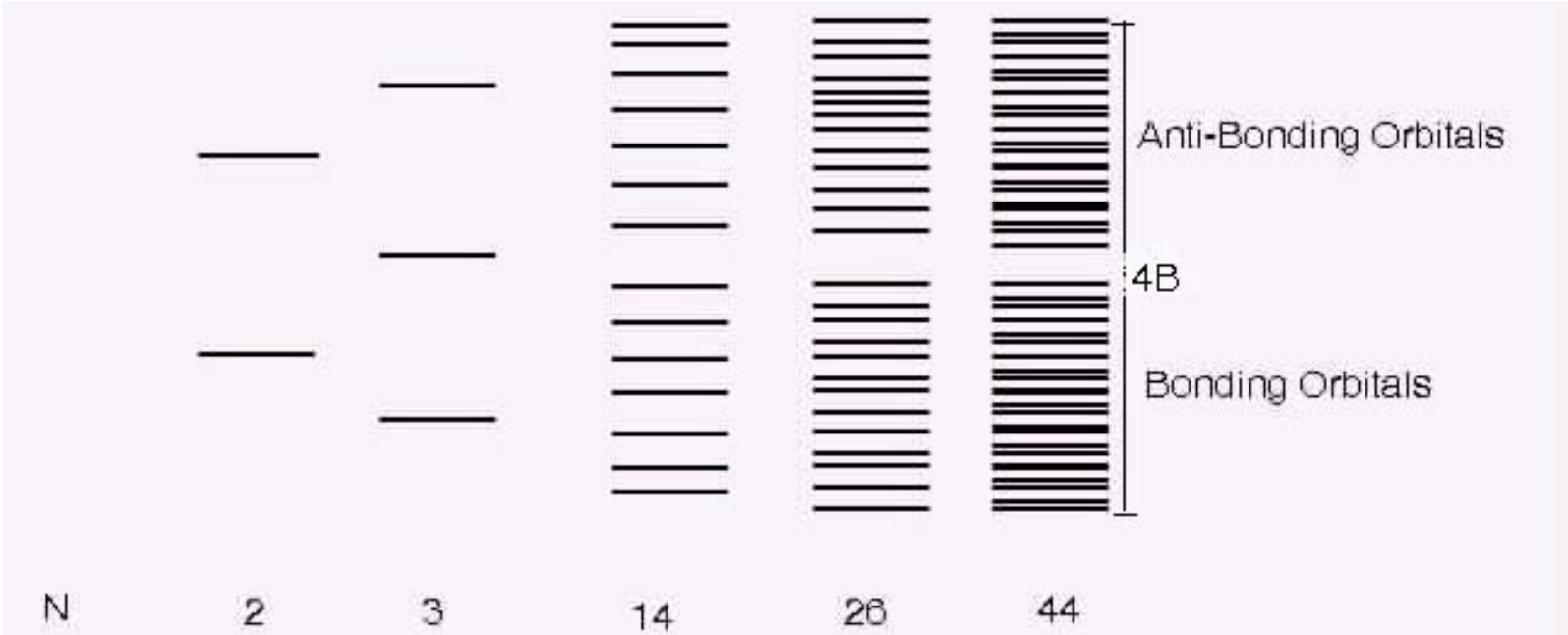



Quantum mechanics & Schrodinger's eqn.

$$H\Psi = E\Psi$$

www.chembio.uoguelph.ca/educmat/ chm729/band/basic2.jpg

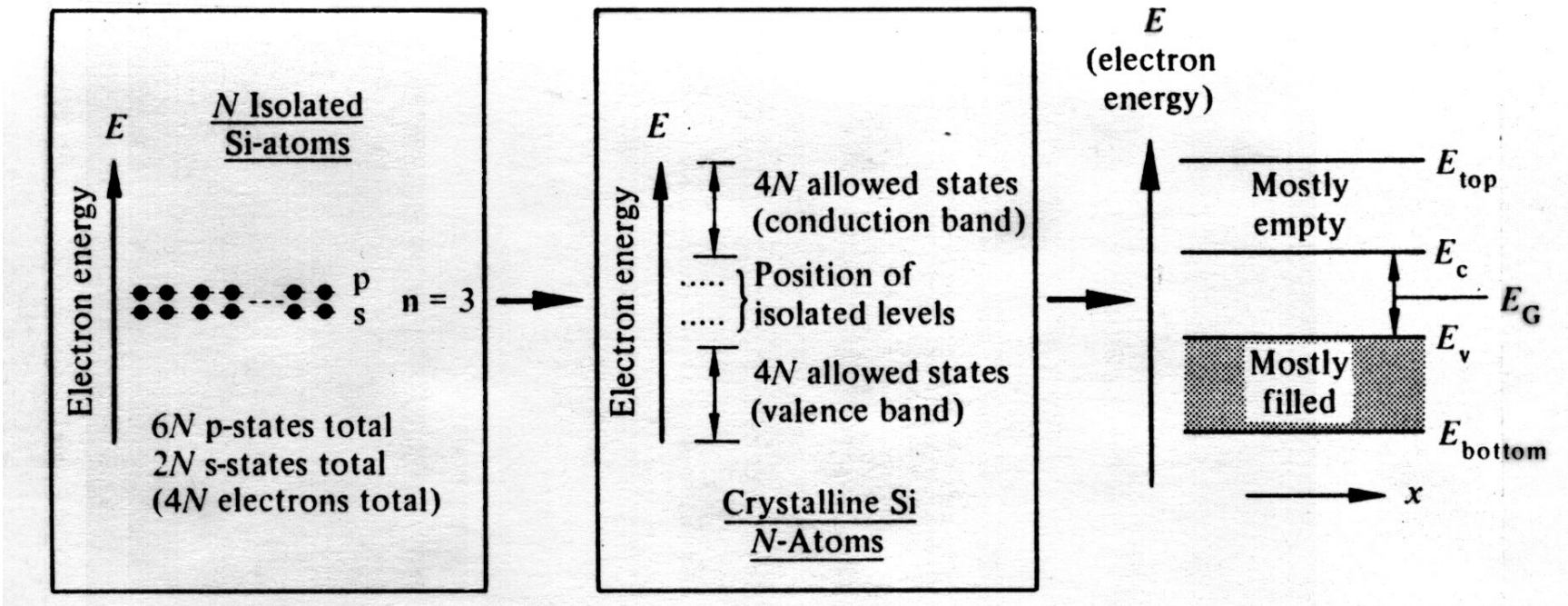
# Semiconductor Models – Energy Band Model




- Energy states bunch up into "bands" and energy states are so close to each other in energy that they are approximately continuous.
- Depending on the energy difference between the bonding and antobonding orbitals a gap opens up between the bands corresponding to the bonding and antibonding orbitals where there are no allowed energy levels

**www.chembio.uoguelph.ca/educmat/ chm729/band/basic2.jpg**

# Energy Band Model



# Band gaps of common semiconductors

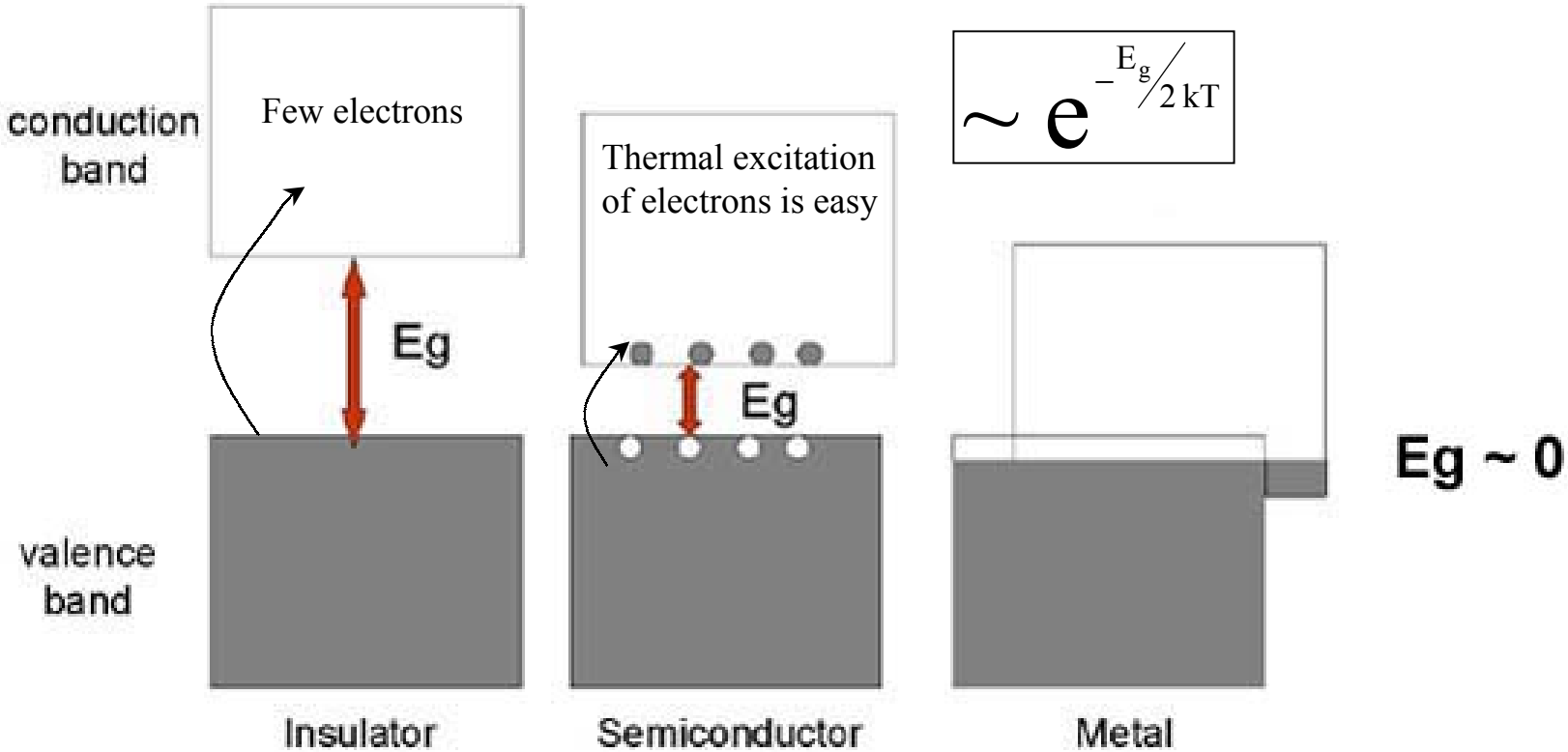
**Periodic table and semiconductors**

| | Group IIB | Group IIIA | Group IVA | Group VA | Group VIA |
|---|---|---|---|---|---|
| 1<br>1*s* | | | | | |
| 2<br>2*s*2*p* | | 5<br>B | 6<br>C | | |
| 3<br>3*s*3*p* | | 13<br>Al | 14<br>Si | 15<br>P | 16<br>S |
| 4<br>4*s*3*d*4*p* | 30<br>Zn | 31<br>Ga | 32<br>Ge | 33<br>As | 34<br>Se |
| 5<br>5*s*4*d*5*p* | 48<br>Cd | 49<br>In | 50<br>Sn | 51<br>Sb | 52<br>Te |

| Element | IV compound | III-V compound | II-VI compound | V-VI compound |
|---|---|---|---|---|
| Si(1.1†) | SiC (2.86 for α structure) | AlP (2.85), GaP (2.26), InP (1.28) | ZnS (3.6), CdS (2.42) | PbS (0.37), PbSe (0.27), PbTe (0.29) |
| Ge (0.67) | | AlAs (2.16), GaAs (1.43), InAs (0.36), AlSb (1.6), GaSb (0.7), InSb (0.18) | ZnSe (2.7), CdSe (1.73), ZnTe (2.25), CdTe (1.58) | |

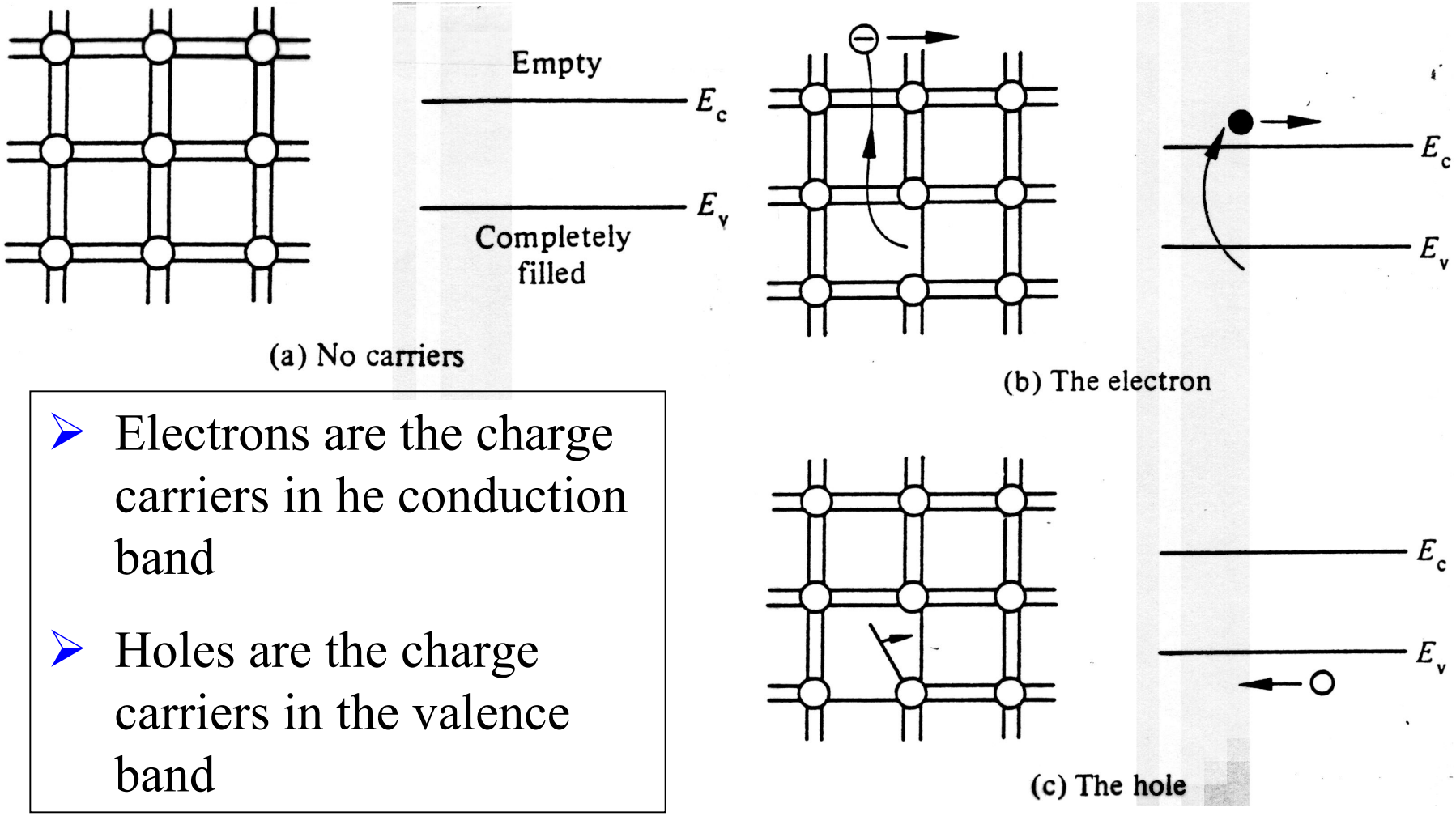
† Energy gap in electronvolts (eV).

# The difference between insulators, semiconductors, and metals in the band theory framework



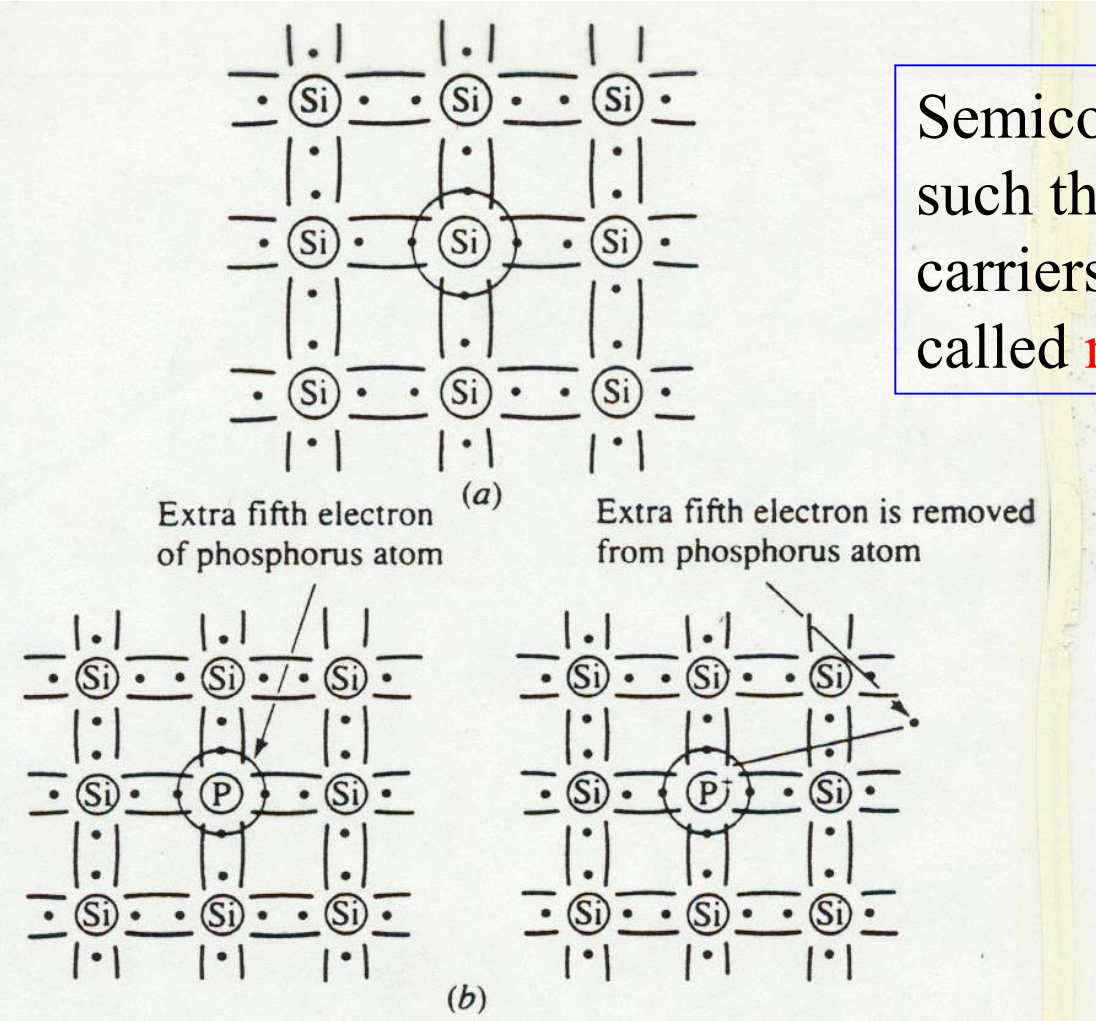

| Gap is very wide<br>~ 8 eV for $SiO_2$<br>~ 5 eV for diamond | thermal excitation is easy kT~0.026 eV<br>~ 1.12 eV for Si | No or very narrow gap |
|---|---|---|

# Charge carriers and intrinsic semiconductor

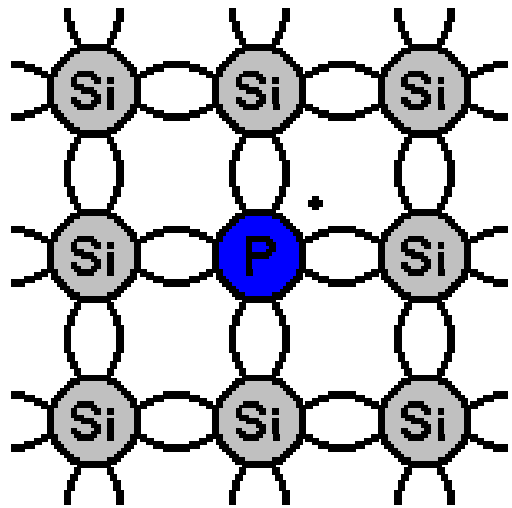



- Electrons are the charge carriers in he conduction band
- Holes are the charge carriers in the valence band

# Doping and Dopants: Manipulating Charge Carrier Densities in Semiconductors – n-type doping

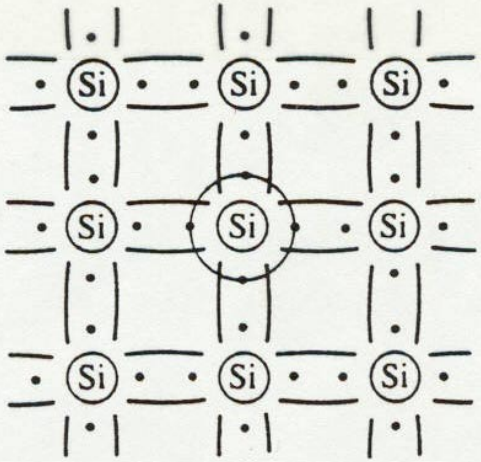



Semiconductors that are doped such that the majority charge carriers are electrons are called n-type semiconductors

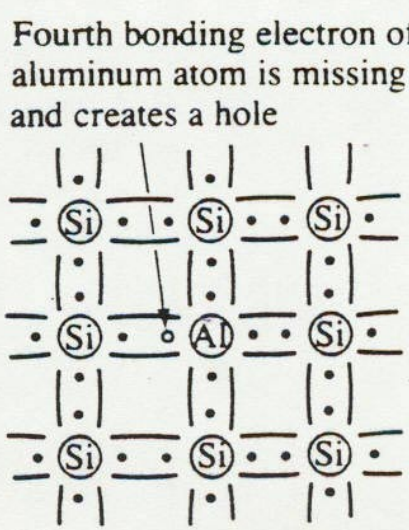


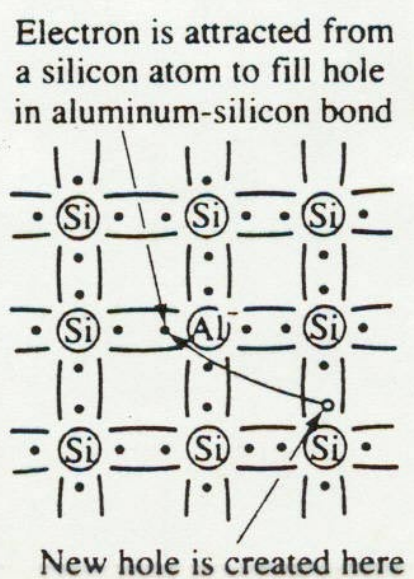

http://www.play-hookey.com/semiconductors/basicstructure.html

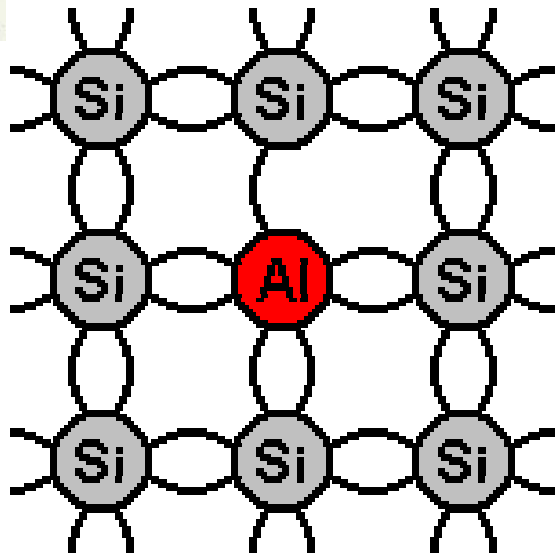
# Doping and Dopants: Manipulating Charge Carrier Densities in Semiconductors – p-type doping




Semiconductors that are doped such that the majority charge carriers are holes are called p-type semiconductors

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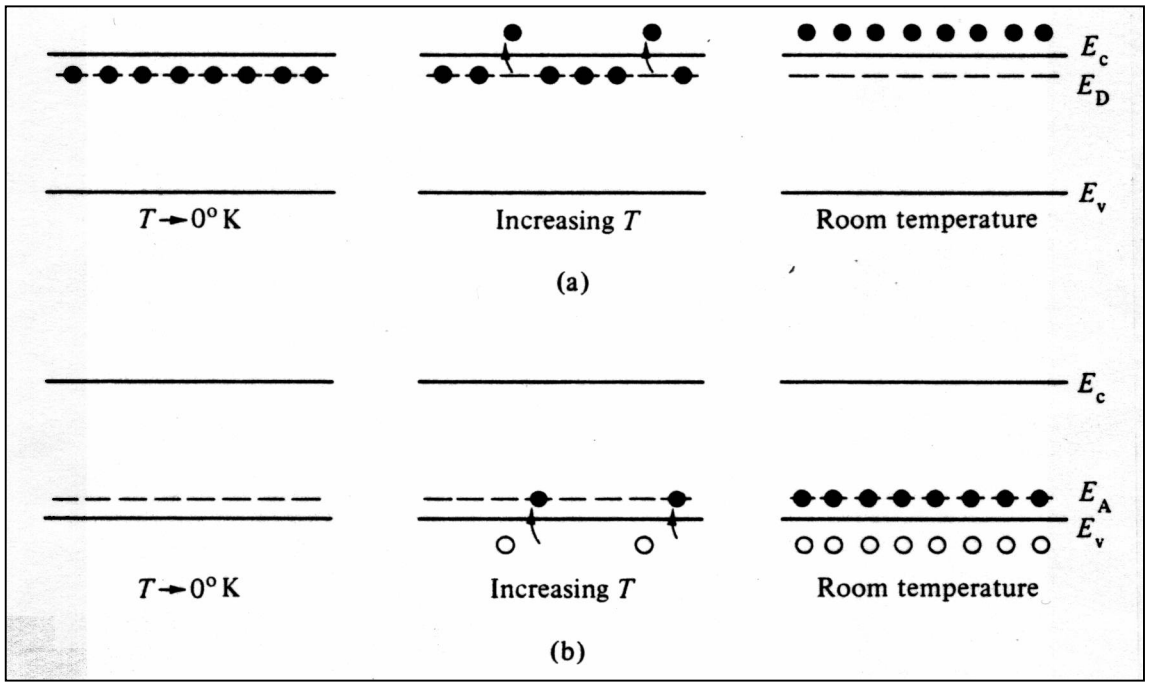
# Visualization of Doping using the energy band model




Dopant-site Binding Energies.

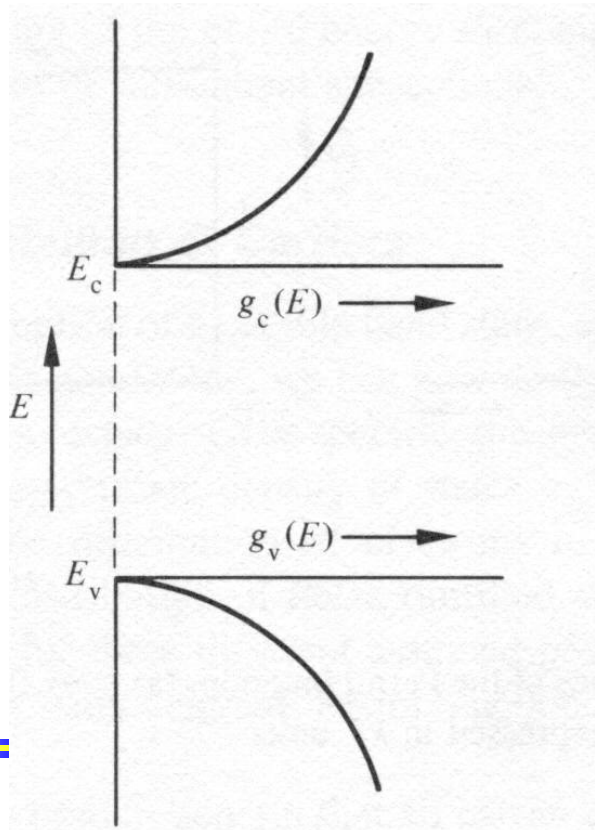
| Donors | $\lvert E_B \rvert$ | Acceptors | $\lvert E_B \rvert$ |
|---|---|---|---|
| Sb | 0.039 eV | B | 0.045 eV |
| P | 0.044 eV | Al | 0.057 eV |
| As | 0.049 eV | Ga | 0.065 eV |
| | | In | 0.16 eV |

Common Silicon Dopants. Arrows indicate the most widely employed dopants.

| Donors (Electron-increasing Dopants) | | Acceptors (Hole-increasing Dopants) | |
|---|---|---|---|
| P← | Column V elements | B← | Column III elements |
| As | | Ga | |
| Sb | | In | |
| | | Al | |

# Density of States

- We talked about formation of bands but did not yet analyze how the allowed states are distributed in energy.
- From quantum mechanics, g(E)dE: # of states $cm^{-3}$ in the range E & E+dE; g(E) has units of $cm^{-3}$ $eV^{-1}$




***Density of states in the conduction band***

$$g_c(E) = \frac{m_n^*}{\pi^2 \hbar^3} \sqrt{2m_n^*(E - E_c)}$$

***Density of states in the valence band***

$$g_v(E) = \frac{m_h^*}{\pi^2 \hbar^3} \sqrt{2m_h^*(E - E_v)}$$

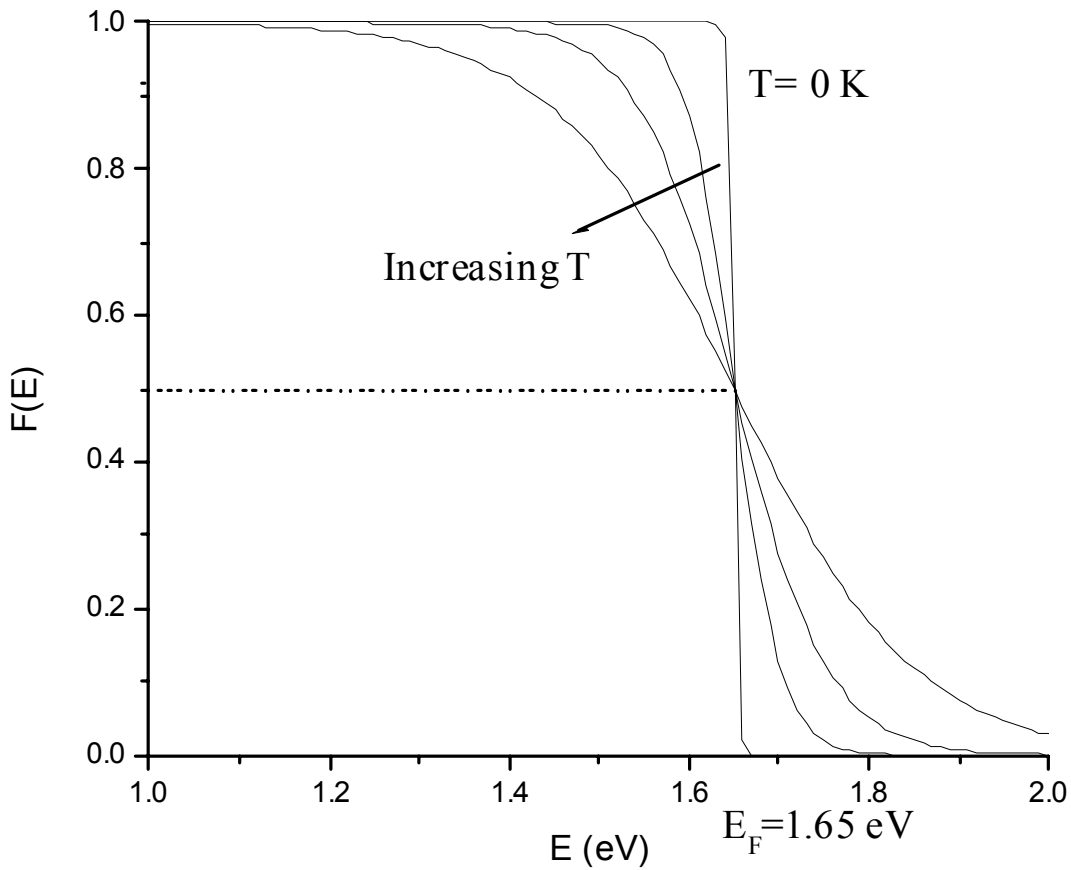
# Fermi Distribution, Fermi Energy, and Fermi Level

- What is the probability that an electronic state with energy E is occupied?
- Answer: Probability is given by Fermi-Dirac Distribution

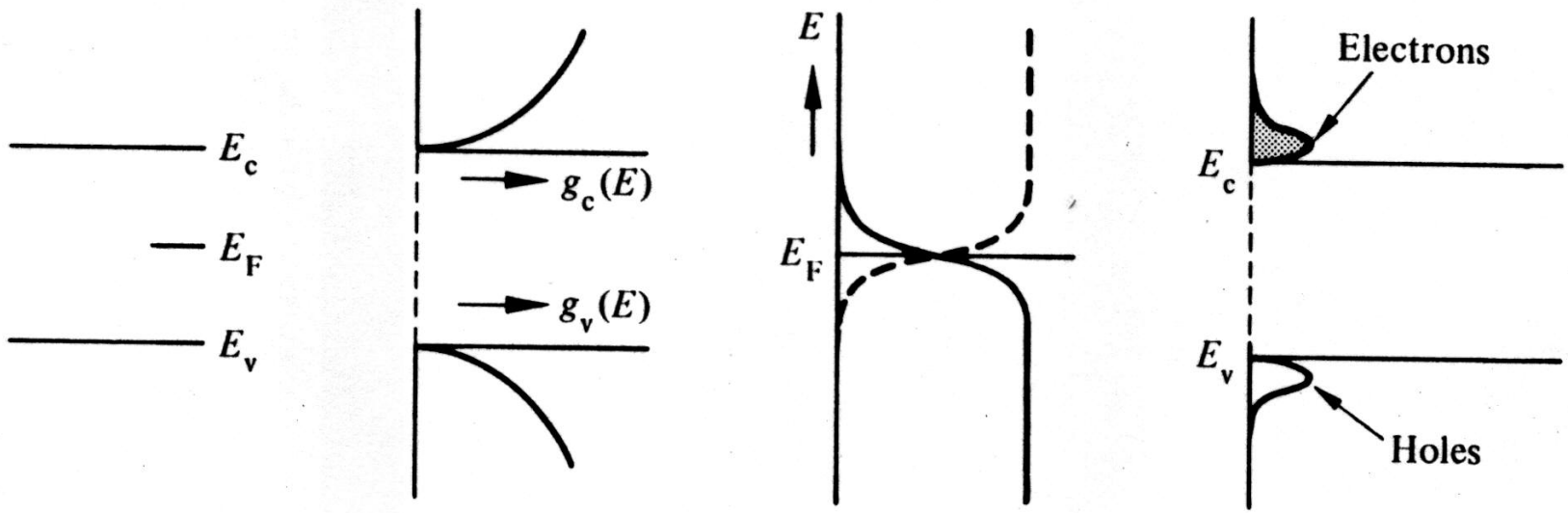
$$F(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

- $E_F$ is a parameter called the Fermi Energy. It is the chemical potential (μ) of the electrons in the semiconductor.
- By definition if $E=E_F$ probability of occupation is ½.
- Comes from a statistical mechanics calculation. Assuming Pauli exclusion principle, it is the most probable distribution on the condition that the total system energy is given.

# Fermi-Dirac Distribution



# Fermi level in an intrinsic semiconductor at T= 0 K is in the middle of the band gap




$$n = \int_{E_c}^{E_{top}} f(E)\, g_c(E)\, dE$$

$$p = \int_{E_{bottom}}^{E_v} (1 - f(E))\, g_v(E)\, dE$$

# Calculation of Charge Carrier Concentrations in Semiconductors

$$n = \frac{\sqrt{2}\left(m_n^* kT\right)^{3/2}}{\pi^2 \hbar^3} \int_0^\infty \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}} \quad where \quad \eta = \frac{E - E_c}{E_F}$$

$$n = \frac{\sqrt{2}\left(m_n^* kT\right)^{3/2}}{\pi^2 \hbar^3} F_{1/2}(\eta_F)$$

Fermi integral of order 1/2

$$n = N_c \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_F)$$

$$N_c = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$$

"Effective" density of conduction band states

$$p = N_v \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_F') \quad where \quad \eta_F' = \frac{E_v - E_F}{E_F}$$

# Charge Carrier Concentrations in Semiconductors – Simplified Expressions

- When $E_F$ is away from the band edges (most cases)

$$E_v + 3kT < E_F < E_c - 3kT$$

- the expressions for n and p simplify to

$$n = N_c e^{(E_F - E_c)/kT}$$

$$p = N_v e^{(E_v - E_F)/kT}$$

- For intrinsic semiconductor $E_i$, the Fermi level for intrinsic semiconductor is close to the midgap and

$$n = p = n_i = N_c e^{(E_i - E_c)/kT} = N_v e^{(E_v - E_i)/kT}$$

# Charge Carrier Concentrations in Semiconductors – Simplified Expressions

- Intrinsic carrier concentration, $n_i$

$$n_i e^{-E_i/kT} = N_c e^{-E_c/kT}$$

$$n_i e^{E_i/kT} = N_v e^{(E_v)/kT}$$

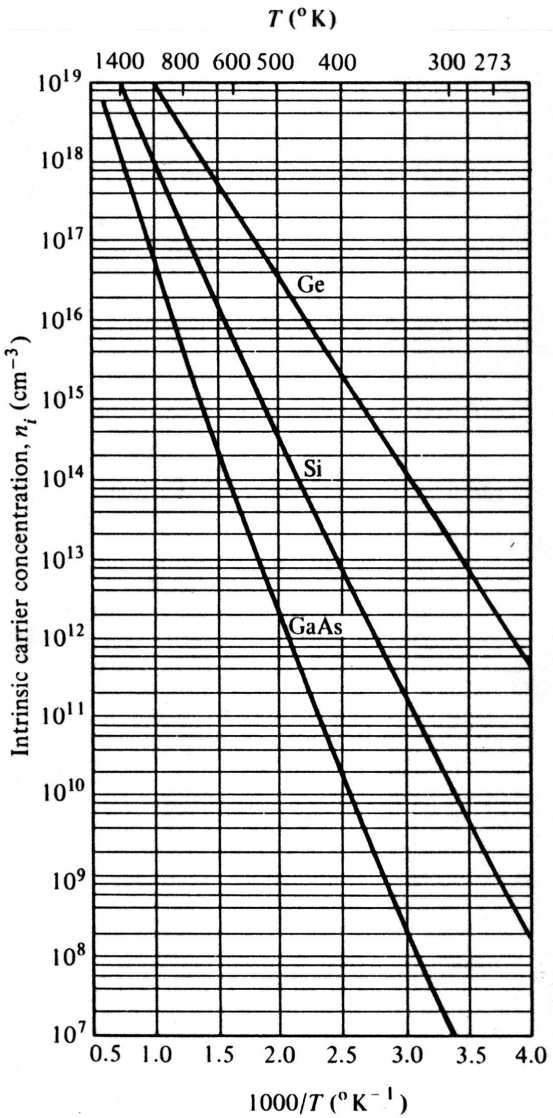
$$n_i^2 = N_v N_c e^{-(E_c - E_v)/kT} \quad \Rightarrow \quad \boxed{n_i = \sqrt{N_v N_c}\, e^{-E_g/2kT}}$$

- Simplified expressions for n and p in terms of $n_i$ and $E_F$

$$n = n_i e^{(E_F - E_i)/kT}$$

$$p = n_i e^{(E_i - E_F)/kT} \quad \Rightarrow \quad np = n_i^2$$

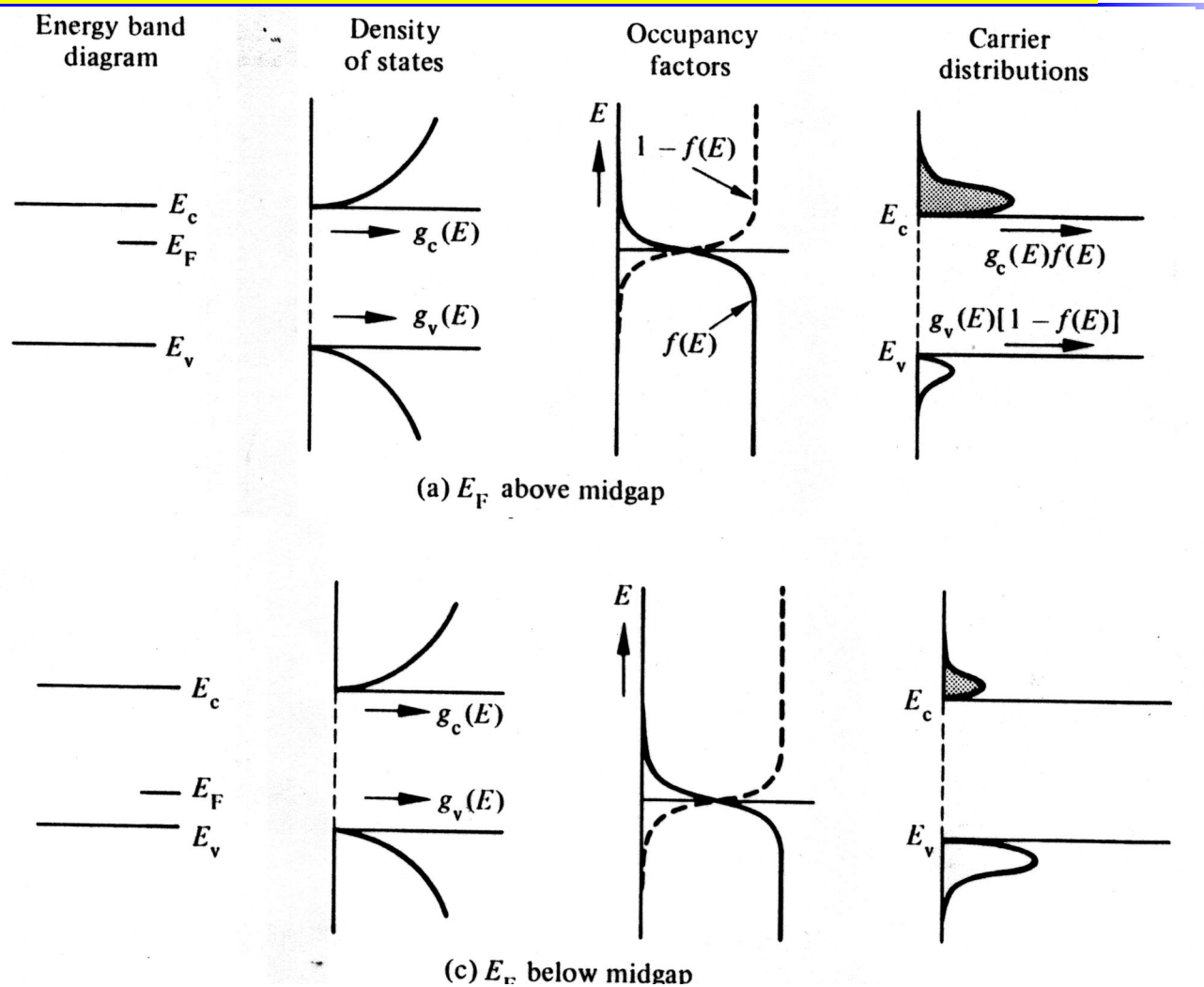
# Intrinsic carrier concentration vs T in Si, Ge, and GaAs




$$n_i = \sqrt{N_v N_c}\, e^{-E_g/2kT}$$

Intrinsic carrier concentration is a material property that depends on temperature.

# Carrier distributions as a function of $E_F$ position



# Carrier Concentration in doped Materials: Manipulating $E_F$ and n and p by doping

- Consider a semiconductor with donor density $N_D$.
- Since $E_C$-$E_D$ is small almost all donors and acceptors will be ionized at room T. Charge neutrality requires that

$$qp - qn + qN_D^+ = 0$$

$$p - n + qN_D = 0$$

- $np = n_i^2$ and elimination of p results in a quadratic equation for n

$$\frac{n_i^2}{n} - n + N_D = 0 \Rightarrow n^2 - N_D n - n_i^2 = 0$$

$$n = \frac{N_D}{2} + \sqrt{\left(\frac{N_D}{2}\right)^2 + n_i^2} \qquad \Rightarrow n \cong N_D \Rightarrow \qquad p = \frac{n_i^2}{N_D}$$

$$N_D \approx 10^{13} - 10^{21}\ cm^{-3} >> n_i \approx 10^{10} cm^{-3} (at\ room\ T)$$

# Carrier Concentration in doped Materials: Manipulating $E_F$ and n and p by doping

- Arguments are similar for a p-type semiconductor and the result is

$$p \cong N_A \quad and \quad n = \frac{n_i^2}{N_A}$$

- "Power of doping": We can manipulate carrier concentrations by manipulating dopant concentrations.
- Processing implications: Need very pure material (ppb)

$$N_{Si} \approx 5 \times 10^{22}\ cm^{-3}$$

$$N_A \ \ or \ \ N_D \approx 10^{13} - 10^{21} cm^{-3}$$

# Intrinsic Fermi level $E_i$

$$n = p$$

$$N_c e^{(E_i - E_c)/kT} = N_v e^{(E_v - E_i)/kT}$$

$$E_i = \frac{E_c + E_v}{2} + \frac{kT}{2} ln\left(\frac{N_v}{N_c}\right) = \frac{E_c + E_v}{2} + \frac{kT}{2} ln\left(\frac{m_p^*}{m_n^*}\right)^{3/2}$$

$$E_i = \frac{E_c + E_v}{2} + \frac{3}{4} kT\, ln\left(\frac{m_p^*}{m_n^*}\right)$$

At room T this term is 0.012 eV for Si

This term is 0.56 eV for Si

- In an intrinsic semiconductor $E_F = E_i$ is ~ @ midgap

# Dependence of $E_F$ on dopant concentration

n-type

$$n = N_D = n_i e^{(E_F - E_i)/kT}$$

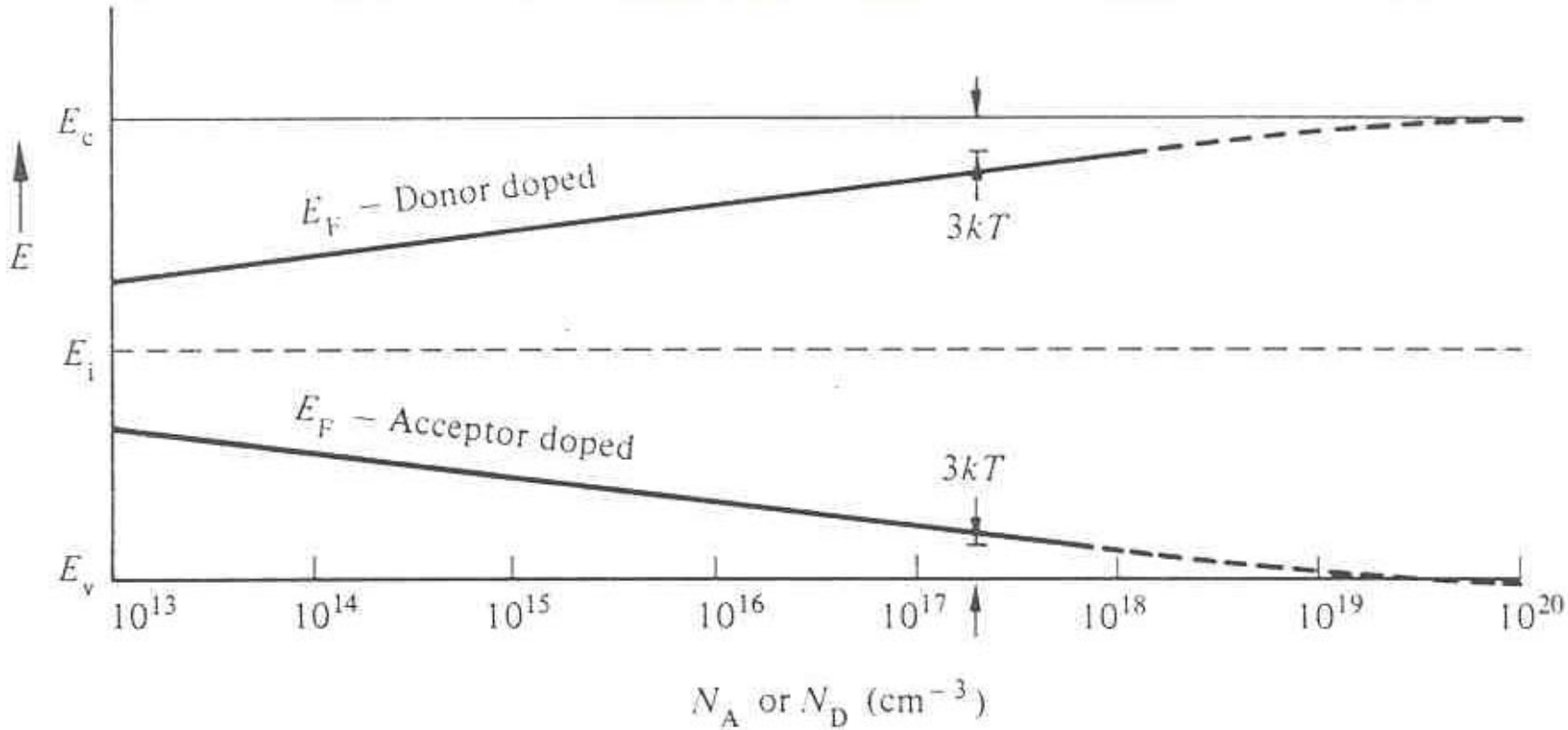
$$E_F - E_i = kT\, ln\left(\frac{N_D}{n_i}\right)$$

p-type

$$p = N_A = n_i e^{(E_i - E_F)/kT}$$

$$E_i - E_F = kT\, ln\left(\frac{N_A}{n_i}\right)$$

# Dependence of $E_F$ on dopant concentration



# T dependence of n and p