ECE 340 Lecture3
Semiconductor Electronics

Spring 2022
10:00-10:50am

Professor Umberto Ravaioli
Department of Electrical and Computer Engineering
2062 ECE Building

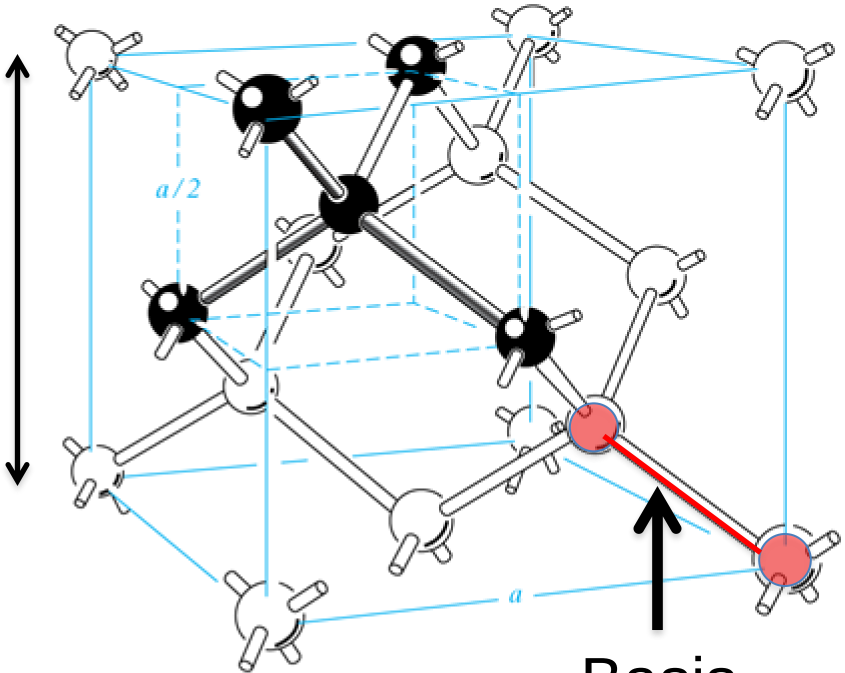
Today’s Discussion

- More on crystals
- Bonding Forces
- Energy Bands

Silicon

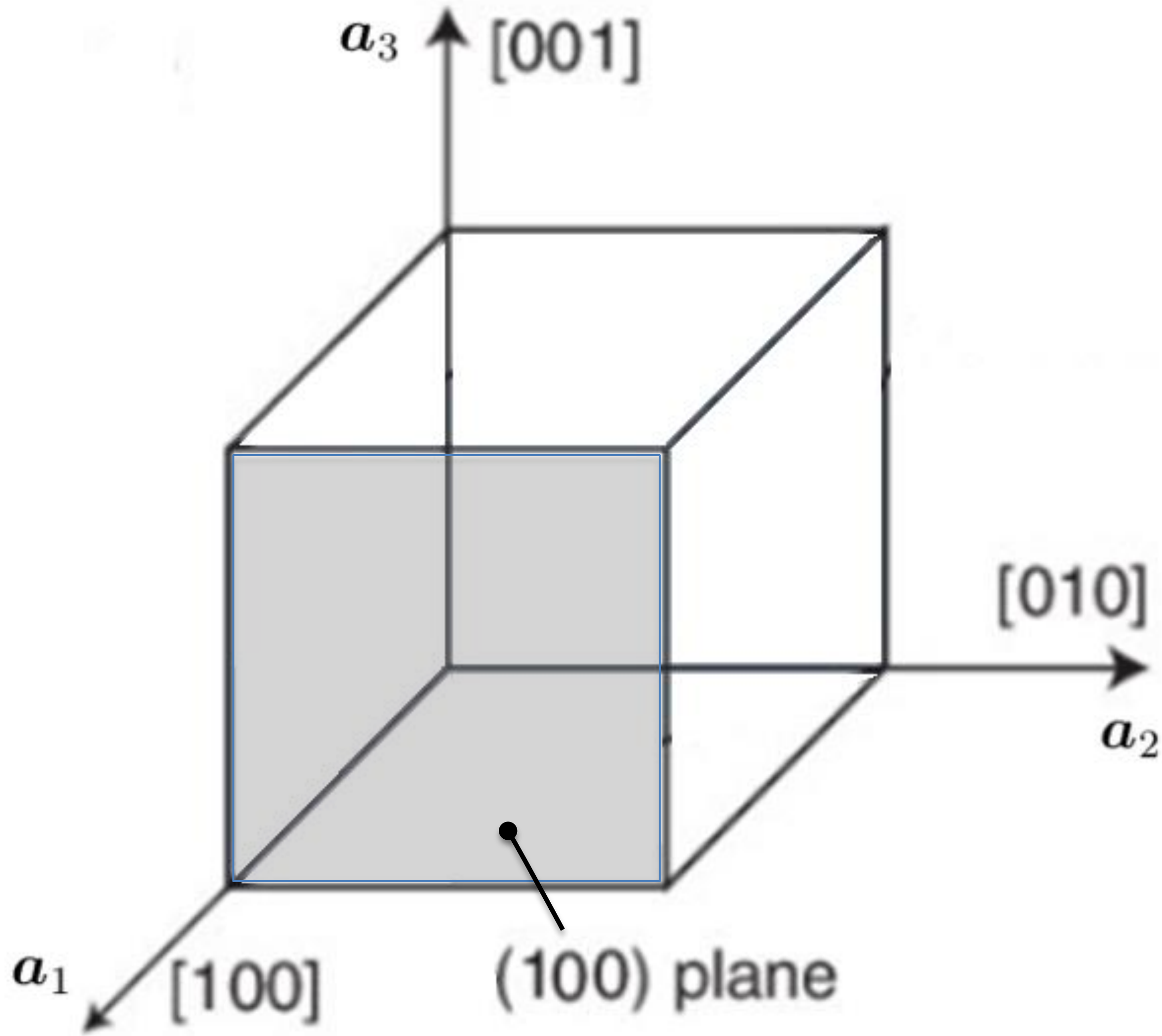
Lattice Constant

a = 5.43 Å

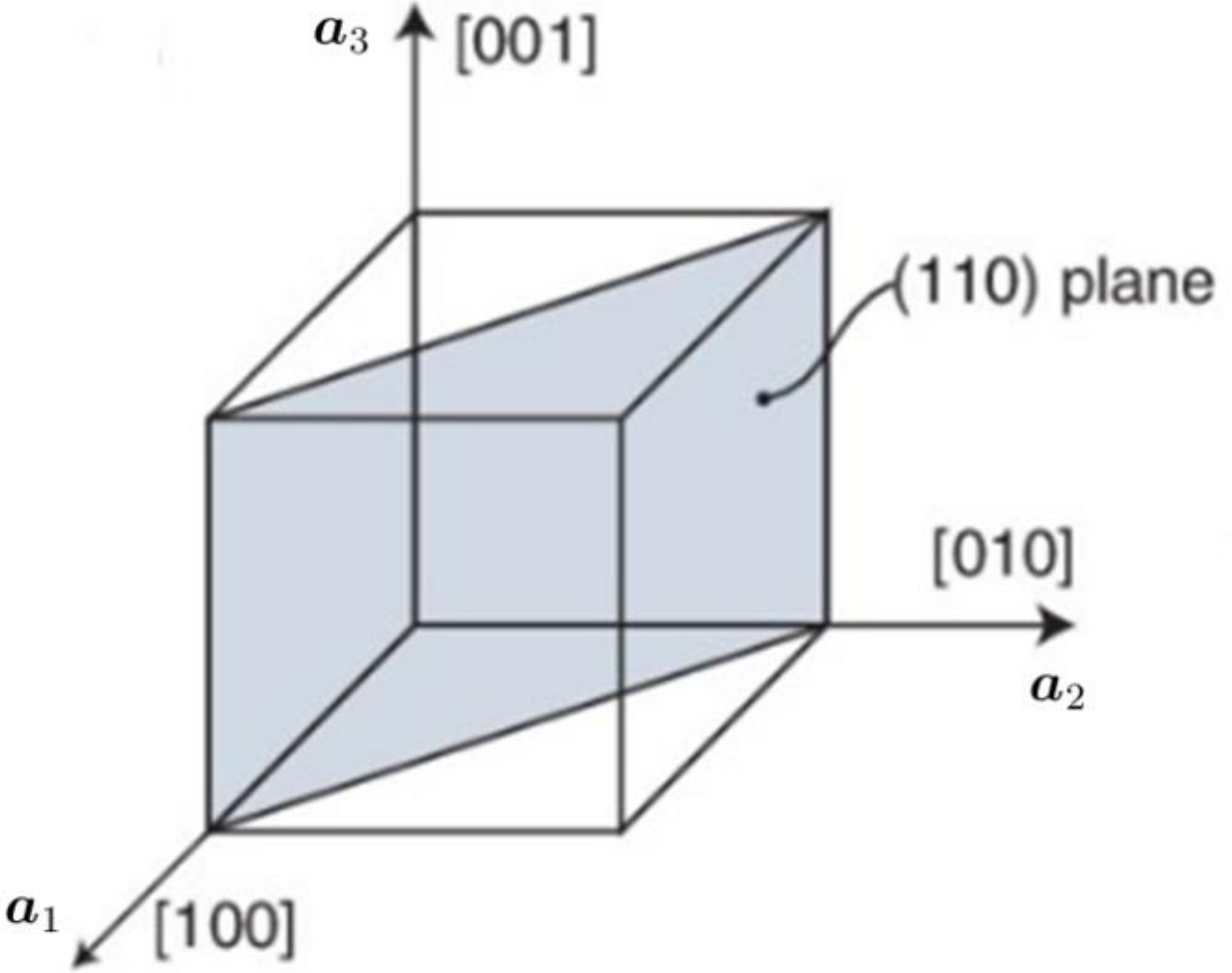


Basis

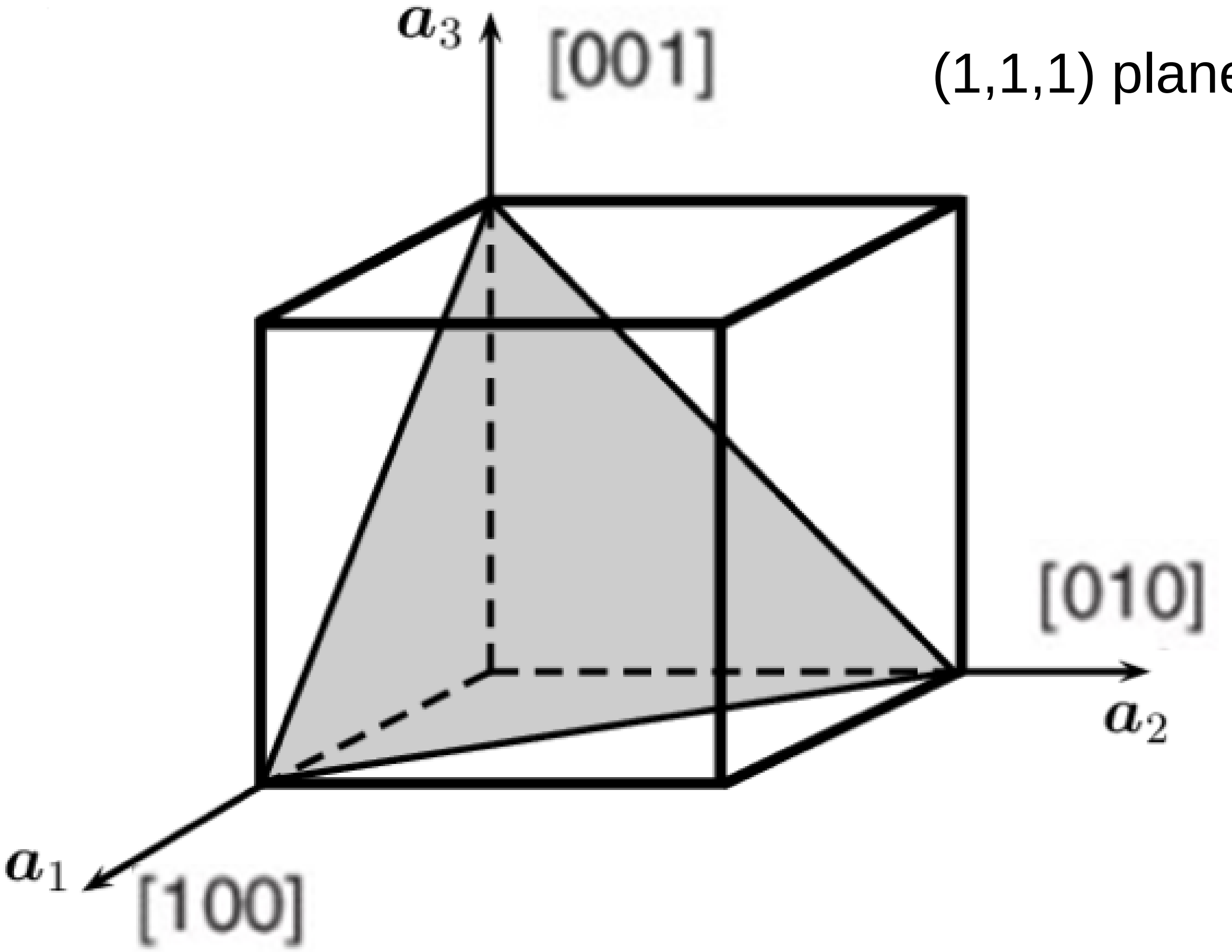
Miller indices



Miller indices



Miller indices



Miller indices

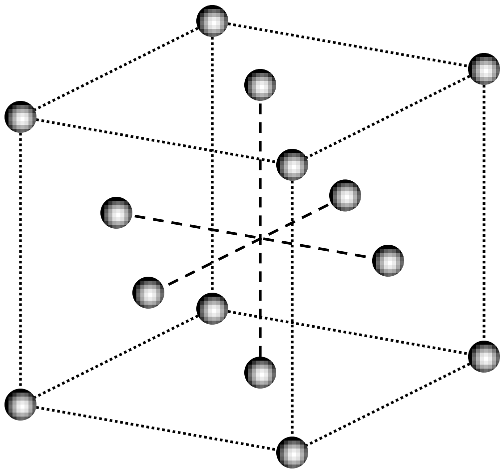
A crystal plane: **(*hkl*)**

Family of equivalent planes: **{*hkl*}**

Crystal direction: **[*hkl*]**
(normal to plane **(*hkl*)** in a cubic lattice)

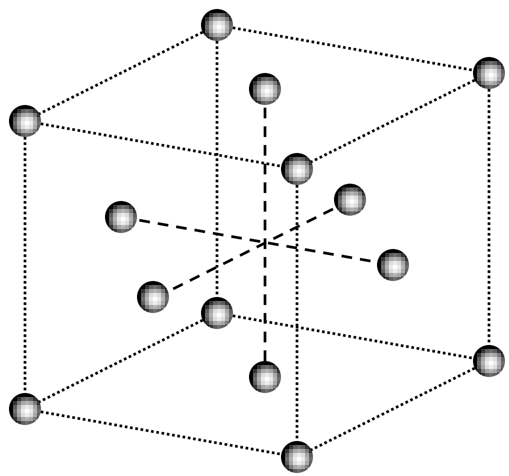
Let’s get to know Silicon better (1)

- How many atoms in the unit cell?
  - Let’s look at the FCC lattice first

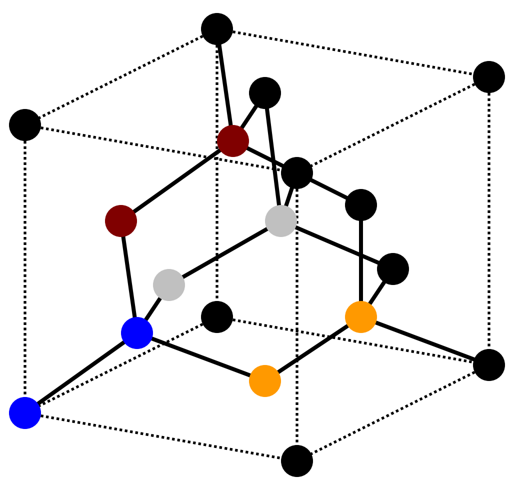


Let's get to know Silicon better (1)

- How many atoms in the unit cell?
  - Let's look at the FCC lattice first
- 4 ATOMS PER CELL

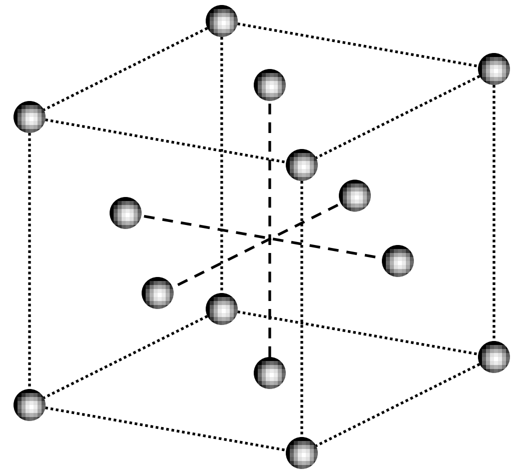


- Now, add the second sub-lattice of the diamond lattice

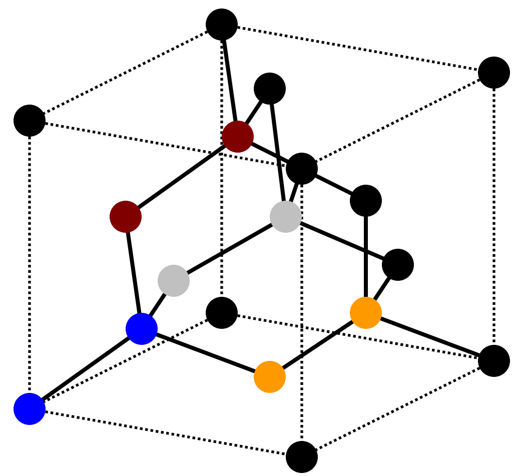


Let's get to know Silicon better (1)

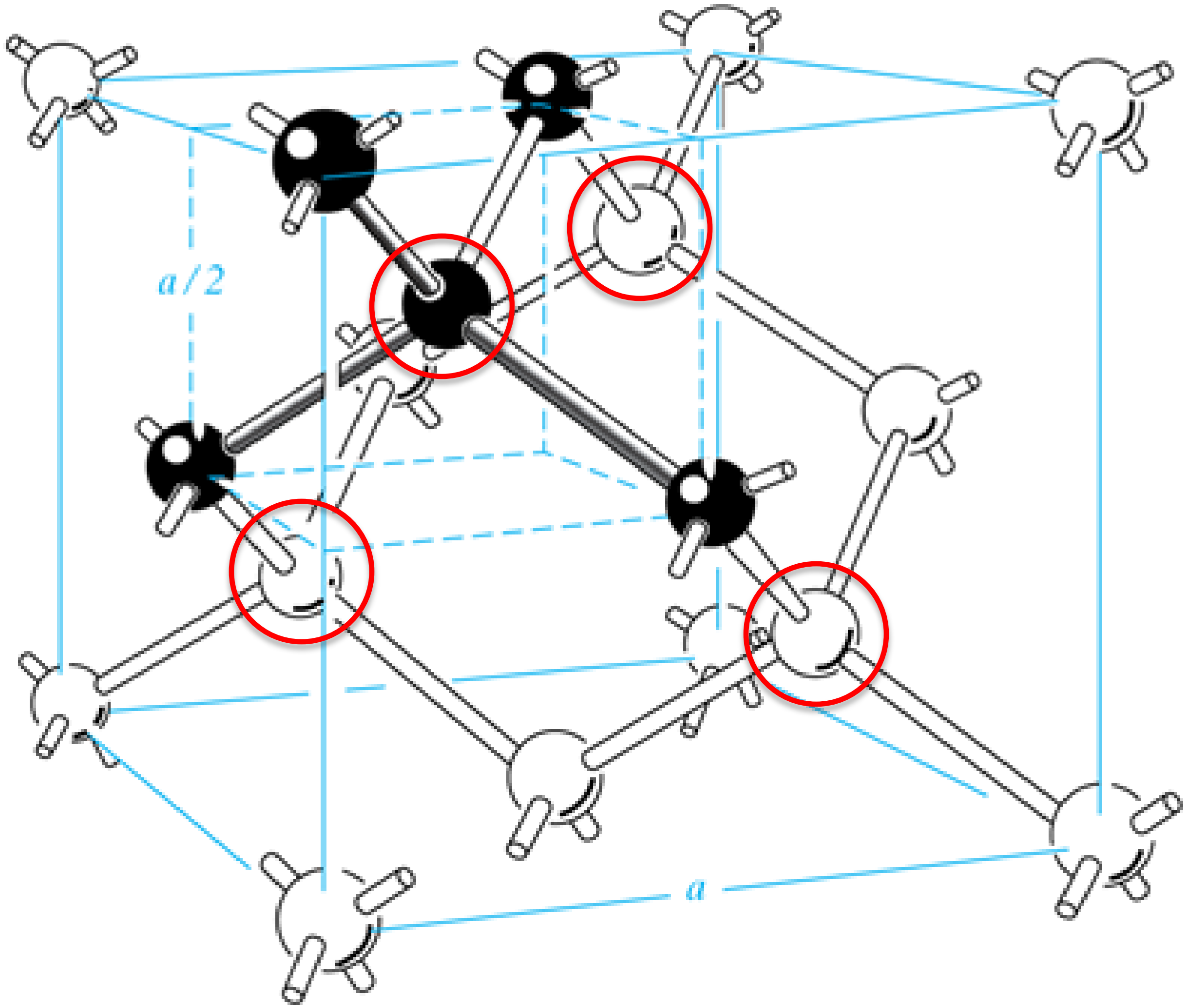
- How many atoms in the unit cell?
  - Let's look at the FCC lattice first
- 4 ATOMS PER CELL



- Now, add the second sub-lattice of the diamond lattice
- 8 ATOMS PER CELL



Let's get to know Silicon better (1)

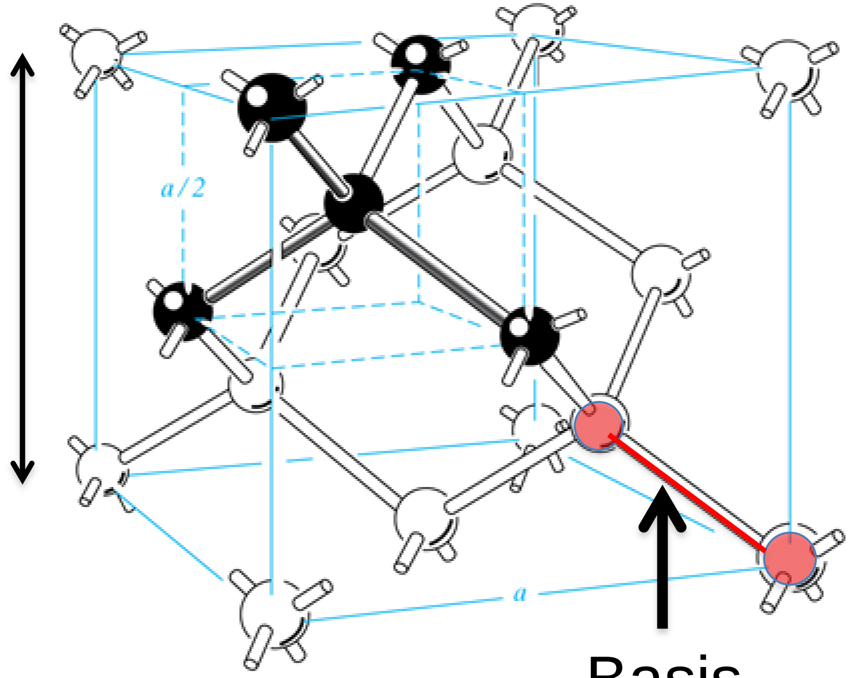


Let's get to know Silicon better (2)

- What is the distance between nearest neighbors?

Lattice Constant

a = 5.43 Å



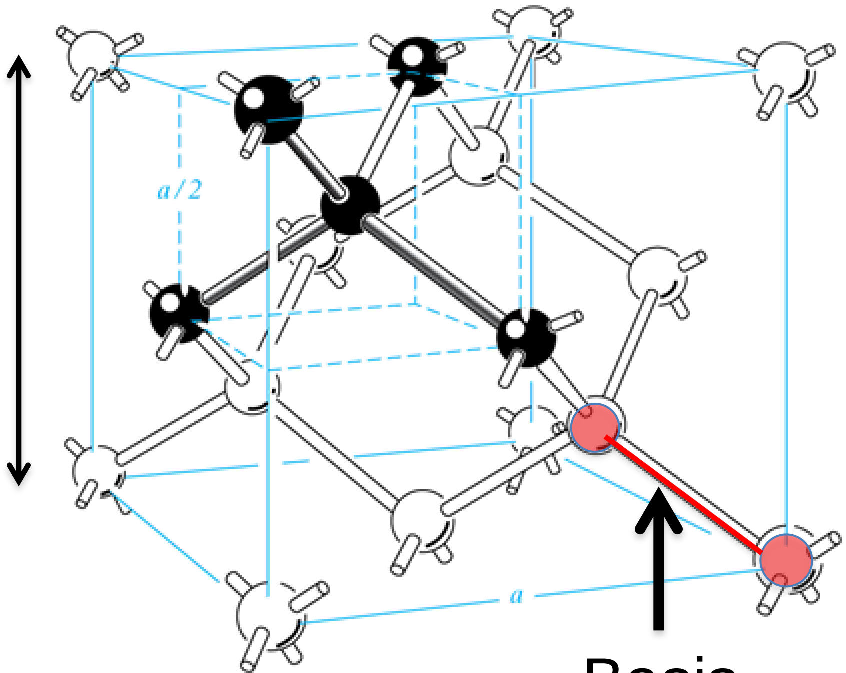
Basis

Let's get to know Silicon better (2)

- What is the distance between nearest neighbors?

Lattice Constant

a = 5.43 Å



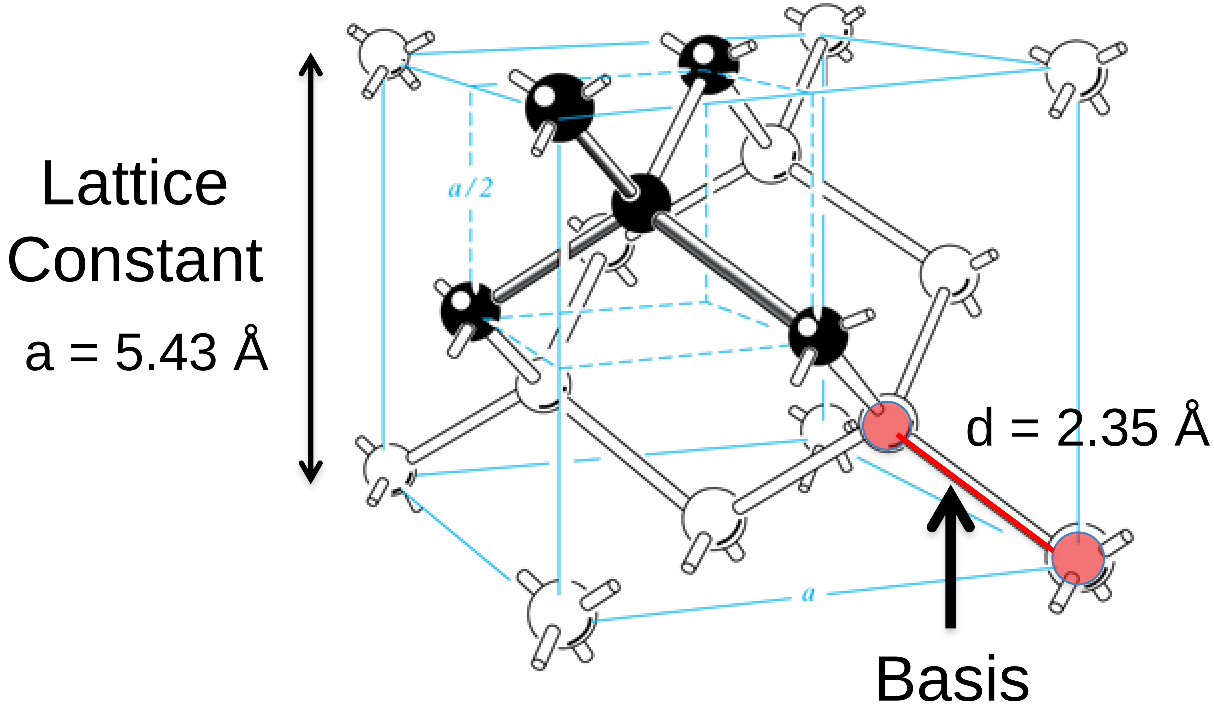
Second atom in basis is offset by (a/4, a/4, a/4)

Diagonal of cube with side a/4

$$d = \frac{\sqrt{3}a}{4} = \frac{1.732 \times 5.43}{4} = 2.35\text{Å}$$

Let’s get to know Silicon better (3)

- What is the packing fraction of Silicon?



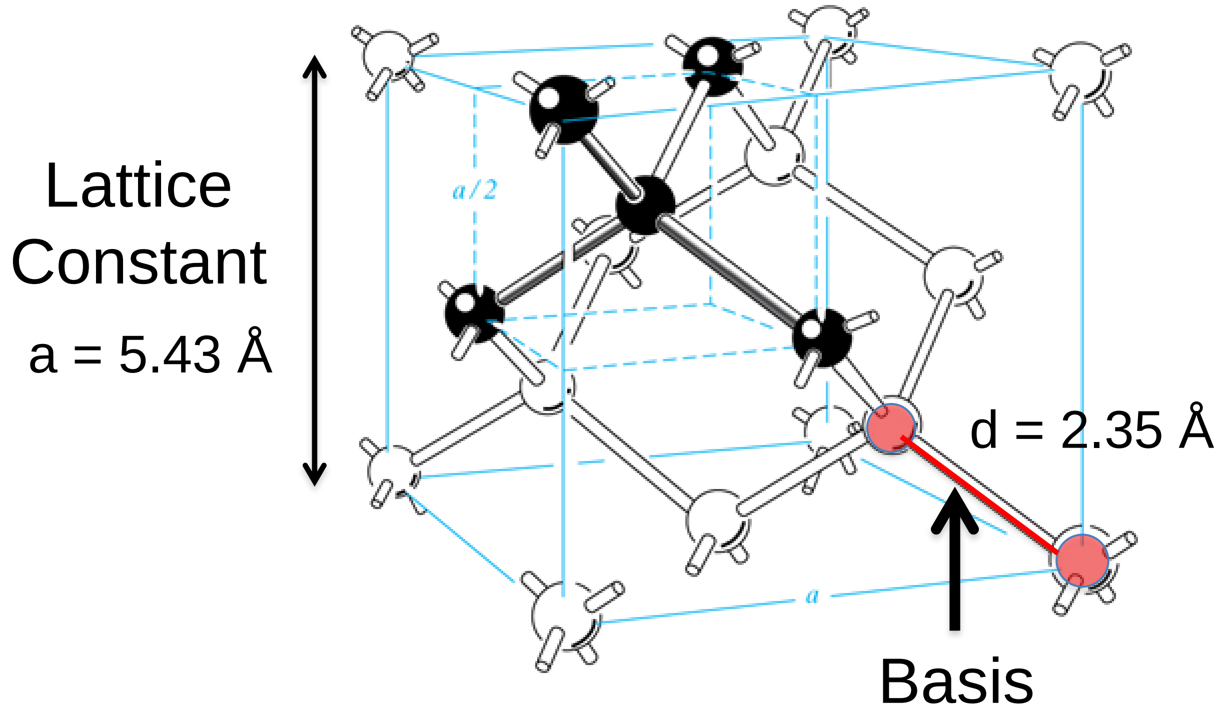
Let’s get to know Silicon better (3)

- What is the packing fraction of Silicon?

Volume of unit cell = a^3 $= 160.1\ \text{Å}^3$

Volume of atom (assume a sphere)

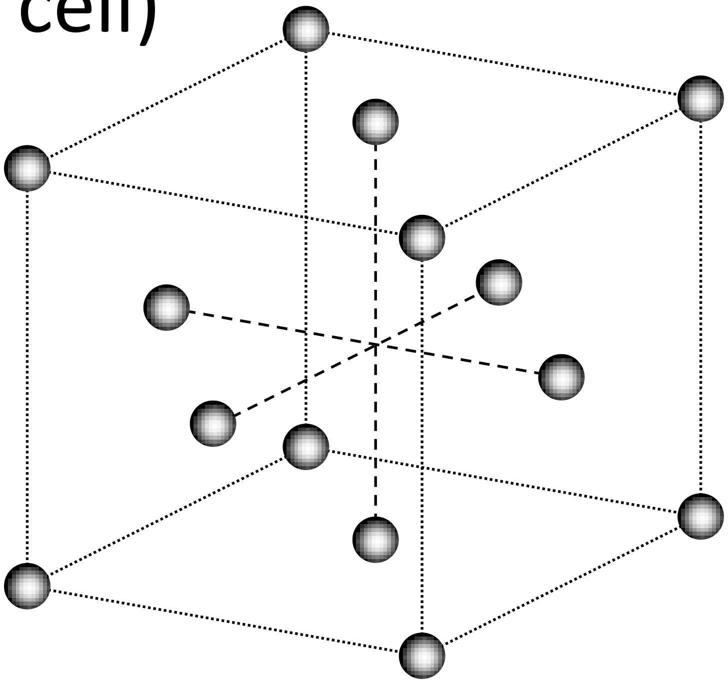
$$\frac{4}{3}\pi\left(\frac{d}{2}\right)^3 = 6.8\ \text{Å}^3$$



Packing fraction = (8 x 6.8)/160.1 = 0.34 = 34%

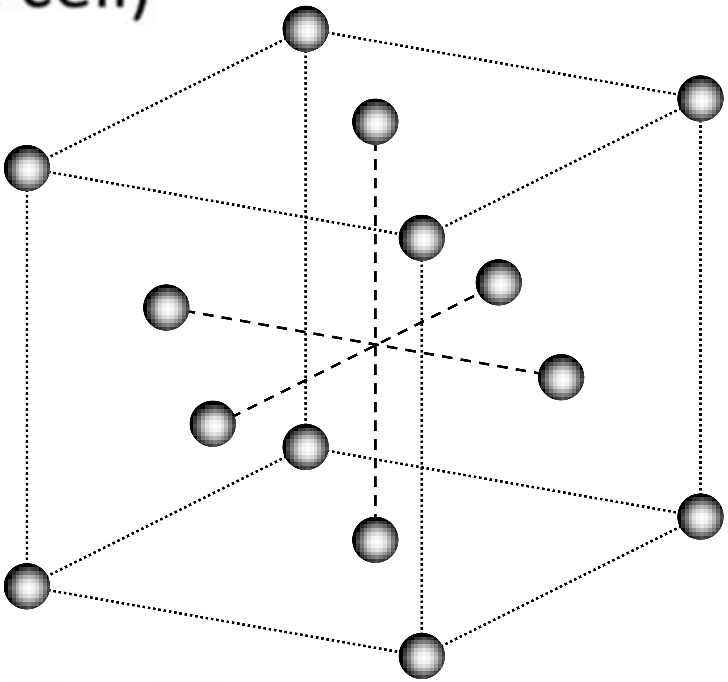
Let's get to know Silicon better (4)

- What is the packing fraction of a simple fcc lattice? (remember: 4 atoms per unit cell)



Let's get to know Silicon better (4)

- What is the packing fraction of a simple fcc lattice? (remember: 4 atoms per unit cell)



Volume of unit cell = a^3

Nearest neighbor distance =

$$d = \frac{a}{2}\sqrt{2}$$

Volume of atom

$$\frac{4}{3}\pi\left(\frac{a}{4}\sqrt{2}\right)^3 = 0.185\, a^3$$

Packing fraction = (4 x 0.185) a^3 / a^3 = 0.74 = 74%

Interesting… that's more than twice than for diamond lattice.

Packing fractions for cubic lattices

- Face-Centered Cubic

$$\sqrt{2}\frac{\pi}{6} = 0.74$$

- Body-Centered Cubic

$$\sqrt{3}\frac{\pi}{8} = 0.68$$

- Simple Cubic

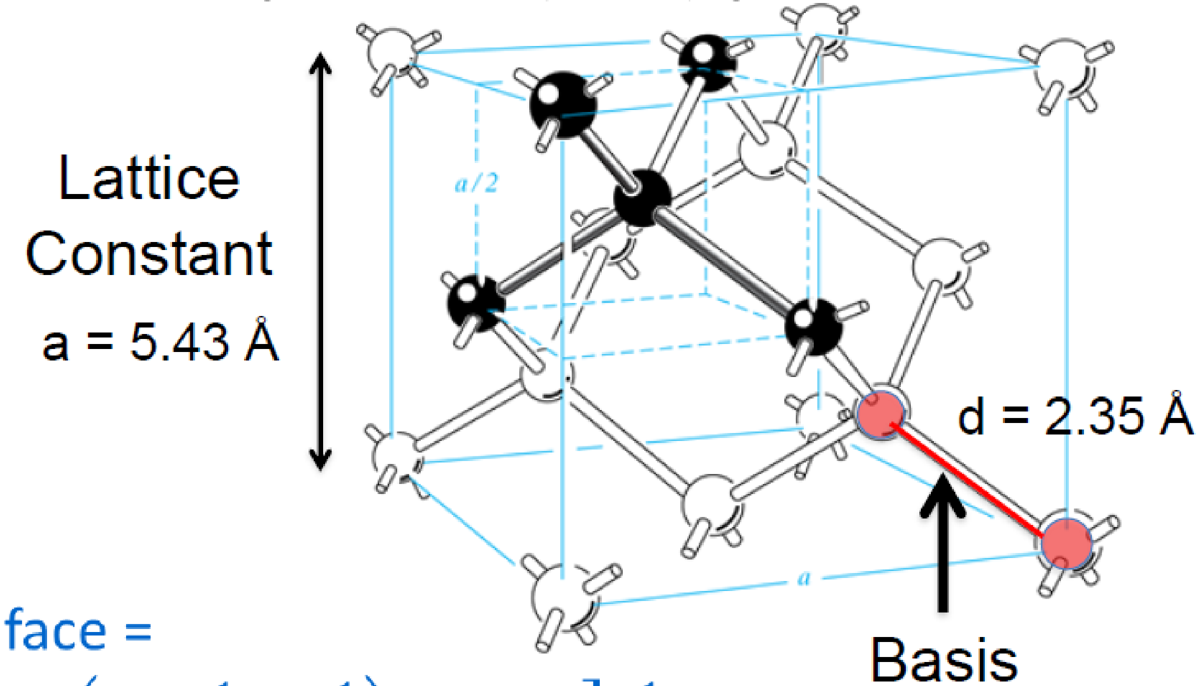
$$\frac{\pi}{6} = 0.52$$

- Diamond Lattice

$$\sqrt{3}\frac{\pi}{16} = 0.34$$

Let's get to know Silicon better (5)

- What is the areal density of the (100) plane?



Areal Density =

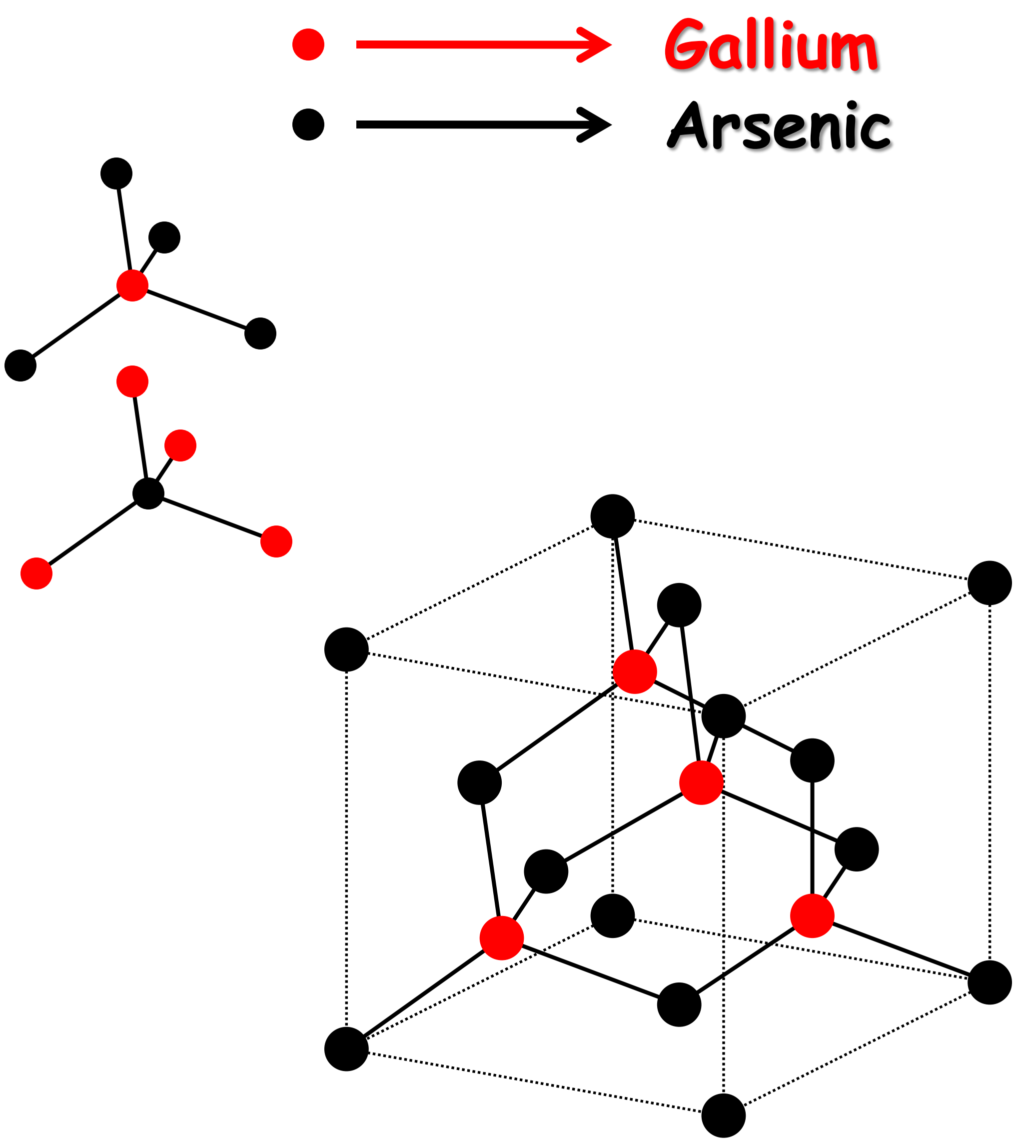
= # Atoms on face/ Area face =

$$= \left[\left(4 \times \frac{1}{8} + \frac{1}{2}\right)_{above\ surface} + \left(4 \times \frac{1}{8} + \frac{1}{2}\right)_{below\ surface}\right] \frac{1}{a^2} = 2/a^2$$

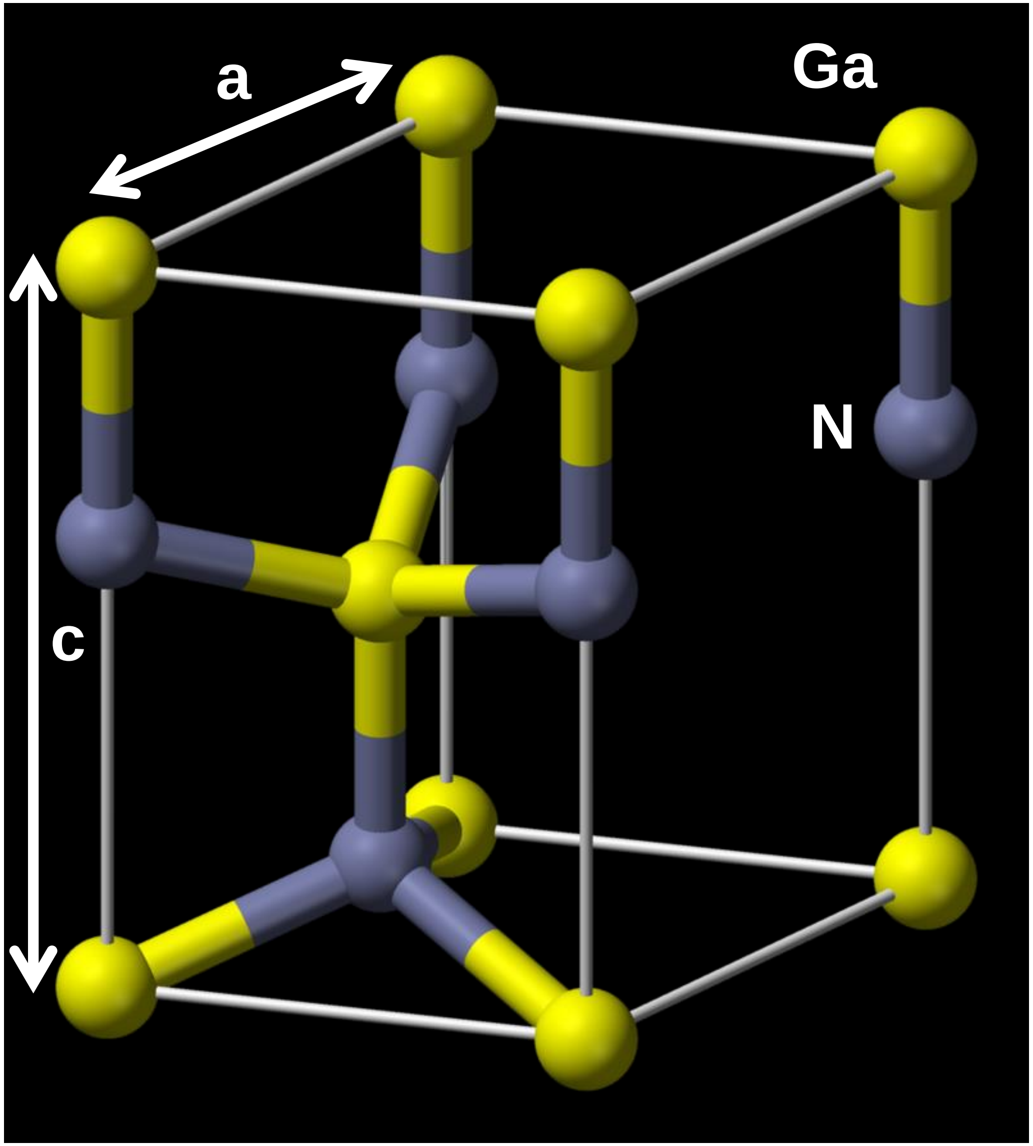
$$= 6.78 \times 10^{18} m^{-2} = 6.78 \times 10^{14} cm^{-2}$$

Compound Semiconductors

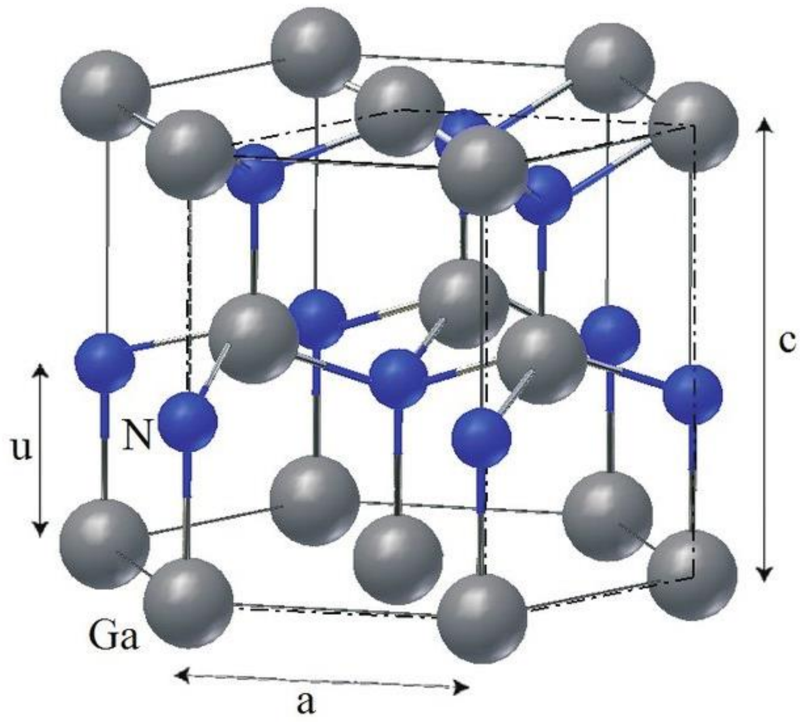
- Many compound semiconductors such as Gallium Arsenide (GaAs) exhibit the **zincblende** crystal structure.
  - The atomic configuration is the same as **diamond**.



Wurtzite Structure

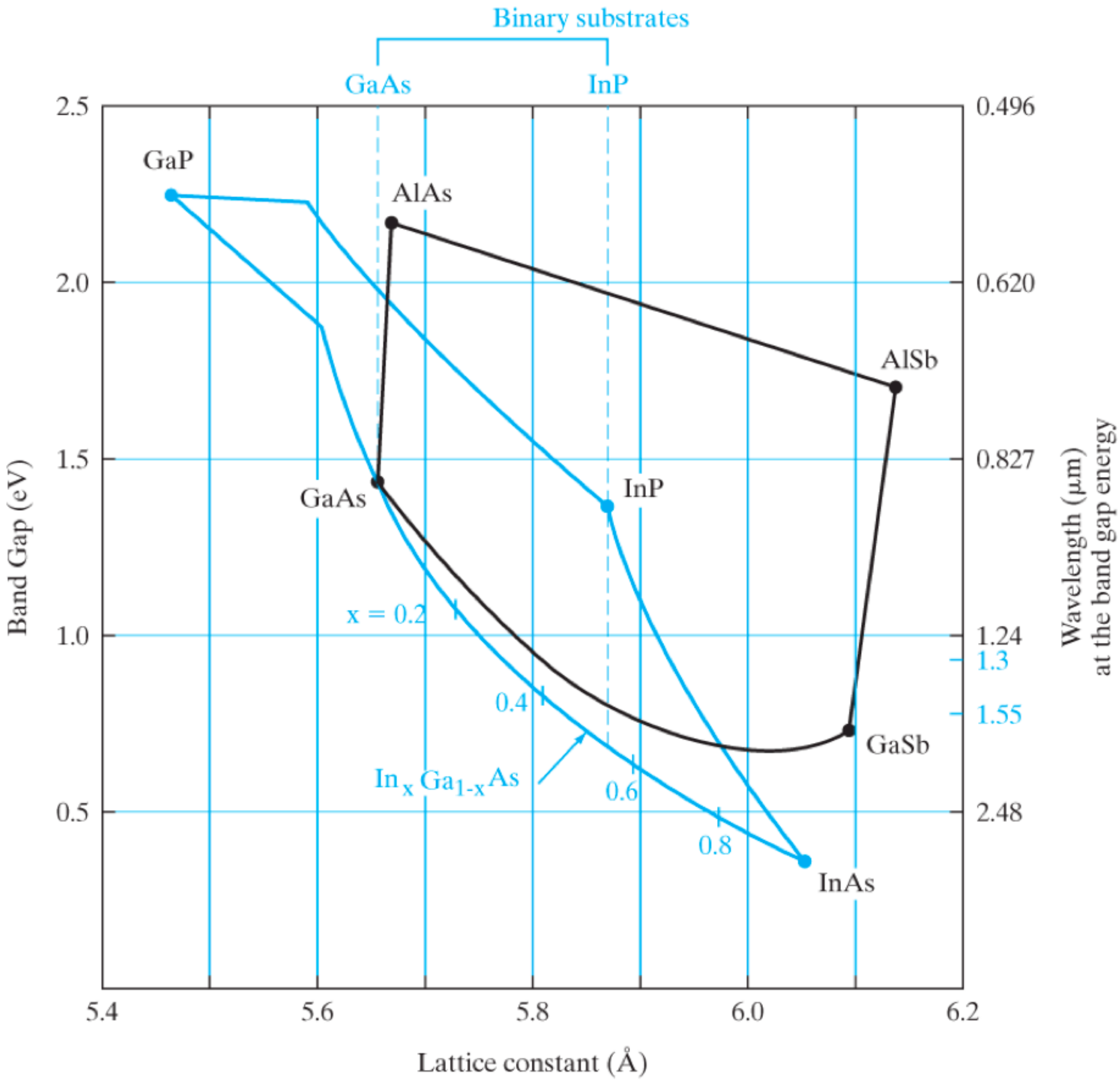


Hoang et al. (2013)



Adapted from Wikipedia, “Wurtzite”

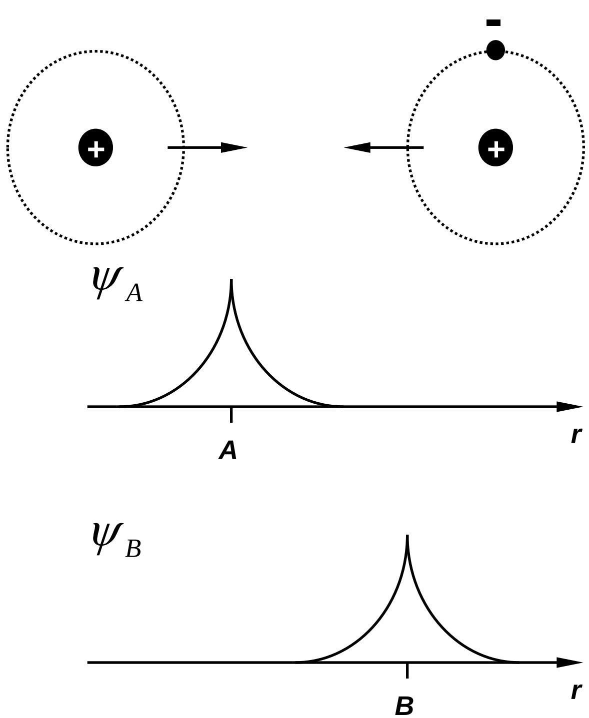
Important Material Systems



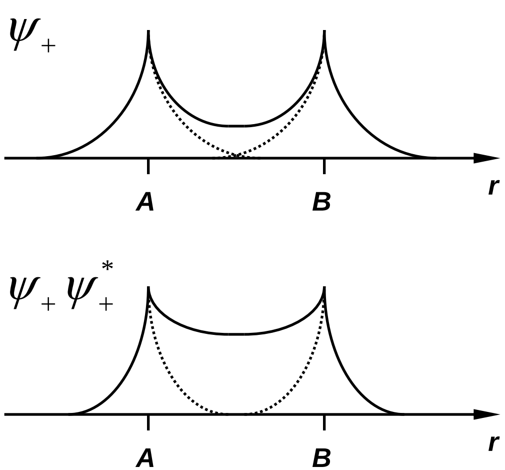
Bonding Forces and Energy Bands

Bonding in Hydrogen atom

- Hydrogen – Consider the case of two atoms A and B with ground state wavefunctions: The resulting molecule is a superposition of the two atomic wavefunctions



$$\psi_{\pm} = \psi_A \pm \psi_B$$

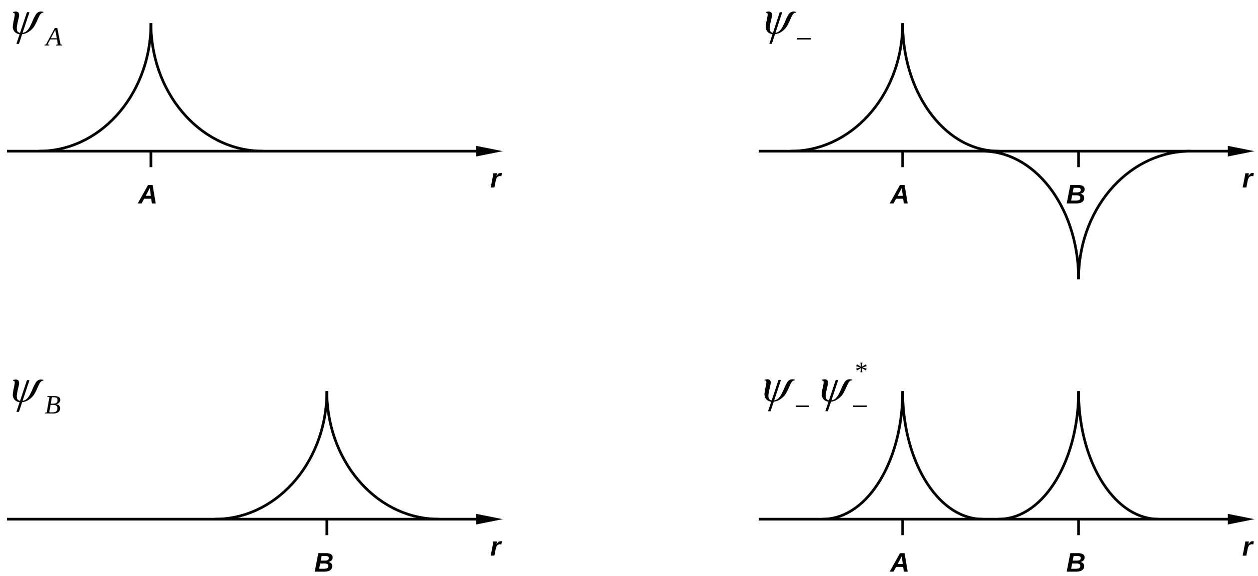


Symmetric State

Bonding in Hydrogen atom

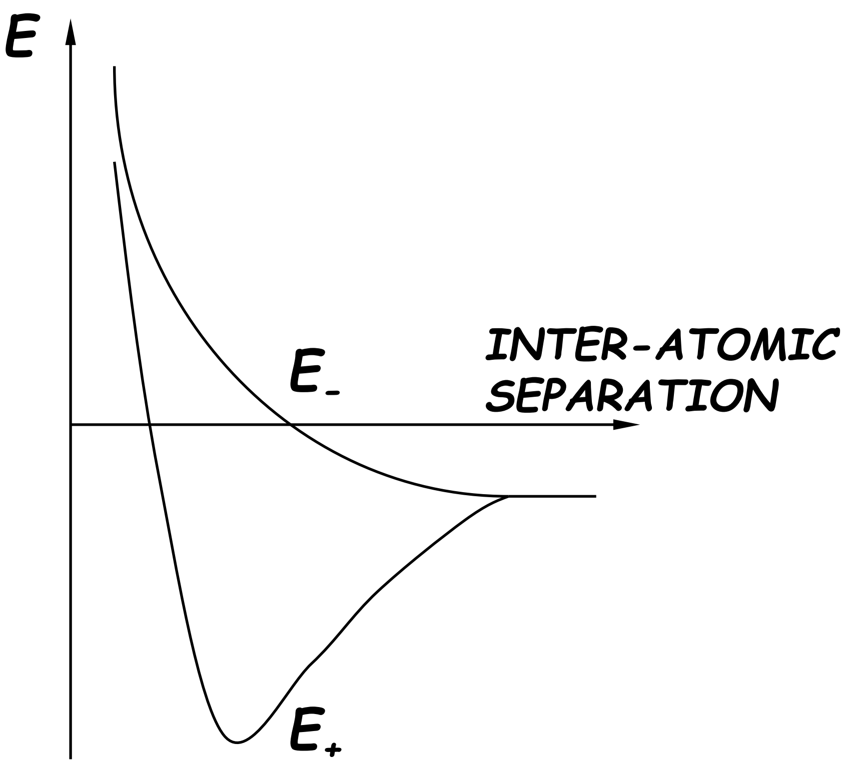
But another combination of wavefunctions exists.

- Antisymmetric wavefunction gives less probability of finding the electron between the two atoms.
  - The symmetric state lies lower in energy.
  - The symmetric state is referred to as the bonding state and the antisymmetric state is referred to as the anti-bonding state.



Bonding in Hydrogen atom

- There is no minimum present in the anti-bonding state indicating the absence of a stable molecular state.
- In the bonding state there is a minimum: stable molecular state



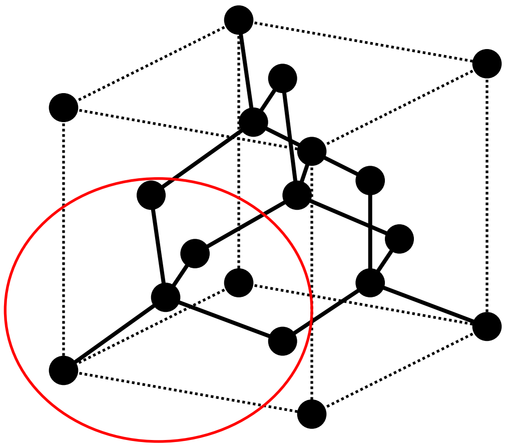
- WHEN ATOMS ARE FAR APART BONDING AND ANTI-BONDING STATES ARE EQUAL IN ENERGY.

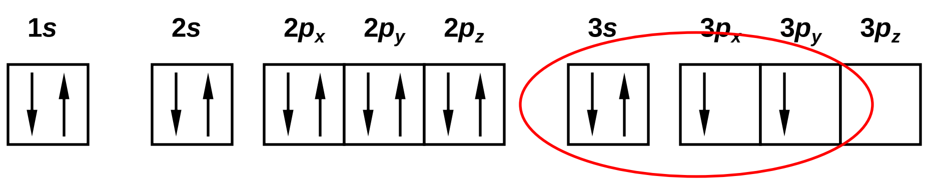
- AS THE INTER-ATOMIC SEPARATION IS REDUCED HOWEVER THE ENERGY OF THE BONDING STATE DECREASES FASTER THAN THAT OF THE ANTI-BONDING STATE.

- THE EXISTENCE OF A MINIMUM ENERGY IN THE BONDING STATE DETERMINES THE EQUILIBRIUM SEPARATION OF THE HYDROGEN ATOMS IN THE MOLECULE .

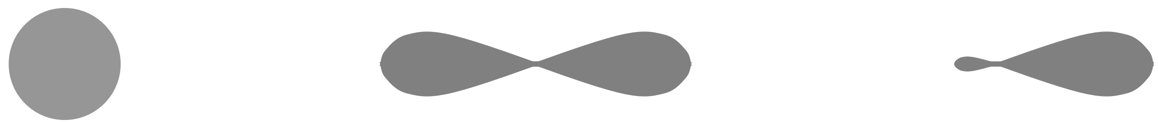
Crystal Bonding

- Each atom shares bonds with 4 other atoms.
- Silicon bonds are covalent, but compound semiconductors have a mix of ionic and covalent bonds.





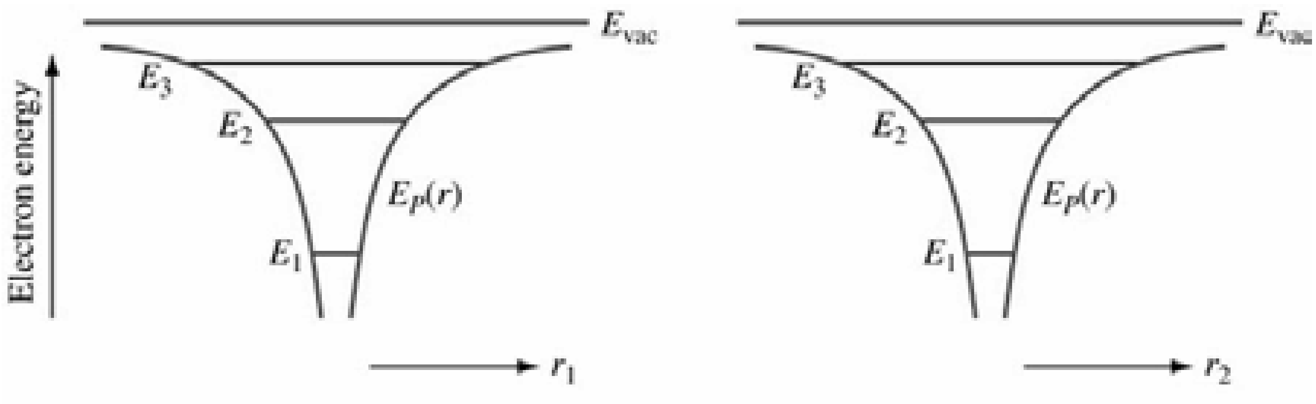
When silicon atoms COMBINE to form a crystal the *s*- and *p*- orbitals HYBRIDIZE to form so-called *sp*^{3} ORBITALS that are mixtures of the *s*- and *p*-orbitals.

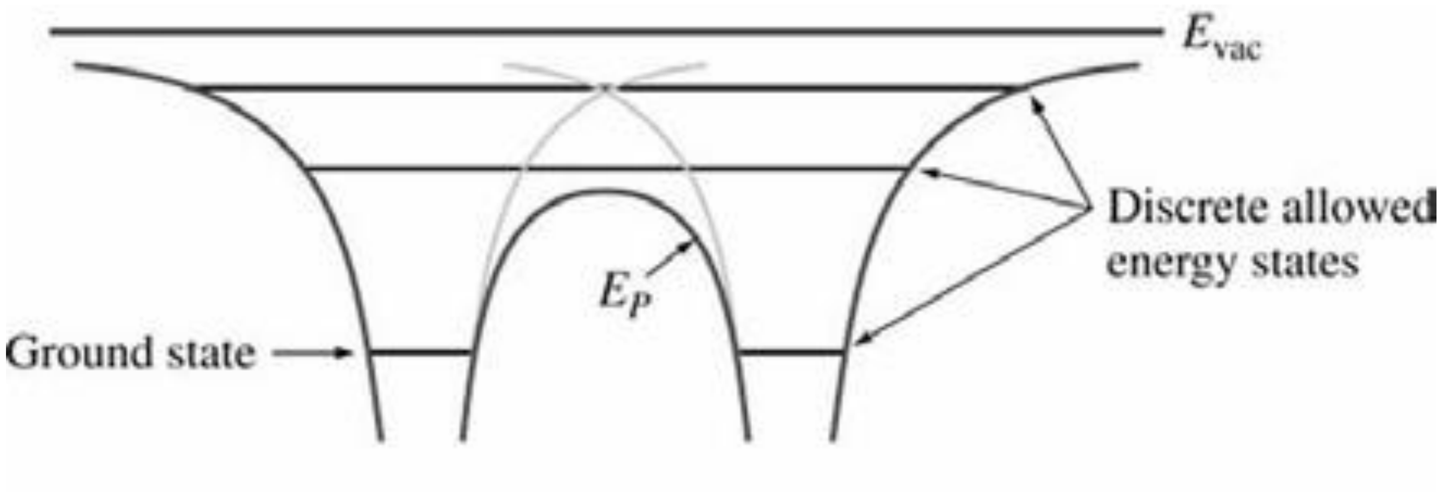


s-ORBITAL | *p*-ORBITAL | *sp*^{3}-ORBITAL

Crystal Bonding

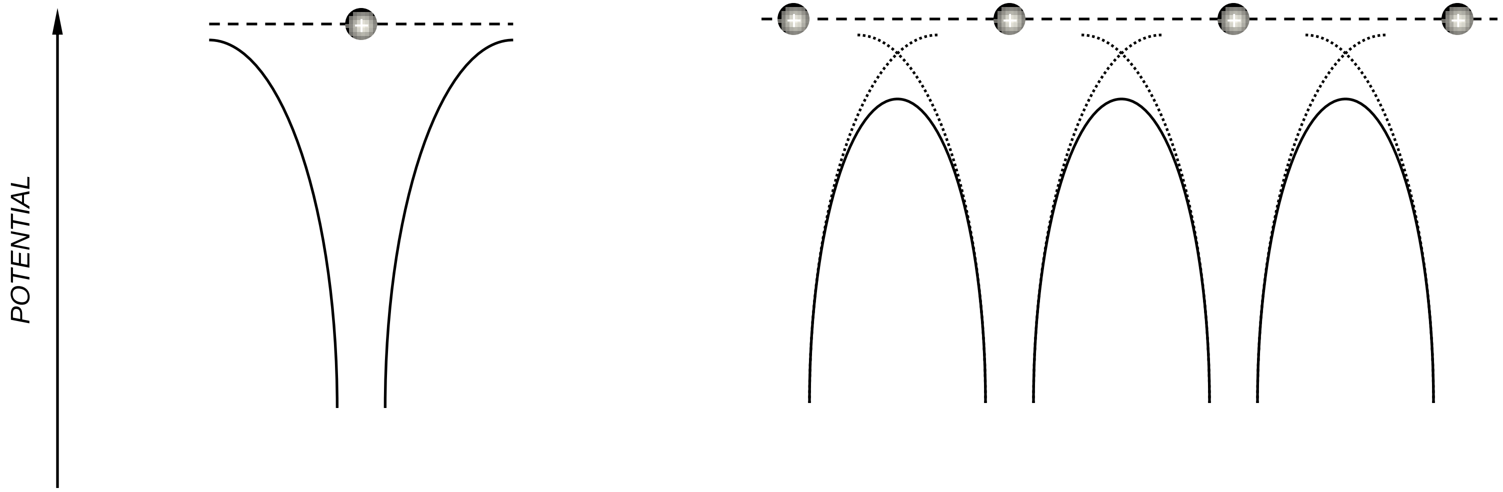
Bring atoms together, the wavefunctions begin to overlap.





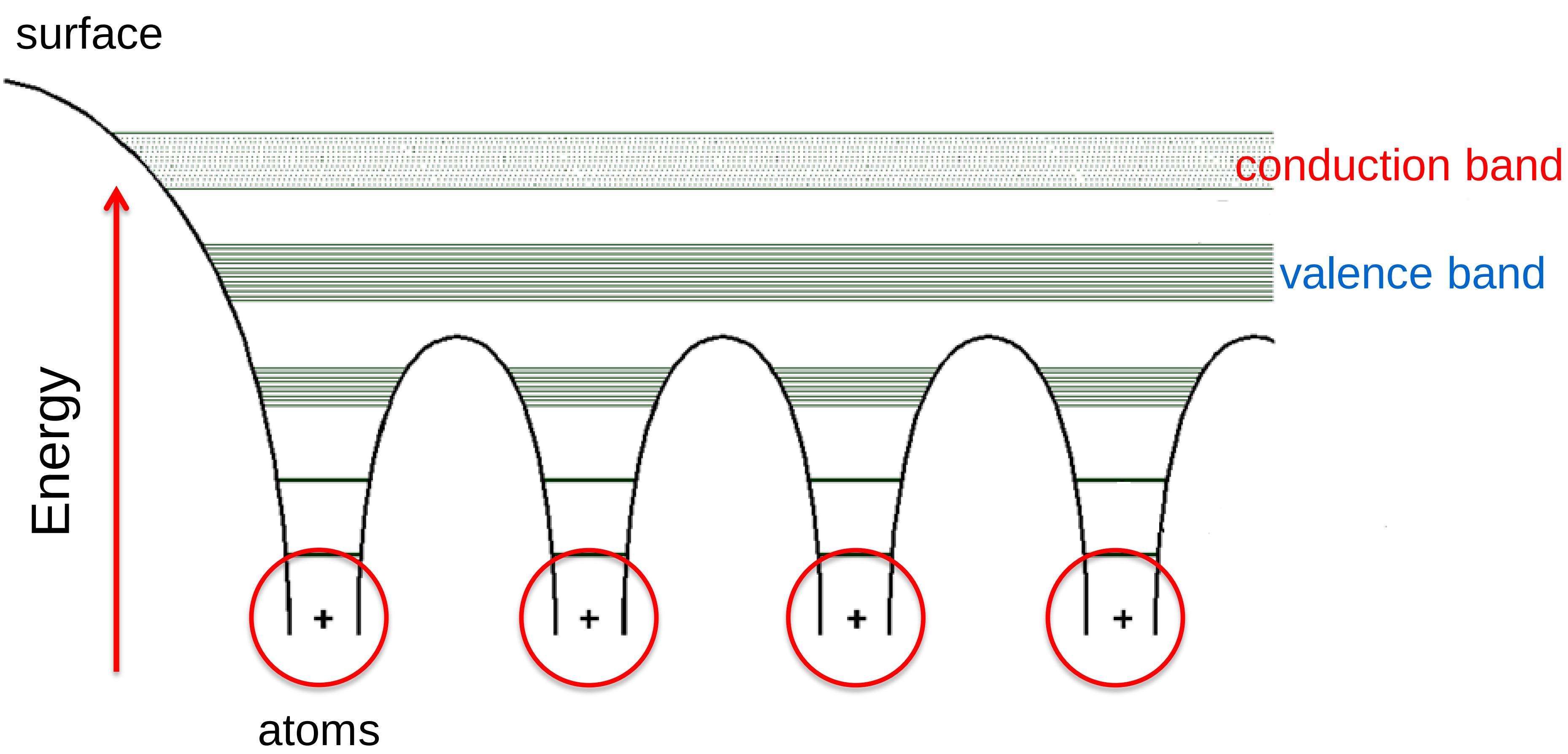
Energy Band Formation

IN A SINGLE ATOM ELECTRONS ARE TRAPPED IN A POTENTIAL WELL

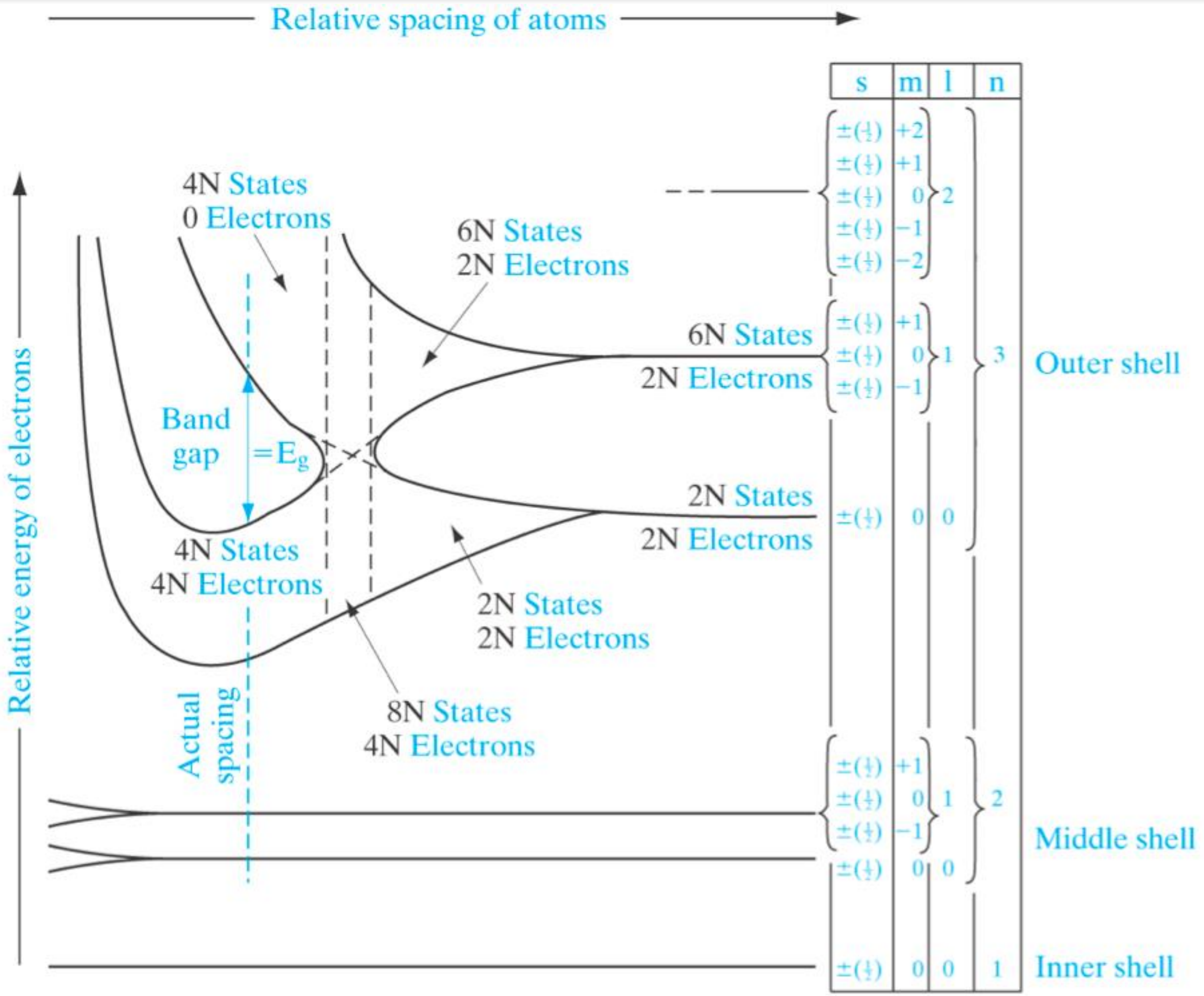


WHEN MANY ATOMS COMBINE AND FORM A CRYSTAL THE ATOMIC POTENTIALS OVERLAP GIVING RISE TO A PERIODIC VARIATION

Energy Band Formation



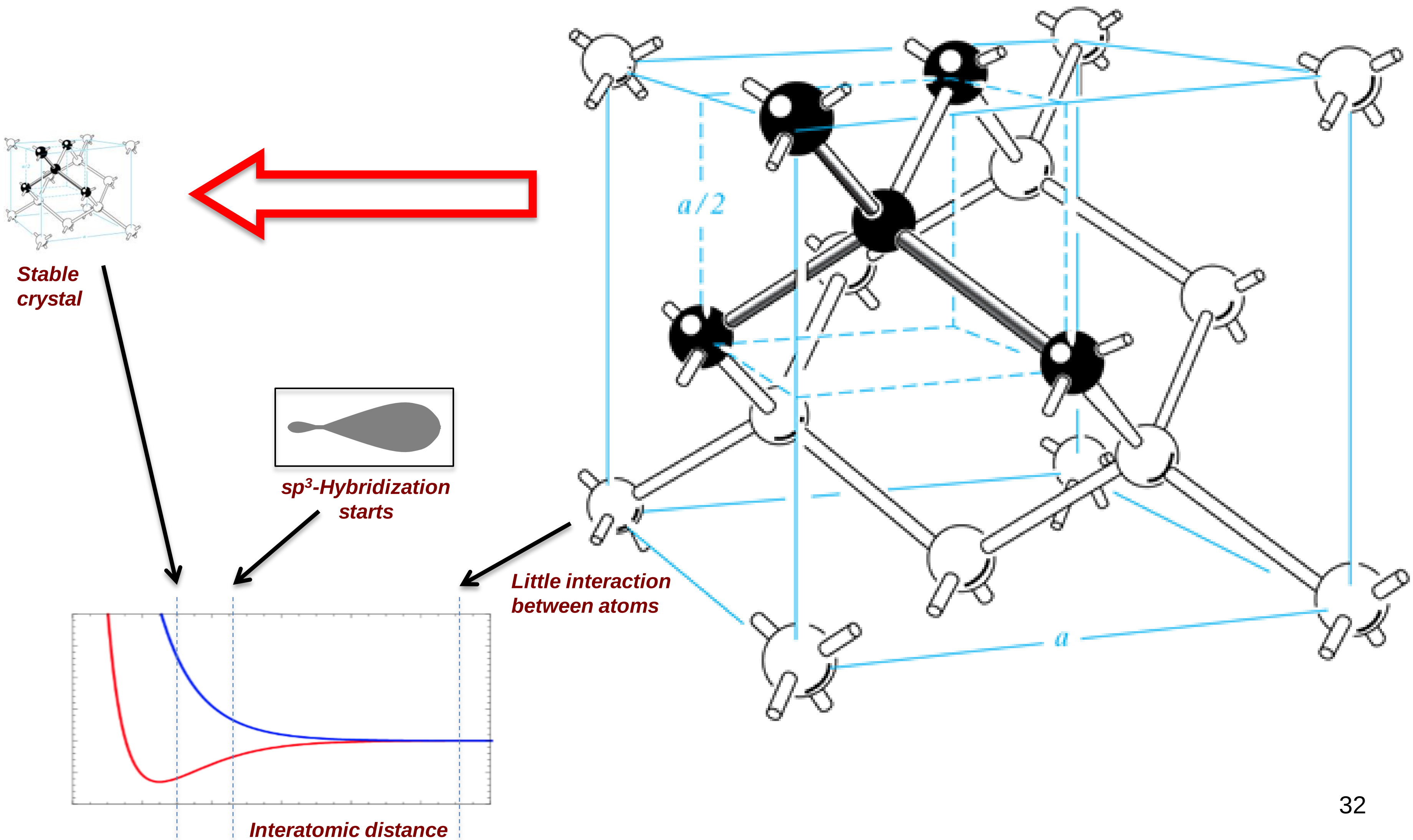
Energy Band Formation



From *Solid State Electronic Devices,* Sixth Edition, by Ben G. Streetman and Sanjay Kumar Banerjee.
ISBN 0-13-149726-X.

Gedanken Experiment

Imagine you start with $a \gg$ and then shrink down to exact size

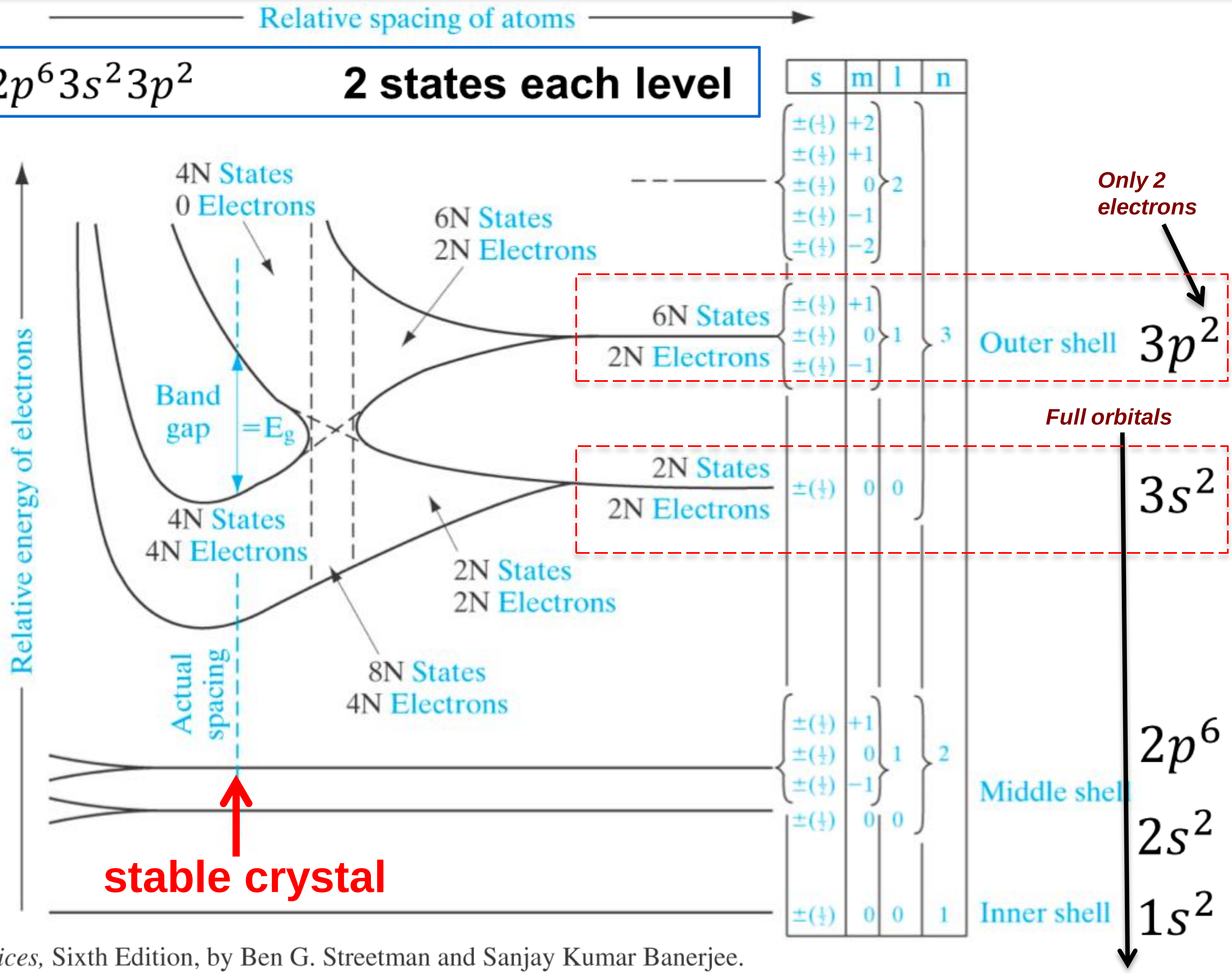


Energy Bands Formation

Silicon – $1s^2 2s^2 2p^6 3s^2 3p^2$ **2 states each level**

Atomic #
Z = 14

N = atoms in crystal



Energy Bands Formation

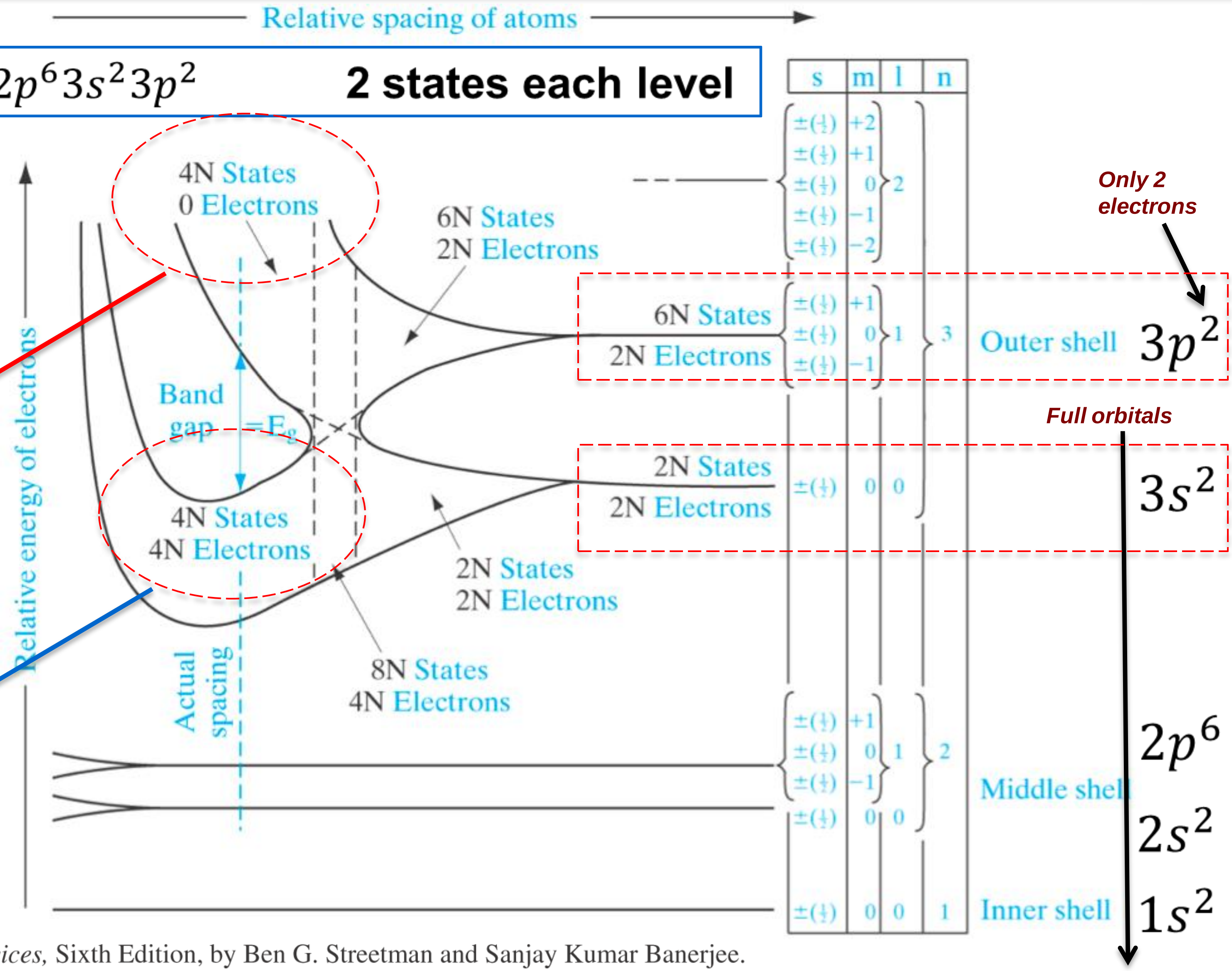
Silicon – $1s^2 2s^2 2p^6 3s^2 3p^2$ **2 states each level**

Atomic #
Z = 14

N = atoms in crystal

no occupation at T = 0K

fully occupied at T = 0K



Energy Band Formation