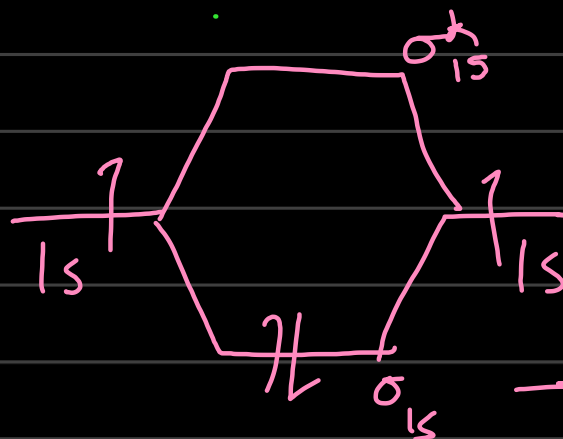# Lecture-11

→ n, l, m , $s = \pm\dfrac{1}{2}$

$$E = f(n) \qquad L = f(l) = \hbar\sqrt{l(l+1)}$$

$$L_z = f(m)$$

$$S = \hbar s = \pm\dfrac{\hbar}{2} \quad \Rightarrow \quad \underline{2s+1 \text{ levels}}$$

LCAO:

Hydrogen:

H_2 is formed. → Net lower energy than individual atoms.

Helium:
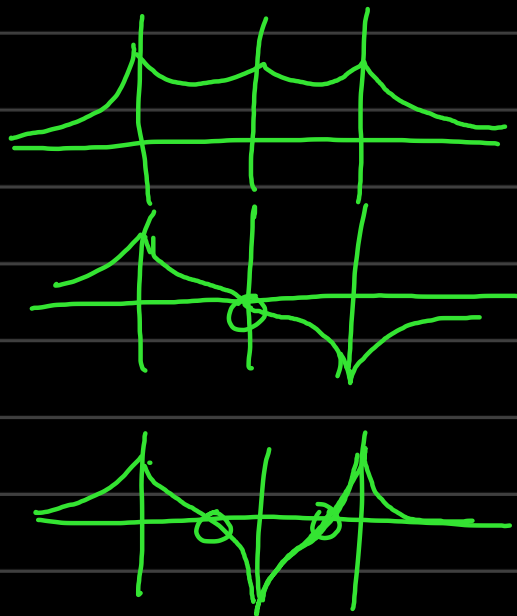

He_2 is not formed. → Net energy higher than sum of individual atoms.

3 hydrogen : H – H – H
               1s   1s   1s

$$\psi_1 = \psi_{1s}(A) + \psi_{1s}(B) + \psi_{1s}(C)$$

$$\psi_2 = \psi_{1s}(A) + \psi_{1s}(B) - \psi_{1s}(C)$$

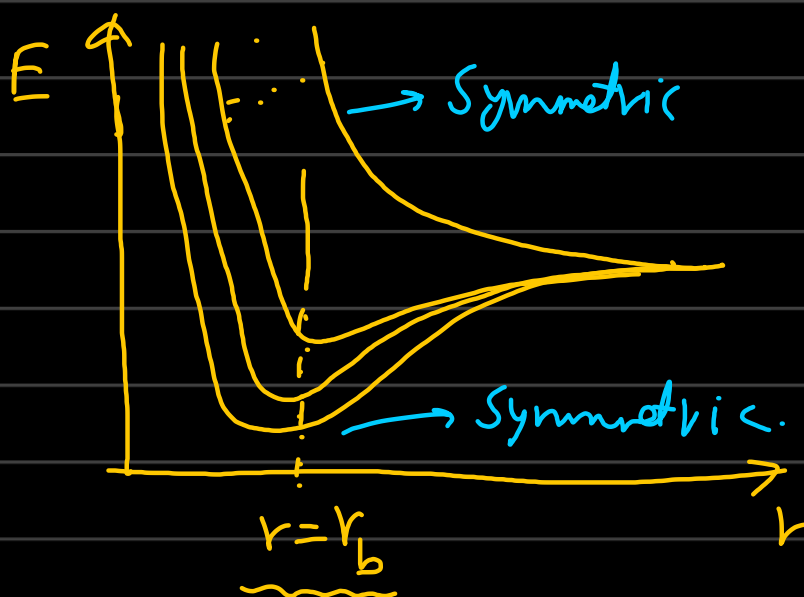$$\psi_3 = \psi_{1s}(A) - \psi_{1s}(B) + \psi_{1s}(C)$$

$$E_3 > E_2 > E_1$$

N – Lithium : Li – Li – Li . . . . .
                2s   2s   2s
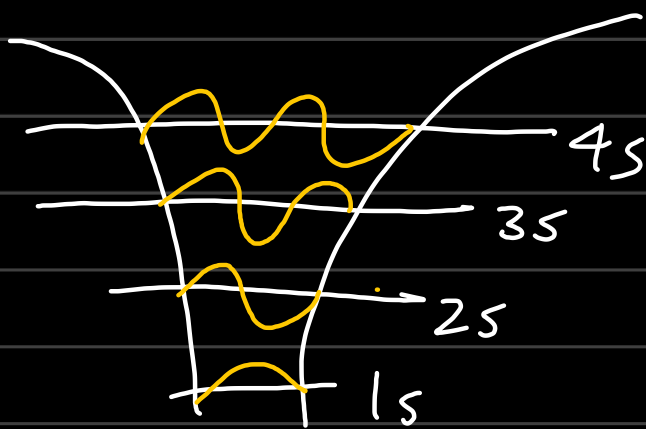

→ Symmetric

→ Symmetric.

$r = r_b$

→ At $r = r_b$: collection infinite energy states
   creates energy bands.

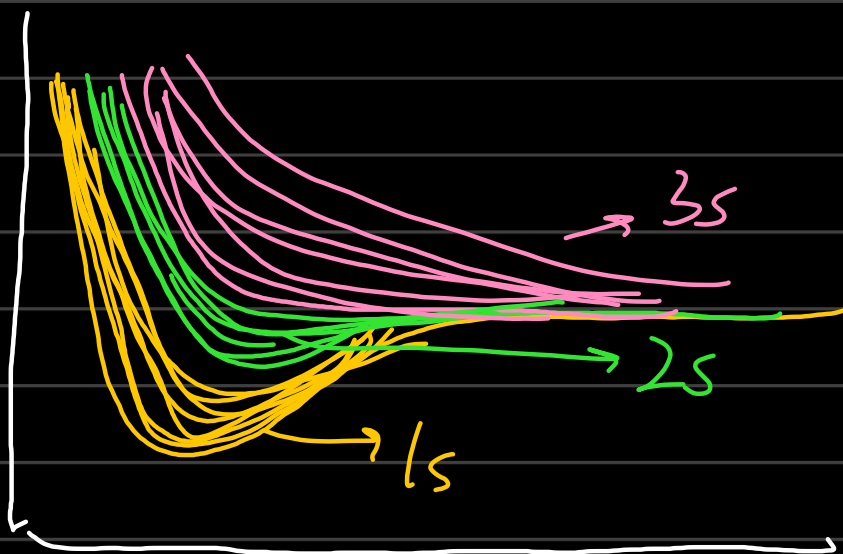→ large no. of discrete energy levels,
results in formation of bands.

→ seems continuous energy spectrum.

✱ No. of occupied states: $\underline{\underline{N/2}}$

→ As n ↑ses, length/size
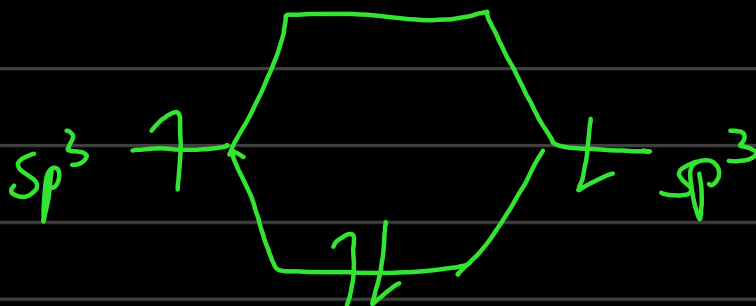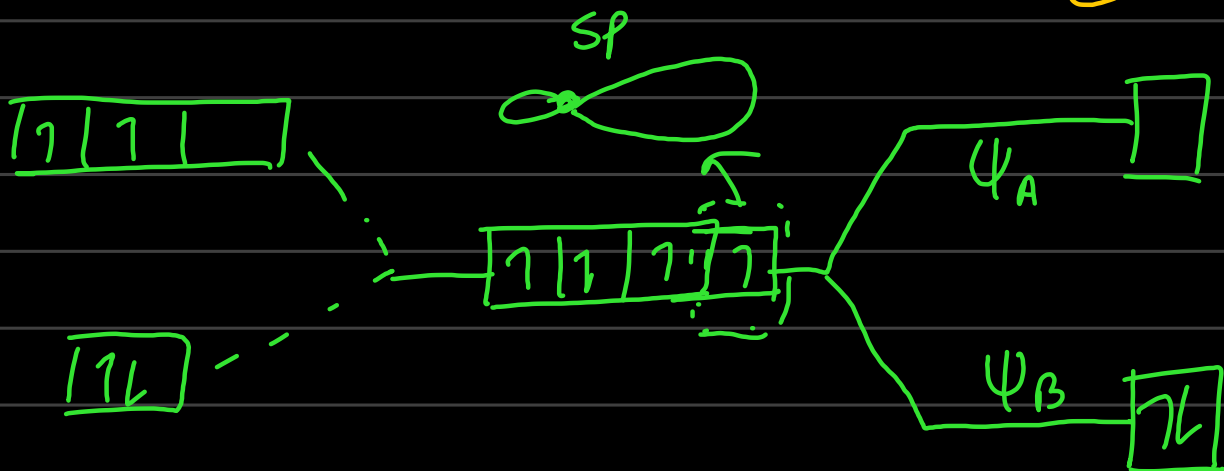of wave functions ↑ses.

→ higher energy.

4s

3s

2s

1s

3s

2s

1s
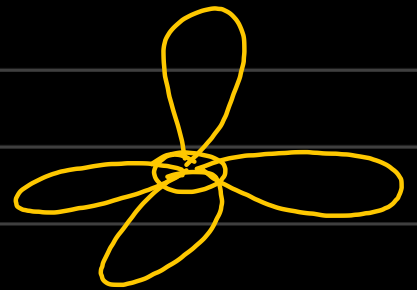
why $E_{2p} \neq E_{2s}$?

Semiconductor:

→ Hybridisation:

$$3s + 3P_x + 3P_y + 3P_z = 4 \ sp^3 \ orbitals$$
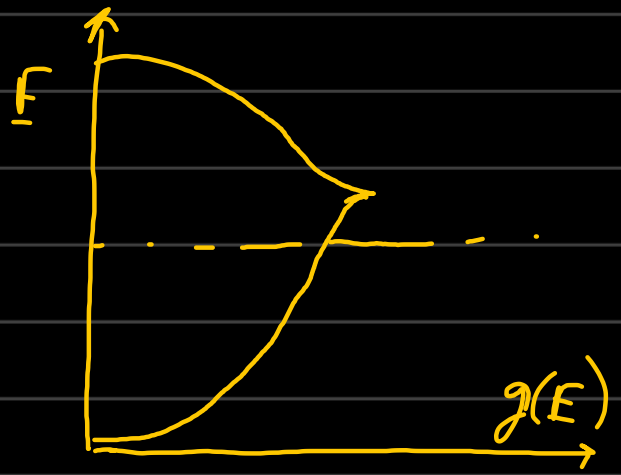

sp^3 ⤢ ⤡ sp^3

Linear combination of 2 sp^3 orbitals when
bonded.

Density of States:

D = density of states

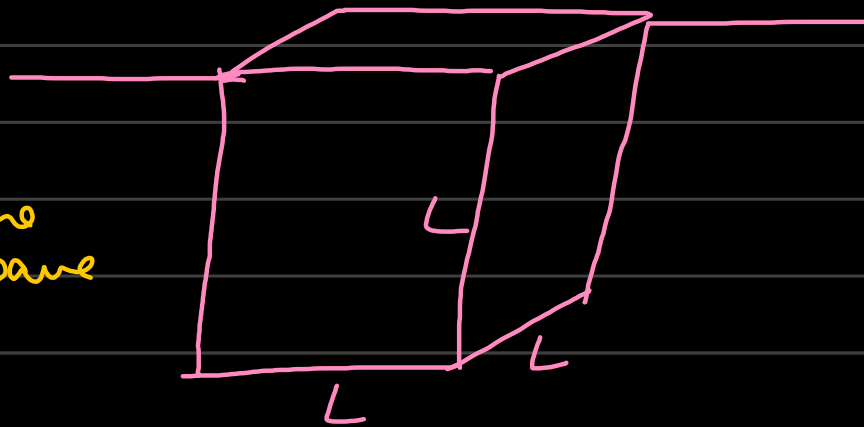↳ total no. of states per unit volume per unit energy.

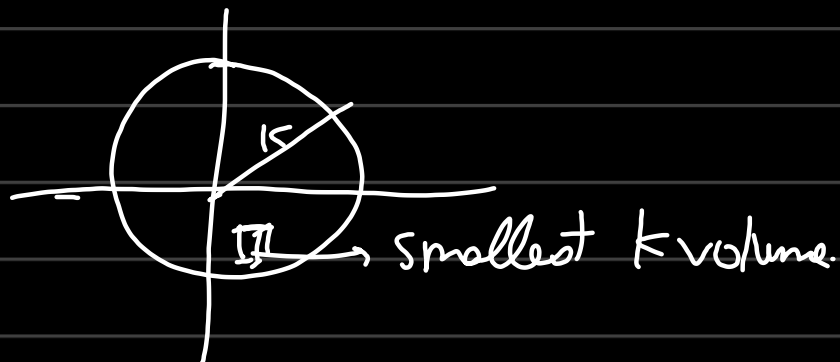$$\boxed{D(E) = \frac{1}{V}\frac{dN}{dE}}$$

↓
fnc of Energy

$V = L^3$ ← vol.

$\psi = Ae^{i(k_x + k_y + k_z)\underset{\sim}{r}}$ → plane wave

$E = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}$

$dE = \frac{\hbar^2 k}{m}dk$

→ smallest k volume.

K is discrete: $k_x = \frac{2\pi n}{L}$; $k_y = \frac{2\pi n}{L}$; $k_z = \frac{2\pi n}{L}$

smallest k volume ⟹ $k_x k_y k_z = \left(\frac{2\pi}{L}\right)^3$

& No. of k points: $\dfrac{\frac{4\pi}{3}k^3}{\left(\dfrac{2\pi}{L}\right)^3}$