1a. Born - Oppenheimer.

The nuclei are regarded fixed at selected positions. S.E. solved for the electronic wavefunction.

b. Hybridization

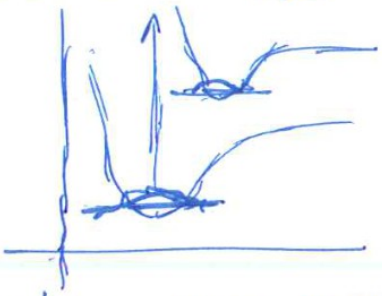
Formation of hybrid orbitals (basis set) out of atomic orbitals. Linear Combination of Atomic Orbitals. e.g. $C(1s^2 2s^2 2p) \rightarrow C(1s^2 2s 2p_x 2p_y 2p_z)$.

c. Frank - Condon

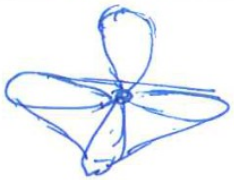
Electronic transitions that are so fast that the locations of the nuclei remain fixed during the transitions.

d. Ground vibrational levels at different inter-nuclear distances
Thus overlap small.

Frank - Condon.



e. In a pure 2-state system you need the "laser" photons to pump the upper level. You never obtain population inversion.

f. sp^3  tetraeder structure.

sp  <u>linear</u> structure.

g.

$E = B(J+1)J$.

$E_{J+1} - E_J = B\{(J+2)(J+1) - J(J+1)\}$.

$= 2B(J+1)$. $= 32$

$E_{J+2} - E_{J+1} = 2B(J+2) = 36$

$\Rightarrow 2B = 4 \Rightarrow B = 2$

$\Rightarrow E_J = 2(J+1)J = 112 \Rightarrow J^2 + J - 56 = 0$

$J = 7$ or $J = -8$ $\Rightarrow$ levels $J = 7, 8, 9$.

h. $B = \frac{\hbar}{4\pi c I} \propto \frac{1}{I}$ $\quad I = \sum_i m_i x_i^2$

m_i larger $\rightarrow$ I larger $\rightarrow$ B smaller.

Energy levels get closer :

For center atom $x_i = 0$ $\rightarrow$ no effect of atomic mass change.

i. $|c\psi|^2 = 1 \Rightarrow |c|^2 \int (6\phi_A^* + 8\phi_B^*)(6\phi_A + 8\phi_B)\, dV$

$|c|^2 \{36|\phi_A|^2 + 64|\phi_B|^2 + 96 \underbrace{\int \phi_A \phi_B\, dV}_{\text{overlap integral } S}\}$

$\Rightarrow |c|^2 \{100 + 96S\} = 1.$

$\Rightarrow c = \sqrt{\frac{1}{100 + 96S}}$

$\psi_N = \frac{3\phi_A + 4\phi_B}{\sqrt{25 + 24S}}$

j. $P(\phi_A) = |\langle \phi_A | \psi_N \rangle|^2 = \frac{9}{25 + 24S}$

$P(\phi_B) = \frac{16}{25 + 24S}$

imbalance $\frac{7}{25 + 24S}$.

k. polar electric dipole moment $\Leftrightarrow$ because of the charge imbalance.

l. bonding $6\phi_A + 8\phi_B = \psi$

antibonding $8\phi_A - 6\phi_B = \psi^*$

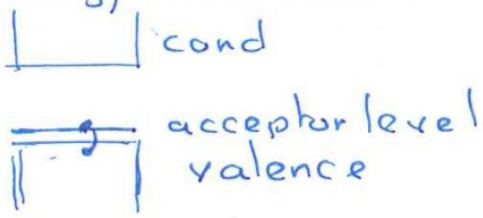
$\Rightarrow \underline{\psi^* \psi = 0}$.

2a use of periodic boundary conditions assumes no direct physical effects due to the boundaries.

b) lattice vibration

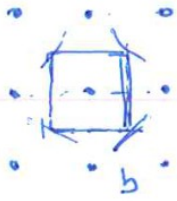
c) system with a band gap; pure no impurities at $T=0$ valence shell filled, conduction band empty, at $T>0$ small fraction of electrons in cond. band. and holes in valence band.

d). acceptor impurity, accepts "easily" electrons from valence band. Energy level close to top of the valence band.
$\Rightarrow$ many holes in valence band
$\Rightarrow$ conducts via hole mobility



e) contact between a donor (n type) and acceptor (p type) semi conductor.
In boundary region depletion (recombination) of majority carriers (electrons or holes).
$\Rightarrow$ space-charge region made up by the fixed impurity ions.

f) square lattice side b



Wigner Seitz cell direct lattice
$A_{ws} = b \times b = b^2$

Brillouin zone cell, reciprocal lattice, square with b spacing $\frac{2\pi}{b}$.

$\Rightarrow A_{B2} = \frac{4\pi^2}{b^2}$.

g). Boundaries $\varphi(0) = \varphi(L) = 0$. for x and y.

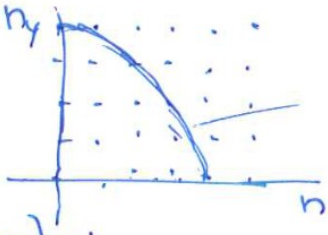
S.E. $\frac{-\hbar^2}{2m}\left\{\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2}\right\} + \underbrace{V}_{=0} = E\varphi.$

$$\frac{+\hbar^2}{2m}\left\{\frac{\pi^2}{L^2} n_x^2 \varphi + \frac{\pi^2}{L^2} n_y^2 \varphi\right\} = \text{Const}\ \varphi$$

h) $$E = \frac{+\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2) = \frac{+\hbar^2\pi^2}{2mL^2} n^2$$

i) n_x and n_y charaterize 1 orbital which accommodates 2 states (spin up and spin down).

$n_x, n_y \geq 0$



$n_F = n_{max}$.

$\Rightarrow$ number of orbitals: ~~$\frac{1}{2}\pi n_F^2$~~ $\frac{1}{4}\pi n_F^2$

$$\Rightarrow \frac{N}{2} = \frac{1}{4}\pi n_F^2 \Rightarrow n_F^2 = \frac{2N}{\pi}$$

$$\Rightarrow E_F = \frac{+\hbar^2 \pi N}{mL^2}$$

j. $\frac{N}{L^2} = 10^{12}\ cm^{-2} \qquad 10^{16}\ m^{-2}.$

$$E_F = \frac{\pi (1.05)^2 10^{-68} \cdot 10^{16}}{9.11 \times 10^{-31}} = \frac{\pi (1.05)^2}{9.11} \times 10^{-21} \left[\frac{J^2 s^2}{kg\, m^2}\right] = [J].$$

$1\ J = 1.6 \times 10^{-19}\ eV \Rightarrow E_F = 2,4\ meV$

k. from ~~k~~i). $N = \frac{mL^2}{\hbar^2 \pi} E$

$$D(E) = \frac{\partial N}{\partial E} = \frac{mL^2}{\hbar^2 \pi}$$

l. $b \rightarrow b/2$. E_F does not depend on lattice distance.
number of electrons increases by a factor of 2 $\Rightarrow N \rightarrow 2N$.

$\Rightarrow E_F \Rightarrow 2E_F$

m. No influence if $d < \lambda_F$ as λ_F is the shortest relevant wavelength.

$\lambda_F = \frac{2\pi}{k_F}$, $k_F = \frac{\pi}{L} n_F = \frac{1}{L}\sqrt{2\pi N}$. (see i for k_F).

So $\lambda_F = L\sqrt{\frac{2\pi}{N}}$.

So, 2D-like if $d < L\sqrt{\frac{2\pi}{N}}$.