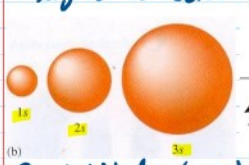
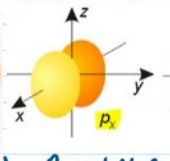
Atoms and Solids

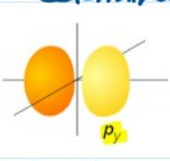
Wednesday, November 4, 2020 6:25 PM

Orbitals

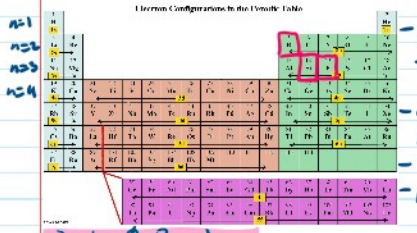
- e^- exist in orbitals around atoms
- orbitals → standing waves on string (nodes)
  - ↳ particular shape & specific energies
- As E↑ Energies get closer
- light emission & absorption determined by energy spacing



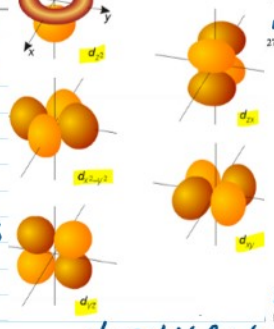




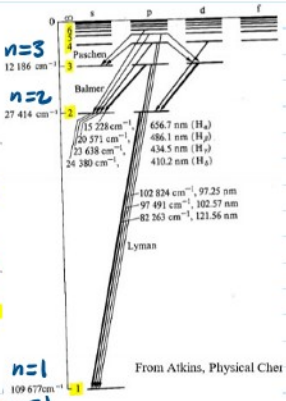
S-orbitals (n=1) P-orbitals (n=2)



- Potential E of e^- due to nucleus: $U = -\frac{q}{4\pi\varepsilon_0 r}$
- allowed E states = orbitals $1s, 2s, 2p, 3s, 3p, 3d, 4s$
- s-orbitals have $\leq 2e^-$
- p-orbitals have $\leq 6e^-$



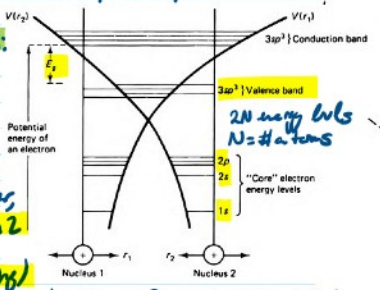
d-orbitals (n=3)



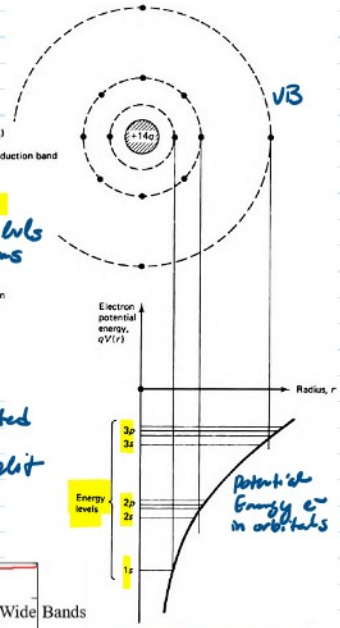
Bands & Bands

- Allowed values of E = Energy levels (n=1, 2, 3)...
- each state can have 2 e^- (opposite spin)
  - ex. Silicon Si: $1s^2 2s^2 2p^6 3s^2 3p^2$
  - when bonding, 3s & 3p orbitals overlap → $3sp^3$

- Formation of E bands:
  - Valence orbitals overlap
  - E levels merge, sharing of valence e^- split into 2 different bands
  - when 2 atoms brought together, each original orbital split in 2 orbitals: lower (bonding) higher (anti-bonding)

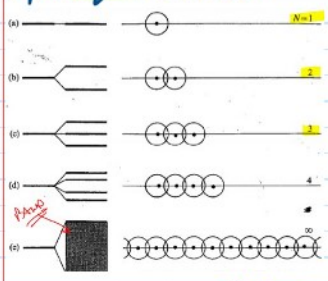


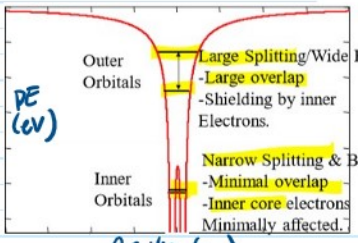
- e^-
- For 1# e^-, bands are formed, associated w/ each orbital
- N identical atoms → orbitals split in N energy levels



2N energy lvls
N = # atoms

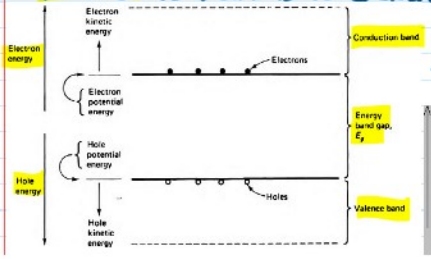
Splitting of E-levels



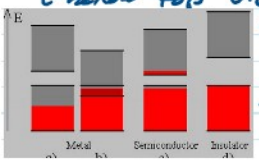


- highest full E band in SC or insulator @ ground = VB
- lowest unoccupied e^- band @ ground = CB

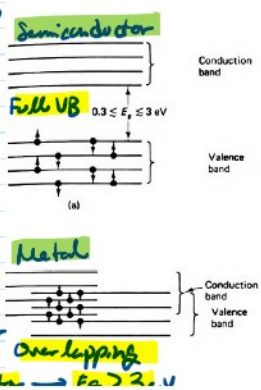
- Top band = Conduction band CB, Bottom band = Valence Band VB
- @ ↑T, some bonds break, if e^- excited & gain PE ≥ E_g, can be excited out of VB to CB
  - ↳ excited e^- depends on T.
- Min E to break Bond & excite e^- from VB → CB = E_g

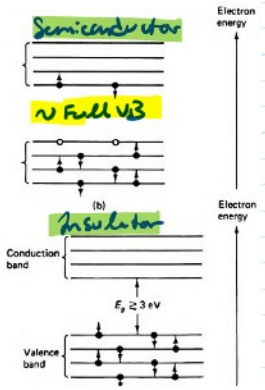


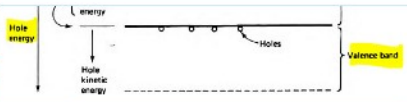
- e^- & holes from band breaking
- E above bottom of CB = e^- KE
  E below top VB = hole KE

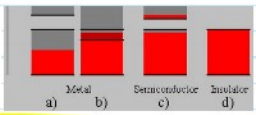


- If band partially full or overlap → metal
- If bands full or empty @ ground, Overlapping





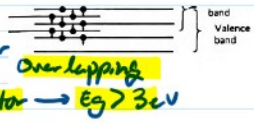


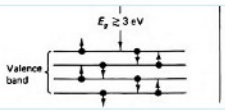


→ metals

- If bands fuller empty @ ground, Overlapping

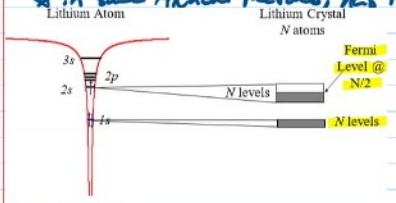
∴ SC or insulator → $E_g > 3eV$





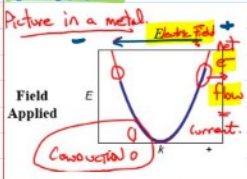
- e⁻ in CB transport charge → carriers
- If E levels closer & E_g ∴ ↑KE, when ↑E_g, VB full & no conduction (insulators)

☆ in some Alkali metals, has Bandgap, but VB not full.



- when e⁻ excited into CB, empty states in VB = holes

Conduction



- Apply field in (-) dir. → pulls (-) charged e⁻ to right ∴ Imbalance ∴ ↑e⁻ to right
- Conduction requires empty & accessible states

- If $\vec{E}$ field applied on e⁻:

← $\vec{E}$ Field

→ $\vec{e}$ accel. $\vec{a} = -\frac{e\vec{E}}{m}$

$v_{drift} = \mu \vec{E}$ → μ = mobility

$\mu = \frac{e\tau}{m^*}$ → effective mass (mass e⁻ inside crystal)

$v_{avg} = \frac{e\vec{E}\tau}{2m^*}$ → τ = avg time btw collisions

- Resistance: collisions of e⁻ & holes w/ impurities in crystal
  - ↳ impurities & vibrating lattice leads to resistance
- Conductivity σ density of carriers in metals, mobility, & charge e⁻

$\sigma = \mu n_0 e$ → carrier speed v (v drift) & applied field: $v = \mu E$