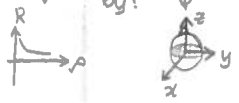
Physics 315

I. Elements

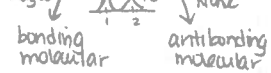
- Periodic table
  - rows: same orbitals (s, p, d, f)
  - columns: charge # (# e^-)
- 4 quantum states
  - 3 has 1
  - ① n
  - ② ℓ = ORB (s, p, d)
  - ③ $m = -\ell \cdots +\ell$
  - spin ↑↓
  - Ruler
    - ① Pauli's (fill lowest)
    - ② Hund's (fill all 1st)
- Wavefunction $\psi_{n,\ell,m}(r,\theta,\phi)$
  - 1st: Radial $R_{n\ell}(\rho)$
  - split into 2nd: spherical $Y_{\ell m}(\theta,\phi)$
  - represented by:



- Energy spectrum
  - lowest: ground state
  - others: excited state
  - E values
    - $E>0$ free state
    - $E<0$ bound state
- Trends:
  - ① Atomic radius (↑R)
  - ② Ionization E (↑IE)
  - ③ e^- Affinity (↑EA)

II. Bonding

- Van der Waals
  - Lennard-Jones ☆
  - $V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$
  - $r<\sigma$: V = repulsive
  - $r>\sigma$: V = attractive
  - ... used to find cohesion energy
  - $\frac{U_{TOT}(R_0)}{N} = 2\epsilon\left[a_{12}\left(\frac{\sigma}{R_0}\right)^{12} - \sigma_6\left(\frac{\sigma}{R_0}\right)^{6}\right]$
- Probability of finding e^- btwn nuclei



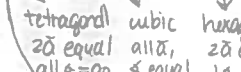
  - maybe bonding molecular → stable
  - NAND antibonding molecular → unstable
- Types of bonds
  - shares e^- → covalent → between non-non or self: H_2
  - H-O, H-F, H-N → H-bond
  - takes/gives e^- → ionic → between metal/non-metal (+)/(−)

III. Crystals

- Crystals = lattice + basis
- lattice: a
- basis: A
  - invariant to translations by lattice vector
  - reciprocal lattice $G_n = n\bar{b}_1$ (1D)
    - used to find Brillouin zone (not for 1D though)
- 3 Types of 2D lattice
  - square: $\bar{a}_1 \perp \bar{a}_2$, $|\bar{a}_1| = |\bar{a}_2|$
  - triangle: $|\bar{a}_1| = |\bar{a}_2|$, 60° ∢
  - oblique: $\bar{a}_1 \neq \bar{a}_2$, ∢ ≠ 60°
- 7 Types of 3D lattices
  - triclinic: all diff $\bar{a}$'s, ∢ ≠ 90°
  - mono'': all diff, 2∢ = 90°
  - orthorombic: all diff, all ∢ = 90°
  - tetragonal: 2$\bar{a}$ equal, all ∢ = 90
  - cubic: all $\bar{a}$, ∢ equal
  - hexagonal: 2$\bar{a}$ equal, 1∢ = 60°, 2∢ = 90°
  - trigonal: all $\bar{a}$ equal, ∢ ≠ 90°
- 4 Types of orthrombics
  - simple
  - base-centered
  - body-centered
  - face-centered

IV. measuring crystals

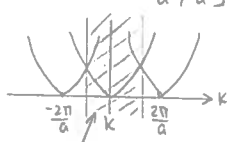
- Laue's condition
  - can only see light scattered off crystals at angles
  - $\bar{G} = \bar{k}_i - \bar{k}_f$ ($\bar{k}_i = \bar{k}_f$ not useful)
  - Intensity is therefore $I(\bar{G}) = |S(\bar{G})|^2$ (S structure factor)
  - $\bar{G} = m_1\bar{b}_1 + m_2\bar{b}_2$
  - $\bar{b}_1 = \frac{2\pi}{a_1}\hat{x}$, $\bar{b}_2 = \frac{2\pi}{a_2}\hat{y}$
- Bragg peak



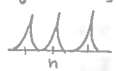
  - ↳ knowing B.P means you know $\bar{G}$ (vector in reciprocal lattice)
- Bragg's condition
  - $2d\sin\theta = n\lambda$
  - maxima corresponds to θ
  - ↓
  - equivalent to Laue's condition

V. Electronic band

- Fermi momentum / E
  - k_F ↓ in ground state
  - e^- CONCENTRATION
  - $E_F = \frac{\hbar^2 k_F^2}{2m}$
- Bloch wavefunctions
  - $\psi_{\bar{k}}(\bar{r}) = e^{ik\bar{r}}u_{\bar{k}}(r)$
  - $\phi(x+Na) = e^{ikNa}\phi(x)$
  - where $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

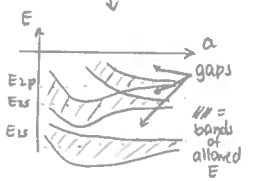


  - Brillouin zone.
- a_B models:
  - $a \gg a_B$: Tight-binding



    - ↓
    - large a/a_B = smaller band
  - $a \ll a_B$: nearly-free e^-

- General evolution of E bands in solids



VI. metals and insulators

- Drude model
  - only for nearly-free e^- or tight-binding models, electronic band ∽ empty
  - ↓
  - assuming non-interacting
  - ↓
  - $C_V = N\frac{3}{2}k_B$ specific heat
- Fermi-Dirac distribution
  - ↓
  - non-interacting fermions
  - $f_{FD}(E) = \frac{1}{e^{\beta(E-\mu)}+1}$
  - ↓
  - Total energy of e^-
  - $U = 2\sum_k E_k f_{FD}(E_k)$
  - $\therefore C_V = 2\nu N k_B \frac{k_B T}{E_F} \sim T$
- Transport properties
  - $R = \frac{V}{I}$
  - T=0: $R=\infty$ (insulators), $R=0$ (metals)
  - Impurities ($T \neq 0$)
  - ↓
  - Scattering states $n \leq 0$: e^{ikna}, Re^{-ikna}
  - $C_n(k) =$ $n>0$: Te^{ikna}
- Diodes / transistors
  - n-doped → w/ e^-
  - p-doped → w/ holes

VII. Phon

- Longitudinal phon
  - ↓ and 2 acoustic phonon modes
  - ↓
  - $w_k \to 0$, $k \to 0$
- chain phonons w/ complicated basis
  - ↓
  - optical phonons
  - ↓
  - excited by light
- Thermal properties
  - $C_V = \left(\frac{dU}{dT}\right)_{N,V}$
  - T=0 → no phonons
  - at low T → # boson is small
  - at high → # phonons is large
- Einstein's model
  - assume E is constant $w_k = \Omega$ for optical phonon's contributions
- Optical properties
  - light strongly couples w/ all ionics
  - light couples w/ covalent w/ partial ionic