1 Atomic Structure

1.1 Energy

$$u_v dv = \frac{8\pi v^2}{c^3} \cdot \frac{hv}{e^{\frac{hv}{K_b T}} - 1} \tag{1}$$

$$E = hv \tag{2}$$

1.2 Photoelectric Effect

$$\frac{1}{2}m_e v_k^2 = E_k = hv - W \tag{3}$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \tag{4}$$

$$R_H = 1.097373 \times 10^7 m^{-1} \tag{5}$$

$$n_1 = 1 \Rightarrow Lyman \tag{6}$$

$$n_1 = 2 \Rightarrow Balmer \tag{7}$$

$$n_1 = 3 \Rightarrow Paschen \tag{8}$$

$$n_1 = 4 \Rightarrow Brackett \tag{9}$$

$$n_1 = 5 \Rightarrow Pfund \tag{10}$$

$$n_2 > n_1 \tag{11}$$

1.3 De Broglie Relationship

$$E^2 = p^2 c^2 + m^2 c^4 \tag{12}$$

for zero rest mass: $E^2 = p^2 c^2 \rightarrow E = pc$ $\tag{13}$

$$hv = h\frac{c}{\lambda} = pc \tag{14}$$

$$\therefore p = \frac{h}{\lambda} \tag{15}$$

1.4 Electron diffraction

$$E_K = eV - \frac{p^2}{2m} \tag{16}$$

$$p = \sqrt{2meV} \tag{17}$$

$$\lambda = \frac{h}{\sqrt{2meV}} \tag{18}$$

$$\lambda = 2d\sin(\theta) \tag{19}$$

$$\sin^2(\theta) = \frac{C}{V}, \text{ Where } C = \frac{h^2}{8med^2} \tag{20}$$

1.5 Bohr Model

$$F_{centripedal} = F_{electric} \tag{21}$$

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \tag{22}$$

$$\therefore v^2 = \frac{e^2}{4\pi\epsilon_0 mr} \tag{23}$$

$$I_{orbit} = n\lambda = 2\pi r \text{ Where n is the quantisation condition} \tag{24}$$

$$\therefore v = \frac{hn}{2\pi mr} \tag{25}$$

$$L = mvr = n\frac{h}{2\pi} = n\hbar \tag{26}$$

As such, allowed radii are described by the expression: $\tag{27}$

$$r_n = \frac{h^2\epsilon_0 n^2}{\pi me^2} = a_{Bohr}n^2 \tag{28}$$

$$r_1 = a_{Bohr} = \frac{h^2\epsilon_0}{\pi me^2} = 5.3 \times 10^{-11}m \tag{29}$$

$$E_k = \frac{1}{2}mv^2 = \frac{e^2}{8\pi\epsilon_0 r} \tag{30}$$

$$E_T = E_k + E_c = \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r^2} = -\frac{e^2}{8\pi\epsilon_0 r} \tag{31}$$

Substiting in r_n gives: $\tag{32}$

$$E_T = -\left(\frac{me^4}{8\epsilon_0^2 h^2}\right) \cdot \frac{1}{n^2} = \frac{-13.6eV}{n^2}, \ 1 \ eV \approx 1.602 \times 10^{-19}J \tag{33}$$

$$\Delta E = E_i - E_f = \frac{me^4}{8\epsilon_0^2 h^2}(\frac{1}{n_f^2} - \frac{1}{n_i^2}) \tag{34}$$

since: $E = hv = h\frac{c}{\lambda}$ $\tag{35}$

$$\frac{1}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \tag{36}$$

1.6   Waves

$$\Psi = Ae^{i(kx-\omega t)} \tag{37}$$

$$k = 2\pi/\lambda \tag{38}$$

$$\omega = 2\pi v \tag{39}$$

$$c = v\lambda = \frac{\omega}{2\pi} \cdot \lambda = \frac{\omega}{\lambda} \tag{40}$$

$$P(x) \propto |\Psi|^2 dx \tag{41}$$

$$\frac{\partial \Psi}{\partial x} = ikAe^{i(kx-\omega t)} = ik\Psi \tag{42}$$

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = i\omega\Psi \tag{43}$$

$$\text{De Broglie: } p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k \tag{44}$$

$$\text{Enstein: } E = hv = h\frac{\omega}{2\pi} = \hbar\omega \tag{45}$$

$$\frac{\partial}{\partial x}\Psi = i\frac{p}{\hbar}\Psi \Rightarrow p\Psi = \{-i\hbar\frac{\partial}{\partial x}\}\Psi \tag{46}$$

$$\frac{\partial}{\partial t}\Psi = -i\frac{E}{\hbar}\Psi \Rightarrow E\Psi = \{i\hbar\frac{\partial}{\partial t}\}\Psi \tag{47}$$

$$\Delta t = \frac{1}{\Delta f} = \frac{h}{\Delta E} \Rightarrow \Delta E \cdot \Delta t \geq h \tag{48}$$

$$\Delta x = \Delta\lambda_{dB} = \frac{h}{\Delta p} \Rightarrow \Delta x \cdot \Delta p \geq h \tag{49}$$

Heisenber's Uncertainty Principle:

It is impossible to specify simultaneously, with precision, both the momentum and the position of a particle.

1.7   Shrodinger's Equation Derivation

$$E = E_k + E_p = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V \tag{50}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V\Psi(x,t) \tag{51}$$

1.8 Time independent Shrodinger's Equation

$$\Psi(x,t) = \phi(t)\psi(t) \tag{52}$$

$$i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V \tag{53}$$

$$\therefore \ i\frac{A}{\hbar}\phi = \frac{\partial\phi(t)}{\partial t} \tag{54}$$

$$\phi(t) = Ce^{-i(\frac{A}{\hbar})t} \Rightarrow \frac{d\phi(t)}{dt} = -i(\frac{A}{\hbar})Ce^{-i(\frac{A}{\hbar})t} \tag{55}$$

By unit analysis: $A = E$ \hfill (56)

$$\therefore \ E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi \tag{57}$$

1.9 Electron in a box

$$V(0) = V(L) = \inf \tag{58}$$

$$V(x) = 0 \ \forall \, x \,|\, 0 < x < L \tag{59}$$

$$\therefore \ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{60}$$

General Solution: $\psi = A\sin(kx) + B\cos(kx)$ \hfill (61)

$$\frac{d^2\psi}{dx^2} = -k^2(A\sin(kx)) + B\cos(kx)) = -k^2\psi \tag{62}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \left(-\frac{\hbar^2}{2m}\right)\cdot(-k^2\psi) = E\psi \tag{63}$$

$$E = \frac{\hbar^2 k^2}{2m} \tag{64}$$

Applying boundary conditions: \hfill (65)

$$\psi(0) = 0 \Rightarrow B = 0 \tag{66}$$

$$\psi(L) = 0 \Rightarrow A = 0 \ or \ \sin(kL) = 0 \tag{67}$$

$$\therefore kL = n\pi, \ n = 1, 2, 3... \tag{68}$$

$$\psi_n = A\sin(\frac{n\pi x}{L}) \tag{69}$$

$$E_n = \frac{h^2}{8mL^2}\cdot n^2 \tag{70}$$

$$1 = \int_0^L A^2\sin^2(\frac{n\pi x}{L})dx \Rightarrow A = \sqrt{\frac{2}{L}} \tag{71}$$

$$\psi_n = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}) \tag{72}$$

$$P_n(x) = \frac{2}{L}\sin^2(\frac{n\pi x}{L})dx \tag{73}$$

1.10   3D

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)\psi + V\psi = E\psi \tag{74}$$

$$\nabla = \left(\frac{d}{dx}+\frac{d}{dy}+\frac{d}{dz}\right) \tag{75}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{76}$$

There are 3 spacial degrees of freedom and 1 spin degree of freedom, therefore there are 4 quantum numbers

n = Principle quantum numbers, $\{n \,|\, n \in \mathbb{N}\}$

ℓ = Orbital quantum number $\{\ell \,|\, 0 \le \ell \le n-1,\ \ell \in \mathbb{W}\}$

m_ℓ = Magnetic quantum number $\{m_\ell \,|\, -\ell \le m_\ell \le \ell,\ m_\ell \in \mathbb{Z}\}$

m_s = Spin quantum number $\{m_s \,|\, m_s \in \{\frac{1}{2}, -\frac{1}{2}\}\}$

2   Bonding and Crystaline Structure

Bond	Action with Charges	ΔE	E_{avg}	Bond Energy
Ionic	Exchange	High	Low	Large
Covalent	Sharing	Low	High	Variable
Metalic	Delocalized Sharing	Low	Low	Variable

2.1   I don't have a good title yet

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n} \tag{77}$$

$$ionic\ character = 1 - e^{-\frac{(X_A - X_B)^2}{4}} \tag{78}$$

$$\frac{\Delta L}{L_0} = \alpha\,(T_2 - T_1) \tag{79}$$

$$APF = \frac{n_a \cdot \frac{4}{3}\pi r_a^3}{a^3} \tag{80}$$

Structure	Coordination Number	Atoms/unit cell	APF
Simple Cubic	6	8	0.52
Body Centered Cubic (BCC)	8	2	.68
Face Centered Cubic	12	4	.74

2.2   Some densities

$$\rho = \frac{nA}{V_c N_a} \tag{81}$$

$$LD = \frac{n_a}{r} \tag{82}$$