NME 220 Molecular and Nanoscale Principles

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Intro to NME

| Driving forces and potentials

Description	Equations
Avogadro's number (Critical parameter of amount of particles to resist fluctuations)	$N_A = 6.02 \times 10^{23}\ \mathrm{mol}^{-1}$
Fick's law $\vec{J}_{AB}\ [\mathrm{mol}/(\mathrm{m}^2\mathrm{s})]$ - diffusive flux $D_{AB}\ [\mathrm{m}^2/\mathrm{s}]$ - binary diffusion coefficient ∇c_A - concentration gradient	$\vec{J}_{AB} = -D_{AB}\nabla c_A$

| Scaling laws

Description	Equations
Power density of engines	$\frac{P}{V} = \frac{Fv}{V}$
Scaling law of power density	$\frac{P}{V} \propto \frac{1}{L}$
Terminal velocity of droplets	$v_t = \frac{2gr^2(\rho_{\mathrm{sphere}} - \rho_{\mathrm{air}})}{9\eta}$
Scaling law of terminal velocity	$v_t \propto L^2$

| Electric transport properties

Description	Equations
Bohr's radius (Critical length scale parameter for discrete excited electronic states)	$a_0 = \frac{4\pi\varepsilon_0(\frac{h}{2\pi})^2}{m_e e^2}$
Ohm's law $\vec{J}$ - electric current density (flux) $\sigma\ [\mathrm{Sm}^{-1}]$ - electric conductivity ∇V - electric potential gradient	$\vec{J} = \sigma\nabla V$
Ohm's law $G_e\ [\mathrm{S} = \Omega^{-1}]$ - electric conductance	$G_e = \frac{1}{R} = \frac{I}{V}$
Mean free path	$\lambda = \frac{k_B T}{\sqrt{2}\pi P d^2}$
Drude model Microscopic description - electric conductivity in 3D σ - electric conductivity λ - mean free path $\overline{c}$ - mean electron gas velocity	$\sigma = \frac{\lambda e^2 n\overline{c}}{6k_B T}$

Description	Equations
Electric conductivity in 1D N_e - transmission probability, # of electronic states (modes) at Fermi level L - length of conuctor	$\sigma = \frac{2e^2 N_e}{hL}$
Electric conductance in 3D	$G_e = \frac{\lambda e^2 n \bar{c}}{6 k_B T} \frac{A}{L} \propto \frac{1}{L}$
Electric conductance in 1D	$G_e = \frac{2e^2}{h} N_e$

Thermo transport properties

Description	Equations
Volumetric heat capacity at constant pressure	$C_V = \rho c_P$
Thermal diffusivity	$\alpha = \frac{k_c}{C_V} = \frac{k_c}{\rho c_P}$
Fourier's law $\vec{q}\ [\mathrm{W m^{-2}}]$ - heat flux $k_c\ [\mathrm{W m^{-1} K^{-1}}]$ - thermal conductivity ∇T - temperature gradient	$\vec{q} = -k_c \nabla T$
Fourier's law $\vec{J}$ - heat flux (?) α - thermal diffusivity ∇T - temperature gradient	$\vec{J} = \frac{\vec{q}}{C_V} = -\alpha \nabla T$
Microscopic description	$k_c = \frac{1}{2} n \bar{c} \lambda k_B$
Thermal conductance in 3D	$G_{th} = k_c \frac{A}{L} \propto \frac{1}{L}$
Thermal conductance in 1D N_{ph} - # of phonons	$G_{th} = \frac{\pi^2 k_B^2 T}{3h} N_{ph}$

Miniaturization effect on surface energy and strain

Description	Equations
Surface stress $\gamma\ [\mathrm{J m^{-2}}]$ - surface energy per area of solid $\gamma\ [\mathrm{F/m}]$ - surface tension of liquid ε - strain $\frac{\partial \gamma}{\partial \varepsilon}$ - stored mechanical energy in solid $(\frac{\partial \gamma}{\partial \varepsilon} = 0)$ for liquid	$f = \gamma + \frac{\partial \gamma}{\partial \varepsilon}$
Surface energy/tension	$\gamma = E_{\text{coh, surface}} - E_{\text{coh, inside}}$
Isotropic pressure f - surface stress D - diameter of particle	$P = \frac{4f}{D}$
Scaling law of elastic strain ε - strain K - bulk modulus	$\varepsilon = -\frac{P}{3K} = -\frac{4}{3} \frac{f}{K} \frac{1}{D} \propto \frac{1}{D}$

Atomic Theory of Matter

Blackbody radiation

Description	Equations
Wein's displacement law $\lambda_{\max}$ - maximum of irradiation spectrum	$\lambda_{\max} T = 2.898 \times 10^{-3}\ \mathrm{m \cdot K}$
Stefan-Boltzmann law $I\ [\mathrm{Wm^{-2}}]$ - radiation power $I_\lambda\ [\mathrm{Wm^{-3}}]$ - spectral irradiation ε - emissivity σ - Stefan-Boltzmann constant	$I = \int_0^\infty I_\lambda \, d\lambda = \varepsilon \sigma T^4$ $(\sigma = 5.67 \times 10^{-8}\ \mathrm{Wm^{-2}K^{-4}})$
Radiation power	$P = IA$
Rayleigh-Jeans' average mode energy of photon	$\langle E \rangle = \frac{1}{2} k_B T$
Rayleigh-Jeans radiation law k_B - Boltzmann's constant	$I_\lambda(\lambda) = \dfrac{2\pi c k_B T}{\lambda^4}$ $I_\nu(\nu) = \dfrac{8\pi \nu^2 k_B T}{c^3}$
Planck's average mode energy of photon	$\langle E \rangle = \dfrac{h\nu}{e^{h\nu / k_B T} - 1}$
Planck's radiation law u - energy density	$u_\lambda(\lambda) = \dfrac{8\pi h c}{\lambda^5} \dfrac{1}{e^{hc/\lambda k_B T} - 1}$ $u_\nu(\nu) = \dfrac{8\pi h \nu^3}{c^3} \dfrac{1}{e^{h\nu / k_B T} - 1}$
Planck's law confirms Stefan-Boltzmann law I - radiation intensity σ - Stefan-Boltzmann constant	$I(\nu) = \sigma T^4$ $\sigma = \dfrac{2\pi^5 k_B^4}{15 c^2 h^3}$
Energy of an EM mode	$E_n = nh\nu$

Photoelectric effect

Description	Equations
Energy of a photon	$\Delta E = h\nu$
Work function f a metal	$\Phi = e\phi$
Photoelectric effect	$E_k = h\nu - e\phi$
Condition for moving free electrons excited by photon	$h\nu \geq e\phi$
Mass-energy equivalence	$E = mc^2$

Wave-particle duality

Description	Equations
Classical linear momentum	$p = mv = \sqrt{2mE}$
Photon linear momentum	$p = \dfrac{h\nu}{c} = \dfrac{h}{\lambda}$
de Broglie wavelength of particle	$\lambda = \dfrac{h}{mv} = \dfrac{h}{\sqrt{2mE_k}}$

Description	Equations
Davisson-Germer experiment (electron diffraction constructive interference)	$n\lambda = 2d\sin\theta$
Bragg's law	$\frac{1}{\lambda} = \frac{n}{2d\sin\theta}$
Bragg-de Broglie relation	$\frac{1}{\lambda} = \begin{cases} \frac{n}{2d\sin\theta} \\ \frac{p}{h} = \frac{\sqrt{2mE}}{h} \end{cases}$

Atomic Model

| Bohr's model of atoms

Description	Equations
Rydberg formula Emission lines of hydrogen R_H - Rydberg constant $n_1 = 1, 2, 3, \dots$ $n_2 > n_1$	$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$ $R_H = 1.097 \times 10^7\ \mathrm{m}^{-1}$
Quantization condition of Bohr's model $n = 1, 2, 3, \dots$ λ - wavelength of electron r - radius of stable shell	$2\pi r = n\lambda$
Energy of electron in each shell $n = 1, 2, 3, \dots$	$E_n = \frac{-m_e e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2}$
Emission and absorption of H atom Emission - $j > 1$ Absorption - $i > j$	$h\nu = \Delta E$ $= -\frac{m_e e^4}{8\varepsilon_0^2 h^2}\left(\frac{1}{n_j^2} - \frac{1}{n_i^2}\right)$ $= -13.6\ \mathrm{eV}\left(\frac{1}{n_j^2} - \frac{1}{n_i^2}\right)$
Reduced mass	$\mu = \frac{m_e m_p}{m_e + m_p}$
Planck's constant	$\hbar = \frac{h}{2\pi}$
Rydberg's constant	$R_H = R_\infty\frac{\mu}{m_e} = \frac{\mu e^4}{8\varepsilon_0^2 h^3 c}$
Bohr radius	$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} \approx 0.053\ \mathrm{nm}$
Reduced Bohr radius	$a_0^* = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2} \approx 0.053\ \mathrm{nm}$
Ionization energy of electron from ground state	$E_I = \frac{-\mu e^4}{8\varepsilon_0^2 h^2} = -13.6\ \mathrm{eV}$

| Dispersion relations

Description	Equations
Wave equation of traveling wave	$u(x,t) = A\sin(kx - \omega t + \phi)$

Description	Equations
Wave number	$k = \frac{2\pi}{\lambda}$
Angular frequency	$\omega = 2\pi\nu = \frac{2\pi}{\lambda}c = kc$
Period	$T = \frac{1}{\nu} = \frac{\lambda}{c}$
Dispersion relation of EM wave	$\omega(k) = ck$
Dispersion relation of particle wave	$\omega(k) = \frac{\hbar}{2m}k^2$

Single slit experiment

Description	Equations
Variables	a - width of the slit L - distance between slit and screen p - integer destructive interference # $p = \pm 1, \pm 2, \pm 3, \dots$
Destructive interference	$\phi = p\lambda = a\sin\theta$
Constructive interference	$\phi = (p + \frac{1}{2})\lambda = a\sin\theta$
Location of destructive interference	$y_p = p\frac{\lambda L}{a}$
Location of constructive interference	$y_p = (p + \frac{1}{2})\frac{\lambda L}{a}$

Double slit experiment

Description	Equations
Variables	δ - path difference of two diffracting waves d - distance between two slits L - distance between slit and screen m - integer constructive interference # $m = 0, \pm 1, \pm 2, \pm 3, \dots$
Constructive interference	$\delta = m\lambda = d\sin\theta$
Destructive interference	$\delta = (m + \frac{1}{2})\lambda = d\sin\theta$
Location of constructive interference	$y_m = m\frac{\lambda L}{d}$
Location of destructive interference	$y_m = (m + \frac{1}{2})\frac{\lambda L}{d}$
Intensity of macroscopic particle and quantum particle with observation	$I = I_1 + I_2$
Intensity of wave and quantum particle	$I = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos\delta$

Heisenberg uncertainty principle

Description	Equations

Description	Equations
Heisenberg uncertainty principle position-momentum form	$\Delta x \Delta p \geq \frac{\hbar}{2}$
Heisenberg uncertainty principle energy-time form	$\Delta E \Delta t \geq \frac{\hbar}{2}$
Macroscopicity	$10^{\mu} \propto \frac{\tau_p}{\tau_e}$

Wave Function

The Schrodinger equation

Description	Equations
Wave function	$\Psi(x,t) = \Psi_0 e^{i(kx-\omega t)}$
Wave function as probability density	$P = \lvert\Psi(x)\rvert^2$
Linear momentum operator	$\hat{p_x} = -i\hbar\frac{\partial}{\partial x} \implies p_x$ as eigenvalue
Time operator	$\hat{t} = -i\hbar\frac{\partial}{\partial t} \implies E$ as eigenvalue
Hamiltonian operator	$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \implies E$ as eigenvalue
Time-dependent wave equation for free particle	$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)$
Time-dependent Schrodinger equation (particle with potential constraint)	$i\hbar\frac{\partial}{\partial t}\Psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi$
Time-independent Schrodinger equation	$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi = E\psi$
Time-independent Schrodinger equation (operator form)	$\hat{H}\psi = E\psi$

Particle in infinite 1D box

Description	Equations
Potential function	$V(x) = \begin{cases} 0 & (0, L) \\ \infty & (-\infty, 0) \cup (L, \infty) \end{cases}$
SE inside the box	$\frac{d^2\psi}{dx^2} + k^2\psi = 0$
General solution	$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$
Quantized wave number	$k_n = \frac{n\pi}{L}$
Quantized momentum	$p_n = \hbar k_n = \frac{n\pi\hbar}{L}$
Quantized energy level	$E_n = \frac{p_n^2}{2m} = \frac{(n\pi\hbar)^2}{2mL^2} = n^2 E_1$

Quantum structures

Description	Equations

Description	Equations
General continuous energy spectrum in non-confined dimensions	$E_i = \frac{\hbar^2 k_i^2}{2m}$
General discrete energy spectrum in confined dimension	$E_{n_i} = \frac{\hbar^2 \pi^2}{2mL^2} n_i^2$
Total energy	$E = E_x + E_y + E_z$
General wave function	$\psi_{n_x}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_x \pi x}{L}\right)$

| The hydrogen atom

Description	Equations
Potential function	$V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$
Energy level of electrons in H atom	$E_n = \frac{-m_e e^4}{8\varepsilon_0^2 h^2} \frac{1}{n^2}$
Wave function of electrons in H atom	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
Principle quantum number	$n = 1, 2, 3, \ldots$
Orbital (angular momentum) quantum number	$l = 0, 1, 2, \ldots, n-1$
Magnetic quantum number	$m_l = -l, \ldots, -1, 0, 1, \ldots, l$
Spin quantum number	$m_s = \frac{1}{2}, -\frac{1}{2}$

Nanoscience & Technology

| Electron transport through 1D quantum wire

Description	Equations
Variables	μ - electrochemical potential of electrode M - mode number (single node: $M = 1$) S - source; D - drain
Electrochemical potential difference between source and drain	$eV_{\text{bias}} = \mu_S - \mu_D$
Current in 1D quantum wire (single mode)	$I = \frac{2q}{h}(\mu_S - \mu_D) = \frac{2q^2}{h} V_{\text{bias}}$
Quantum conductance (single mode)	$G_Q = \frac{2q^2}{h} \approx 7.75 \times 10^{-5}\ \text{S}$
Quantum resistance (single mode)	$R = \frac{h}{2q^2} \approx 12.9\ \text{k}\Omega$
Current in 1D quantum wire (multi-mode)	$I = \frac{2qM}{h}(\mu_S - \mu_D) = \frac{2q^2 M}{h} V_{\text{bias}}$
Quantum conductance (multi-mode)	$G_Q = \frac{2q^2 M}{h}$
Quantum resistance (multi-mode)	$R = \frac{h}{2q^2 M}$

Particle in finite 1D box

Description	Equations
Finite potential	$V(x) = \begin{cases} V & (-\infty, 0) \cup (L, \infty) \\ 0 & (0, L) \end{cases}$
Wave number	$k = \sqrt{\frac{2mE}{\hbar^2}}$
Modified wave number	$k' = \sqrt{\frac{2m}{\hbar^2}(V - E)}$
Wave function on the left	$\psi_1(x) = C_1 e^{ik'x}$
Wave function in the middle	$\psi_2(x) = A_1 \sin(kx) + A_2 \cos(kx)$
Wave function on the right	$\psi_3(x) = C_2 e^{-ik'x}$

Tunneling effect

Description	Equations
Wave number	$k = \sqrt{\frac{2mE}{\hbar^2}}$
Modified wave number	$k' = \sqrt{\frac{2m}{\hbar^2}(V - E)}$
Wave function on the left	$\psi_1(x) = \psi_{\text{incid}}(x) + \psi_{\text{refl}}(x)$ $\psi_{\text{incid}}(x) = Ae^{ikx}$ $\psi_{\text{refl}}(x) = Be^{-ikx}$
Wave function in the barrier	$\psi_2(x) = Ce^{ik'x} + De^{-ik'x}$
Wave function on the right	$\psi_3(x) = \psi_{\text{trans}}(x) = Fe^{ikx}$
Transmission probability	$T(L, V, E) = \frac{\lvert\psi_{\text{trans}}(x)\rvert^2}{\lvert\psi_{\text{incid}}(x)\rvert^2}$ $\approx 16\frac{E}{V}\left(1 - \frac{E}{V}\right)e^{-k'L}$ $\approx \frac{1}{2}e^{2k'L}$
Work function with trapezoidal approximation at junction	$\Phi = \frac{1}{2}(\Phi_1 + \Phi_2 - \lvert eV_{\text{bias}}\rvert)$
Tunnel current $D_s(E_F)$ - density of states at Fermi level	$I_t \propto V_{\text{bias}} D_s(E_F) \exp\left(-\sqrt{\frac{8m}{\hbar^2}(\Phi - E)}L\right)$

Energy discretization of nanoparticles

Description	Equations
Spacing between energy levels	$\Delta E = \frac{4}{3}\frac{E_F}{N_e}$
Energy level and thermal noise	$\Delta E \begin{cases} \ll k_B T & \text{not quant. confined, continuous} \\ > k_B T & \text{quant. confined, discrete} \end{cases}$
Conductor-insulator classification	$\Delta E = \frac{4}{3}\frac{E_F}{N_e} = k_B T$

Description	Equations
Number of electrons that can have discrete energy level	$N_e < \frac{4}{3}\frac{E_f}{k_B T}$

Single electron box

Description	Equations
Variables	t - tunnel; g - gate; c - charging
Total capacitance	$C_{\text{dot}} = C = C_t + C_G$
Gate voltage	$V_G = \frac{q_1}{C_t} + \frac{q_2}{C_G}$
System energy	$E_{\text{sys}} = \frac{q_1^2}{2C_t} + \frac{q_2^2}{2C_G}$
Charging energy	$E_c = \frac{e^2}{2C}$
Quantum kinetic energy V - volume of QD $D_s(E)$ - density of states	$E_k = \frac{1}{VD_s(E_F)}$
Electron addition energy	$E_a = E_c + E_k$
Thermal noise requirement of single electron box (Coulomb blockade)	$E_c \gg k_B T$ $E_c > 10 k_B T$
Quantum noise requirement of single electron box	$R_t \gg \frac{h}{e^2} \approx 25.8\text{k}\Omega$
RC time constant	$\tau = R_t C$
Gibbs free energy	$\mathcal{F} = H - TS$
Gibbs free energy at equilibrium (Coulomb parabola potential)	$\mathcal{F}(n, V_G) = \frac{(C_G V_G - ne)^2}{2C} \propto V_G^2$
Coulomb parabola potential conditions	$\mathcal{F} = \begin{cases} 0 & \text{if } C_G V_G = ne \\ E_c & \text{if } C_G V_G = (n+1)e \end{cases}$
Capacitance of quantum dots d - diameter	$C_{\text{dot}} = G\varepsilon\varepsilon_0 d$
Geometric factor	$G = \begin{cases} 2\pi & \text{sphere} \\ 4 & \text{disc} \end{cases}$

Single electron transistor

Description	Equations
Charging energy	$E_c = \frac{e^2}{2C_{\text{dot}}}$
Charging energy Q_0 - polarization charge ne - uncompensated electrons	$E_c = \frac{(Q_0 - ne)^2}{2C_{\text{dot}}}$
Charging voltage	$V_g = \frac{E_c}{e} = \frac{e}{2C_{\text{dot}}}$

Description	Equations
Capacitance of quantum dot	$C_{\text{dot}} = C_{t_1} + C_{t_2} + C_G$

Electronic Structure of Molecules

The hydrogen atom (revisited)

Description	Equations
Potential function	$V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$
Energy level of electrons in H atom	$E_n = \frac{-m_e e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} = -13.6\ \text{eV}\frac{1}{n^2}$
Bohr radius	$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} \approx 0.053\ \text{nm}$
Wave function	$\psi(\mathbf{r}) = R(r)Y(\theta,\phi)$
Angular component of wave function	$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$
Wave function in ground state	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
Wave function in $n,0,0$ state	$\psi_{n00} = \frac{R_n(r)}{\sqrt{4\pi}}$
Probability density function	$\rho_{nlm} = \lvert\psi_{nlm}\rvert^2 = \psi\psi^*$
Radial probability density	$P_{nl}(r) = \lvert R_{nl}\rvert^2 r^2$
Number of radial nodes	$n - l - 1$

Angular momentum

Description	Equations
Angular momentum operator in z direction	$\hat{L}_z = i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$
Orbital angular momentum in z direction	$L_z = m_l\hbar$
Angular momentum magnitude operator	$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$
Orbital angular momentum	$L = \hbar\sqrt{l(l+1)}$
Spin angular momentum in z direction	$S_z = m_s\hbar$
Spin angular momentum	$S = \hbar\sqrt{s(s+1)}$
Total angular momentum in z direction	$J_z = m_j\hbar$
Total angular momentum	$J = \hbar\sqrt{j(j+1)}$
spin angular momentum quantum number	$s = \frac{1}{2}, m_s = \pm\frac{1}{2}$
Spin-orbit coupling	$j = l \pm s$
Energy degeneracy considering spin	$2n^2$

Bonding in molecules

Description	Equations
Bonding (symmetric linear combination)	$\psi_g = \psi_1 + \psi_2$
Anti-bonding (asymmetric linear combination)	$\psi_u = \psi_1 - \psi_2$

Electronic states

Note: the mass here are electron mass.

Description	Equations
Fermi-Dirac distribution	$f(E) = \dfrac{1}{\exp\left(\dfrac{E - E_f}{k_B T}\right) + 1}$
Fermi energy in 3D at 0 K	$E_F = \dfrac{\hbar^2 k_F^2}{2m} = \dfrac{\hbar^2}{2m}\left(3\pi^2 n_e\right)^{2/3}$
Fermi wave number in 3D at 0 K	$k_F = \frac{1}{\hbar}\sqrt{2mE_F} = \left(3\pi^2 n_e\right)^{1/3}$
Fermi velocity approximation in 3D	$v_F = \dfrac{\hbar k_F}{m} = \dfrac{\hbar}{m}(3\pi^2 n_e)^{1/3}$
Wavelength in 3D at 0 K	$\lambda_F = \dfrac{2\pi\hbar}{m v_F}$
Density of states (general)	$D_s(E) = \dfrac{dN}{dE}\dfrac{1}{V}$
Density of states in 3D at 0 K	$D_s^{\mathrm{3D}}(E) = \dfrac{8\sqrt{2}\pi m^{3/2}}{h^3}\sqrt{E}$
Density of states in 2D at 0 K $(0 < E < E_1)$	$D_s^{\mathrm{2D}}(E) = \dfrac{4\pi m}{h^2}$
Density of states in 1D at 0 K	$D_s^{\mathrm{1D}}(E) = \dfrac{\sqrt{2m}}{h}\dfrac{1}{\sqrt{E}}$
Density of states in 0D at 0 K	$D_s^{\mathrm{0D}}(E) = 2$
Number density of electron (general)	$n_e(E) = \dfrac{N}{V} = \displaystyle\int_0^\infty f(E)D(E)\,dE$
Number density of electron in 3D at 0 K	$n_e^{\mathrm{3D}} = \dfrac{16\sqrt{2}\pi m^{3/2}}{3h^3}E_F^{3/2}$
Number density of electron in 2D at 0 K	$n_e^{\mathrm{2D}} = \dfrac{4\pi m}{h^2}E_F$
Number density of electron in 1D at 0 K	$n_e^{\mathrm{1D}} = \dfrac{2\sqrt{2m}}{h}\sqrt{E_F}$
Number density of electron in 0D at 0 K	$n_e^{\mathrm{0D}} = 2E_F$

Semiconductor carriers

Description	Equations
Band gap	$E_g = E_c - E_v$
Density of state of electrons (conduction band)	$D_c(E) = \dfrac{8\sqrt{2}\pi m_e^{*3/2}}{h^3}\sqrt{E - E_c}$
Density of state of holes (valance band)	$D_v(E) = \dfrac{8\sqrt{2}\pi m_h^{*3/2}}{h^3}\sqrt{E_v - E}$

Description	Equations
Fermi-Dirac distribution for electrons	$f(E) = \frac{1}{1 + \exp(\frac{E - E_F}{k_B T})}$
Fermi-Dirac distribution for holes	$1 - f(E)$
Boltzmann approximation	$E - E_F \gg k_B T$
Effective density of state of electrons in 3D	$N_c^{\mathrm{3D}} = N_{e,\mathrm{eff}} = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}$
Effective density of state of holes in 3D	$N_v^{\mathrm{3D}} = N_{h,\mathrm{eff}} = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2}$
Effective density of state in 2D (use appropriate mass)	$N^{\mathrm{2D}} = \frac{m^* k_B T}{\pi \hbar^2}$
Effective density of state in 1D (use appropriate mass)	$N^{\mathrm{1D}} = \sqrt{\frac{m^* k_B T}{2\pi \hbar^2}}$
Effective density of state in 0D (use appropriate mass)	$N^{\mathrm{0D}} = 2$
Electron (carrier) density	$n_e(E) \approx N_{e,\mathrm{eff}} \exp\left(-\frac{E_c - E_F}{k_B T}\right)$
Hole (carrier) density	$n_h(E) \approx N_{h,\mathrm{eff}} \exp\left(-\frac{E_v - E_F}{k_B T}\right)$
Intrinsic carrier density	$n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2k_B T}\right)$
Exciton separation distance	$a_{\mathrm{ex}} = a_0 \frac{\varepsilon}{m_{\mathrm{ex}}/m_e}$

Semiconductor doping

Description	Equations
Variables	oc - open circuit bi - built-in sc - short circuit
Solar cell conductivity μ - electron mobility	$K \propto \mu n_i$
Open-circuit voltage (p-n solar cells) N_a - donor atom concentration Δn - excess electrons generated by photons (photocurrent) $q = e$ - elementary charge	$V_{\mathrm{oc}} = \frac{E_{\mathrm{HL}}}{q} = \frac{E_{F_n} - E_{F_p}}{q} = \frac{k_B T}{q} \ln\left(\frac{(N_a + \Delta n)\Delta n}{n_i^2}\right) \approx \frac{k_B T}{q} \ln\left(\frac{I_{ph}}{I_0}\right)$
Built-in voltage (p-n diode)	$V_{\mathrm{bi}} = \frac{E_{F_n} - E_{F_p}}{q} = \frac{k_B T}{q} \ln\left(\frac{N_a N_d}{n_i^2}\right)$
Relationship between open circuit and built-in voltages	$V_{\mathrm{oc}} < V_{\mathrm{bi}}$ $V_{\mathrm{bi}} = V_{\mathrm{oc}} + \frac{2k_B T}{q}$

Description	Equations
Depletion width	$w = \sqrt{\frac{2\varepsilon_r\varepsilon_0(N_a+N_d)}{qN_aN_d}V_{\text{eff}}}$
Fill factor	$\text{FF} = \frac{P_{\max}}{V_{\text{oc}}I_{\text{sc}}}$
Efficiency	$\eta = \frac{P_{\max}}{P_{\text{in}}} = \frac{(\text{FF})V_{\text{oc}}I_{\text{sc}}}{P_{\text{in}}}$

Molecular Modes and Energetic Properties

Energy: Electronic $\gg$ Vibrational $\gg$ Rotational $\gg$ Thermal noise (k_BT) $\gg$ Translational

| Vibration modes of diatomic molecules

Description	Equations
Spring potential	$V(x) = \frac{1}{2}k_sx^2$
Frequency of quantum harmonic oscillator $m_1 \gg m_2 = m$	$\nu = \frac{1}{2\pi}\sqrt{\frac{k_s}{m}}$
Energy levels of quantum harmonic oscillators	$E_n = (n+\frac{1}{2})h\nu$ $n = 0, 1, 2, \dots$
Zero-point energy	$E_0 = \frac{1}{2}h\nu$
Equidistant energy levels	$\Delta E_{\text{vib}} = h\nu_{\text{vib}}$
Reduced mass	$\mu = \frac{m_1m_2}{m_1+m_2}$
Frequency of quantum harmonic oscillator m_1 m_2	$\nu = c\tilde{\nu} = \frac{1}{2\pi}\sqrt{\frac{k_s}{\mu}}$
Vibrational wave number of quantum harmonic oscillator	$\tilde{\nu} = \frac{1}{\lambda} = \frac{1}{2\pi c}\sqrt{\frac{k_s}{\mu}}$
Wave number of quantum harmonic oscillator	$k_\lambda = \frac{2\pi}{\lambda} = \frac{1}{c}\sqrt{\frac{k_s}{\mu}}$
Dissociation energy D_e and actual dissociation energy D_0	$D_0 = D_e + \frac{1}{2}h\nu$
Morse potential r_e - equilibrium position, bond length a - inverse width of Morse potential	$V(r) = D_e(1-e^{-a(r-r_e)})^2$ $a = \sqrt{\frac{k_s}{2D_e}} = \omega\sqrt{\frac{\mu}{2D_e}}$
Vibrational temperature	$\Theta_{\text{vib}} = \frac{h\nu}{k_B}$
Vibrational energy	$E_{\text{vib}} = k_B\Theta_{\text{vib}}$

| Rotational modes of diatomic molecules

Description	Equations
Angular velocity (frequency)	$\omega = 2\pi\nu$
Linear velocity	$v_i = r_i\omega$
Moment of inertia	$I = m_1r_1^2 + m_2r_2^2 = \mu R^2$

Description	Equations
Kinetic energy of rigid rotor	$E_k = \frac{1}{2} I \omega^2$
Rotational constant	$B = \frac{\hbar^2}{2I}$ $\tilde{B} = \frac{B}{hc} = \frac{h}{8\pi^2 cI}\ [\mathrm{cm}^{-1}]$
Rotational temperature	$\Theta_{\mathrm{rot}} = \frac{B}{k_B} = \frac{\hbar^2}{2Ik_B}$
Rotational energy	$E_{\mathrm{rot}} = k_B \Theta_{\mathrm{rot}}$
Energy of rigid rotor	$E_J = J(J+1)\frac{\hbar^2}{2I}$ $= J(J+1)B$ $= J(J+1)k_B\Theta_{\mathrm{rot}}$
Probability of being in a particular rotational energy state	$f_J = (2J+1)\exp(-J(J+1)\Theta_{\mathrm{rot}}/T)$
Energy for absorption	$\Delta E_{\mathrm{rot}}^{J\to J-1} = 2B(J+1)$
Energy for emission	$\Delta E_{\mathrm{rot}}^{J\to J+1} = 2BJ$
Separation between transitions	$\Delta(\Delta E_{\mathrm{rot}}^{J\to J-1}) = \Delta(\Delta E_{\mathrm{rot}}^{J\to J+1}) = 2B$
Non-degenerate translational energy level in 1D	$E_n^{\mathrm{1D}} = \frac{n^2h^2}{2mL^2}$
Non-degenerate translational energy level in 3D	$E_n^{\mathrm{3D}} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$

Polyatomic molecules

Degree of freedom	Linear molecule with n atoms	Nonlinear molecule with n atoms
Translational	3	3
Rotational	2	3
Vibrational	$3n-5$	$3n-6$

Description	Equations
Intensity of IR vibrational signal	$I_{\mathrm{IR}} \propto \left(\frac{du_D}{d\xi}\right)^2$
Rotational motion energy	$E_J = \frac{J(J+1)\hbar^2}{2I}$ $J = 0, 1, 2, \dots$
Degeneracy of rotational motion energy	$g_J = 2J+1$
Moment of inertia	$I = \sum_{i=1}^{n} m_i(x_i - x_{cm})^2$

Lattice vibration and phonon

Description	Equations

Description	Equations
Harmonic potential	$V(r_i - r_j) = \sum_{i,j} \frac{1}{2} m\omega^2 (r_i - r_j)$
Energy of phonon (lattice vibration) in 3D	$E^{\mathrm{3D}}_{n_x,n_y,n_z} = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega$ $n = 0, 1, 2, \dots$
Debye frequency Upper limit of dispersion frequency n - atom number density	$\omega_D = 6\pi^2 n c_{\mathrm{sound}}^3$