ChemE 2200 - Physical Chemistry II for Engineers - Spring 2025

Part 1 - Applied Quantum Chemistry

lec	date	topics	reading
Q1	Wed 1/22	Course Overview. Recap of Quantum Theory and Quantum Chemistry. The hydrogen atom (review): Atomic orbital wave-functions shapes and energies	McQuarrie & Simon: 6.1, 6.2, 6.4, 6.5, 6.6, and 6.7.
Q2	Wed 1/22	The Interaction of Electromagnetic Radiation and Matter: photon-induced transition probabilities, the hydrogen atom spectrum. Multi-electron atoms: Pauli Exclusion Principle, Hund's Rules, anti-symmetric and symmetric wavefunctions, Grotrian Diagrams.	McQuarrie & Simon: 8.1, 8.5, 8.6, 8.9, 8.10, and 8.11.
Q3	Fri 1/24	Chemical bonds: Molecular orbitals from Linear Combinations of Atomic Orbitals, Molecular-Orbital Energy-Level Diagrams.	McQuarrie & Simon: 9.1, 9.2, 9.3, 9.5, 9.6, 9.7, 9.8, 9.9, 9.10, 9.11, 9.12, and 9.13. Duncan, *Molecular Orbitals.*
Q4	Mon 1/27	The Electromagnetic Spectrum and Associated Transitions. Molecular spectroscopy overview. Rotational transitions and microwave spectroscopy. Targeted microwave heating for therapy.	McQuarrie & Simon, 5.8, 5.9, 13.1, 13.2, 13.11, and 13.12.
Q5	Wed 1/29	The Interaction of Electromagnetic Radiation with Matter, cont'd. Vibrational Transitions and Infrared Spectroscopy. Selective dissociation of target molecules.	McQuarrie & Simon, 5.1 – 5.7.
Q6	Fri 1/31	The Interaction of Electromagnetic Radiation with Matter, cont'd. Vibrational-Rotational Spectroscopy. Electronic transitions.	McQuarrie & Simon, 13.3 and 13.13.
Q7	Mon 2/3	The Interaction of Electromagnetic Radiation with Matter, cont'd. Electronic Transitions. Vertical transition probabilities. Molecular dissociation vs fluorescence vs phosphorescence.	McQuarrie & Simon, 13.6 – 13.7.
Q8	Wed 2/5	The Interaction of Electromagnetic Radiation with Matter, cont'd. The fates of electronic excited states, continued.	McQuarrie & Simon,15.1-15.2.
Q9	Fri 2/7	Electronic Properties of Solids: The Free-Electron Model for Solids. Fermi levels.	Duncan, *Electrons in Solids*, pp. 1-10.
Q10	Mon 2/10	Free-Electron Model, continued: Electrical Conductivity of Metals and Superconductors. The Band Theory for Solids; the Kronig-Penney Model. Why energy band gaps?	Duncan, *Electrons in Solids*, pp. 11-15.
Q11	Wed 2/12	Electronic Properties of Insulators and Semiconductors. Doping for electronic devices. Photodetector design.	Duncan, *Electrons in Solids*, pp. 15-18.

Part 2 - Chemical Thermodynamics

lec	date	topics	reading
T1	Fri 2/14	Classical Thermodynamics. 1st law of thermodynamics: internal energy, heat, and work. Pressure-volume work. Adiabatic, isothermal, isobaric, and isochoric Processes. State functions vs. path functions.	McQuarrie & Simon, Chp 19.1-19.5
	Mon 2/17	*No lecture – February Break*	
T2	Wed 2/19	Analysis of adiabatic expansion. Molecular interpretations of heat and work. Internal energy U vs enthalpy H.	McQuarrie & Simon, Chp 19.6-19.8

T3	Fri 2/21	Joule-Thomson Expansion. Calculating enthalpy changes. Designing a refrigerant	McQuarrie & Simon, exercises 19-52 and 22-48.
T4	Mon 2/24	Calculating Enthalpy for Pure Substances. Calculating enthalpy changes for chemical reactions. Entropy, *S*, state function for spontaneous change. Calculating entropy changes for isothermal, isobaric, isochoric, and adiabatic processes.	McQuarrie & Simon, Chapter 19.9-19.12, 20.1-20.3.
T5	Wed 2/26	2nd Law of Thermodynamics – $\Delta S > 0$ for spontaneous processes. Calculating entropy changes for isolated systems: (1) Heat flow from hot to cold. (2) Gas expansion from high pressure to low pressure. (3) Gases mixing and (4) Vaporization. Entropy and statistical probability.	McQuarrie & Simon, Chapter 20.4-20.6
T6	Fri 2/28	Heat Engines and Heat Pumps. The Carnot cycle. The Rankine, Otto, and Diesel cycles.	McQuarrie & Simon, Chapter 20.7.
T7	Mon 3/3	Analysis with combined 1st and 2nd Laws. The 3rd Law of Thermodynamics.	McQuarrie & Simon, Chapter 21.1-21.5
T8	Wed 3/5	Calculating Entropy Change of Chemical Reactions, ΔS_{rxn}. Spontaneity. The Helmholtz energy, *A*, and maximum work.	McQuarrie & Simon, Chapter 21.9, 22.1-22.3.
T9	Fri 3/7	The Gibbs Energy, *G*. The Parameters of Thermodynamics – Physical Observables and Theoretical Concepts. The Maxwell relations and 'useful' relations.	McQuarrie & Simon, Chapter 22.2-22.3.
T10	Mon 3/10	The Gibbs-Helmholtz Equation. Solid-liquid-gas phase equilibria. The chemical potential, μ.	McQuarrie & Simon, Chapter 22.3-23.8.
T11	Wed 3/12	The Thermodynamics of Chemical Equilibrium: Extent of reaction, ξ. Reactant quotient and equilibrium constant.	McQuarrie & Simon, Chapter 26.1-26.6.
T12	Fri 3/14	The Thermodynamics of Chemical Equilibrium: The temperature dependence of ΔG. Coupling reactions to lower spontaneity temperature. Ellingham diagrams.	McQuarrie & Simon, Chapter 26.7.

Part 3 - Chemical Kinetics

lec	date	topics	reading
K1	Mon 3/17	Introduction to Chemical Kinetics. Reaction-coordinate energy-level diagrams. Kinetics vs thermodynamics. Reaction rate orders.	McQuarrie & Simon: 28.1. Atkins: 25(intro).
K2	Wed 3/19	Determining Rate Equations from Experimental Data. Method of initial rates and isolation method. Integrated rate equations - 1^{st}-order, 2^{nd}-order, and n^{th} order reactions. Method of half-lives.	McQuarrie & Simon: 28.2-28.4.
K3	Fri 3/21	Rate Equation Nomenclature. Rate equations and rate constants. Reversible reactions and equilibration.	McQuarrie & Simon: 28.5. Atkins: 25.3-5.
K4	Mon 3/24	Reversible Reactions, cont'd. Temperature dependence of reaction rates - Arrhenius theory. Arrhenius parameters from experimental data. Typical activation energies and prefactors.	McQuarrie & Simon: 28.7. Atkins: 25.6.
K5	Wed 3/26	Reaction Mechanisms. Deriving rate equations from a sequence of elementary steps. Analysis of $A \rightarrow B \rightarrow C$.	McQuarrie & Simon: 29.1-29.2.

K6	Fri 3/28	Reaction Mechanisms, cont'd. Analysis of A → B → C, cont'd. Reactive intermediates and the steady-state approximation. How to identify a reactive intermediate.	McQuarrie & Simon: 29.3-29.4. Atkins: 25.7 (pp. 778-81).
K7	Mon 4/7	Reaction Mechanisms, cont'd. Analysis of A ↔ B → C and A ↔ B ↔ C. Preequilibrium approximation. Why is "pre-equilibrium" a misnomer?	McQuarrie & Simon: 29.5. Atkins: 25.7 (pp. 782-4). .
K8	Wed 4/9	Example Applications of the Steady-State Approximation and Pre-Equilibrium Approximation. Unimolecular decomposition and the Lindemann mechanism.	McQuarrie & Simon: 29.6. Atkins: 25.8.
K9	Fri 4/11	Chain Reactions - the Rice-Herzfeld Mechanism for the Dehydrogenation of Ethane.	McQuarrie & Simon: 29.7. Atkins: 26.1.
K10	Mon 4/14	Chain Reactions, cont'd. Photochemical reactions. quantum yield, the ozone cycle for UV absorption, Beer-Lambert law. The CFC cycle for ozone depletion.	McQuarrie & Simon: 15.8. Atkins: 26.11, 26.12.
K11	Wed 4/16	Photochemical Reactions, cont'd. Isotope separation, ultrapurification and photolithography. Negative and positive resists.	Atkins: 26.4.
K12	Fri 4/18	Polymerization. Polymer properties, kinetics of chain polymerization, stepwise polymerization.	Atkins: 26.3.
K13	Mon 4/21	Polymerization, cont'd. kinetics of stepwise polymerization. Catalysis. General properties of catalytic cycles. Mechanism of enzyme-catalyzed biomolecular reactions. The metabolic cycle. Michaelis-Menten reactions and Hanes plots.	McQuarrie & Simon: 29.8, 29.9. Atkins: 26.2, 26.5, 26.6.
K14	Wed 4/23	Homogeneous Catalysis. Acid-catalyzed dissociation in hydrocarbons. Metal-salt catalyzed partial oxidation: the Wacker process for ethylene to acetaldehyde.	McQuarrie & Simon: 31.6, 31.7. Atkins: 28(intro)-28.1, 28.3-28.4.
K15	Fri 4/25	Homogeneous Catalysis. Autocatalysis Heterogeneous Catalysis. Truncated solids and solid acids.	McQuarrie & Simon: 31.8, 31.10. Atkins: 28.6.
K16	Mon 4/28	Heterogeneous Catalysis, cont'd. Thermodynamics of adsorption - the Langmuir isotherm, associative and dissociative adsorption.	
K17	Wed 4/30	Heterogeneous Catalysis, cont'd. Rate equations for surface reactions, the Langmuir-Hinshelwood mechanism.	McQuarrie & Simon: 30-10, 27.1-27.4.
K18	Fri 5/2	Heterogeneous Catalysis, cont'd. Devising mechanisms for surface reactions.	
K19	Mon 5/5	The Kinetics of Slope Day.	

References:

McQuarrie & Simon, *Physical Chemistry - A Molecular Approach* (University Science Books, 1997)

P. W. Atkins and J. de Paula, *Physical Chemistry*, 7th ed. (Freeman, 2002)