

Introduction to Physical Chemistry

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Key concepts, scope, and foundational principles

1. What Is Physical Chemistry?

Aspect	Description
Definition	The branch of chemistry that studies how matter behaves on a molecular and atomic level and how chemical reactions occur, using the principles of physics.
Goal	Connect macroscopic observations (temperature, pressure, color) with microscopic phenomena (molecular motion, energy changes, quantum states).
Core Disciplines	• Thermodynamics – energy & equilibrium • Chemical Kinetics – reaction rates • Quantum Chemistry – electronic structure • Statistical Mechanics – linking microscopic states to macroscopic properties • Spectroscopy – interaction of matter with electromagnetic radiation

2. Historical Milestones

Year	Scientist	Contribution
1789	Lavoisier	Established the law of conservation of mass; laid the groundwork for quantitative chemistry.
1803	J. Willard Gibbs	Formulated the concept of <i>chemical potential</i> and phase rule.
1854	Rudolf Clausius	Introduced the concept of entropy (S) and the second law of thermodynamics.
1869	Dmitri Mendeleev	Developed the periodic table, showing systematic trends that physical chemistry later explained.
1905	Albert Einstein	Explained Brownian motion, providing evidence for atomic theory.
1926	Erwin Schrödinger	Presented the wave equation, founding quantum mechanics.

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Year	Scientist	Contribution
1935	Linus Pauling	Applied quantum mechanics to chemical bonding (valence bond theory).
1960s–70s	Various	Development of modern computational chemistry (Hartree-Fock, DFT).

3. Fundamental Principles

3.1 Thermodynamics

1. First Law (Energy Conservation)

$$\Delta U = q + w$$

- ΔU : change in internal energy
- q : heat exchanged
- w : work done on the system

2. Second Law (Entropy)

$$\Delta S_{\text{univ}} \geq 0$$

- Spontaneous processes increase the entropy of the universe.

3. Gibbs Free Energy

$$\Delta G = \Delta H - T\Delta S$$

- $\Delta G < 0$: reaction is spontaneous at constant T and P.

3.2 Chemical Kinetics

- **Rate Law:** $\text{rate} = k [A]^m [B]^n$
- **Arrhenius Equation:** $k = A e^{-E_a/RT}$
- **Reaction Mechanisms:** elementary steps, intermediates, transition states.

3.3 Quantum Chemistry

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- **Schrödinger Equation** (time-independent):

$$\hat{H}\psi = E\psi$$

- **Orbitals & Energy Levels:** solutions give molecular orbitals, bond order, and spectra.
- **Approximations:** Hartree-Fock, post-HF methods, Density Functional Theory (DFT).

3.4 Statistical Mechanics

- **Partition Function (Q):** links microscopic states to macroscopic thermodynamic quantities.

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