

Lecture 15 “Modern trends and tasks of physical chemistry”

Goal of the lecture: To explore the current directions, challenges, and interdisciplinary applications of physical chemistry in modern science and technology, focusing on how new experimental and computational methods expand our understanding of molecular structure, dynamics, and energy transformations.

Brief lecture notes: **Physical chemistry** is a branch of science that connects **physics and chemistry**, providing the theoretical foundation for understanding the behavior of matter and energy on an atomic and molecular level. Traditionally, it has included topics such as **thermodynamics, kinetics, electrochemistry, and quantum chemistry**. In the 21st century, physical chemistry has evolved far beyond classical theories. New experimental tools and computational technologies have enabled scientists to study chemical phenomena with **atomic precision**, leading to advances in **nanotechnology, materials science, environmental chemistry, and biophysics**.

Modern physical chemistry plays a crucial role in addressing global challenges, such as **clean energy production, climate change, drug design, and sustainable materials development**.

1. Major Modern Trends in Physical Chemistry

1. Computational and Theoretical Chemistry

The development of **quantum chemical methods** and **molecular modeling** allows researchers to simulate chemical reactions, predict molecular properties, and visualize electron distributions. Techniques such as **Density Functional Theory (DFT)** and **Molecular Dynamics (MD)** are widely used to study reaction mechanisms, catalysis, and nanostructures.

Supercomputers and AI-assisted modeling make it possible to design new materials before they are synthesized in the lab.

2. Nanochemistry and Surface Science

Understanding the behavior of matter at the **nanoscale (1–100 nm)** has become a key research direction. Physical chemistry provides the tools to study **surface energy, adsorption, catalysis, and quantum effects** that dominate at this scale.

Nanostructured materials, such as **graphene, quantum dots, and metal nanoparticles**, have found use in electronics, sensors, and medicine.

3. Electrochemistry and Energy Conversion

The search for renewable and sustainable energy sources has led to intense research in **electrochemical systems** such as **fuel cells, batteries, and supercapacitors**. Physical chemistry helps understand charge transfer, ion transport, and electrode kinetics, enabling the design of efficient and durable energy storage devices.

4. Spectroscopy and Photochemistry

Modern **spectroscopic techniques** (IR, Raman, NMR, UV–Vis, XPS) allow precise identification of chemical structures and real-time monitoring of reaction dynamics.

In **photochemistry**, light is used to drive chemical transformations, playing an

essential role in **solar energy conversion**, **artificial photosynthesis**, and **photoelectrocatalysis**.

5. Environmental and Green Physical Chemistry

Physical chemistry contributes to solving environmental problems through **CO₂ capture**, **pollution control**, and the design of **green catalytic systems** that minimize energy consumption and waste. Computational chemistry helps predict the fate of pollutants and develop sustainable materials.

6. Biophysical and Medicinal Chemistry

Physical chemistry principles are applied to biological systems to study protein folding, enzyme kinetics, and molecular recognition. Techniques like calorimetry, spectroscopy, and molecular docking are vital for understanding drug–target interactions and designing new pharmaceuticals.

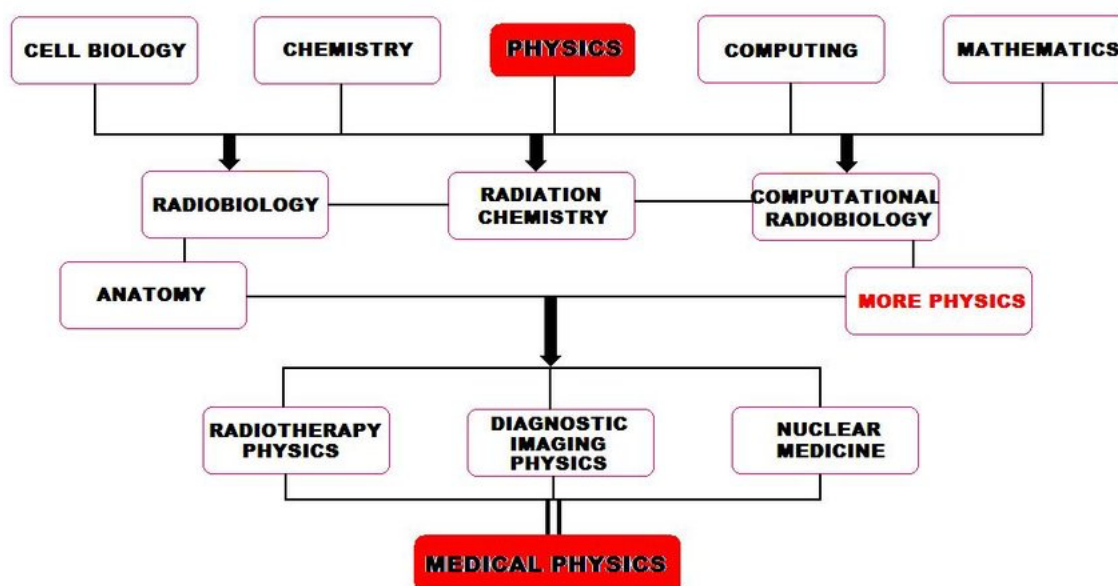


Figure 1 – Interdisciplinary connections of modern physical chemistry

Physical chemistry serves as the central bridge connecting molecular science with physics, biology, and materials research.

2. Emerging Research Areas

Research Area	Description	Applications
Computational chemistry	Simulates molecular systems and reaction mechanisms	Drug design, materials modeling
Nanomaterials	Study of particles and surfaces at the nanometer scale	Catalysis, energy storage, sensors
Quantum thermodynamics	Application of quantum principles to energy processes	Quantum computers, molecular engines
Soft matter physics	Study of polymers, gels, and colloids	Biomedical materials, coatings

Photochemical energy conversion	Harnessing solar energy for chemical fuel production	Artificial photosynthesis, photovoltaics
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3. Current Challenges and Tasks of Physical Chemistry

Despite its progress, physical chemistry faces several key scientific and technological challenges:

- **Bridging scales:** Linking atomic-level behavior to macroscopic properties remains difficult.
- **Complex systems:** Understanding dynamic, disordered, or biological environments where traditional models fail.
- **Data-driven chemistry:** Developing AI and machine learning tools to handle large data sets from simulations and experiments.
- **Sustainability:** Designing materials and reactions that reduce energy use and environmental impact.
- **Integration:** Combining theoretical predictions with real-time experimental observations.

Meeting these challenges will enable the development of **smart materials**, **clean energy systems**, and **precise molecular technologies** for future industries.

4. The Role of Physical Chemistry in Society

Physical chemistry has a profound impact on modern life. It underlies:

- The **development of new energy materials** (batteries, fuel cells, solar cells).
- **Environmental protection** through efficient catalytic and separation processes.
- **Advances in medicine**, including drug design, imaging, and nanomedicine.
- **Technological innovation**, from semiconductors to sustainable chemical manufacturing.

Thus, physical chemistry is not only a theoretical discipline but also a **driving force of modern technology and sustainability**.

Table 1 – Comparison of Traditional and Modern Physical Chemistry

Aspect	Traditional Physical Chemistry	Modern Physical Chemistry
Focus	Thermodynamics, kinetics, equilibrium	Nanoscience, computational modeling, energy systems
Tools	Analytical equations, classical experiments	Supercomputers, spectroscopy, AI algorithms
Scale	Bulk matter	Atomic and nanoscale phenomena
Approach	Isolated systems	Complex, dynamic, and interactive systems
Applications	Industry and basic research	Renewable energy, nanomedicine, environmental tech

Questions for self-control

1. What are the main modern trends in physical chemistry research?
2. How has computational chemistry changed the way scientists study molecules?
3. Explain the role of physical chemistry in the development of sustainable energy technologies.
4. What are the current challenges facing physical chemistry in the 21st century?
5. Describe how physical chemistry connects with biology, materials science, and environmental studies.

Literature:

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