

8 Jul 2024 (Mon)
Theme: Catalysis in applications

**Thematic lecture 4:**

***Catalysis in Drug Discovery and Development*** by Assistant Prof Zhu Ye

Abstract: Catalysis stands as a cornerstone in the realm of drug discovery and development, revolutionizing the way chemists synthesize new pharmaceutical compounds. This seminar covers the intricate roles of catalysis in expediting drug discovery processes, from the initial stages of compound synthesis to the final stages of formulation. Participants will gain insights into the latest advance in catalytic methodologies, including transition metal catalysis, organocatalysis, and enzymatic catalysis, and their pivotal contributions to accelerating discovery of biologically active molecules and enhancing reaction efficiency in drug development. Furthermore, the seminar spotlights emerging trends and transformative potential of catalysis in driving sustainable approaches to meet the evolving challenges in pharmaceutical research.

**Introduction**

1. Overview of Drug Discovery and Development
  - Stages of drug discovery process
  - Importance of efficiency and specificity during drug discovery process
  - The role of chemical synthesis in drug discovery process
2. Catalysis as an indispensable tool in synthesis
  - General principles of catalysis
  - Types of catalysts (homogeneous, heterogeneous, biocatalysts)

**Role of Catalysis in Drug Discovery**

1. Enhancing Reaction Efficiency
  - Acceleration of chemical reactions
  - Reduction of reaction times and costs
  - Diversification of chemical structures
2. Selectivity and Specificity
  - Improving the selectivity of chemical reactions
  - Importance of regioselectivity and stereoselectivity in pharmaceuticals

**Types of Catalysis Used in Drug Discovery**

1. Homogeneous Catalysis
  - Metal-based catalysts (precious metals and nonprecious metals)
  - Applications in cross-coupling reactions
2. Heterogeneous Catalysis
  - Catalyst supports and surface reactions
  - Hydrogenation and oxidation reactions
3. Biocatalysis
  - Enzymatic catalysis
  - Applications in chiral synthesis and complex molecule formation

### **Case Studies in Catalysis for Drug Discovery**

1. Successful Drug Synthesis
  - Analysis of types of catalytic processes involved
  - Examples of drugs synthesized using catalytic methods
2. Challenges and Solutions
  - Common challenges in catalytic drug synthesis
  - Innovations and advancements addressing these challenges

### **Catalysis in Drug Development**

1. Process Optimization
  - Role of catalysis in scaling up production
  - Optimization of reaction conditions for large-scale synthesis
2. Quality Control and Consistency
  - Ensuring purity and consistency of the final product
  - Role of catalysts in achieving high-quality standards
3. Regulatory Considerations
  - Compliance with regulatory guidelines
  - Impact of catalytic processes on regulatory approval

### **Future Directions and Innovations**

1. Advances in Catalytic Methods
  - Emerging catalytic technologies (photocatalysis, electrocatalysis)
  - Impact of these advances on drug discovery
2. Integration of Catalysis with Computational Methods
  - Use of computational chemistry in catalyst design
  - Predictive modelling and high-throughput screening
3. Sustainability and Green Catalysis
  - Role of catalysts in promoting environmentally friendly and sustainable processes
  - Integration of green chemistry principles in drug development by reducing waste and energy consumption

### **Conclusion and Outlook**

1. Summary of the role and impact of catalysis in drug discovery and development
2. Importance of continued research and innovation for future breakthroughs of catalytic methods in pharmaceuticals