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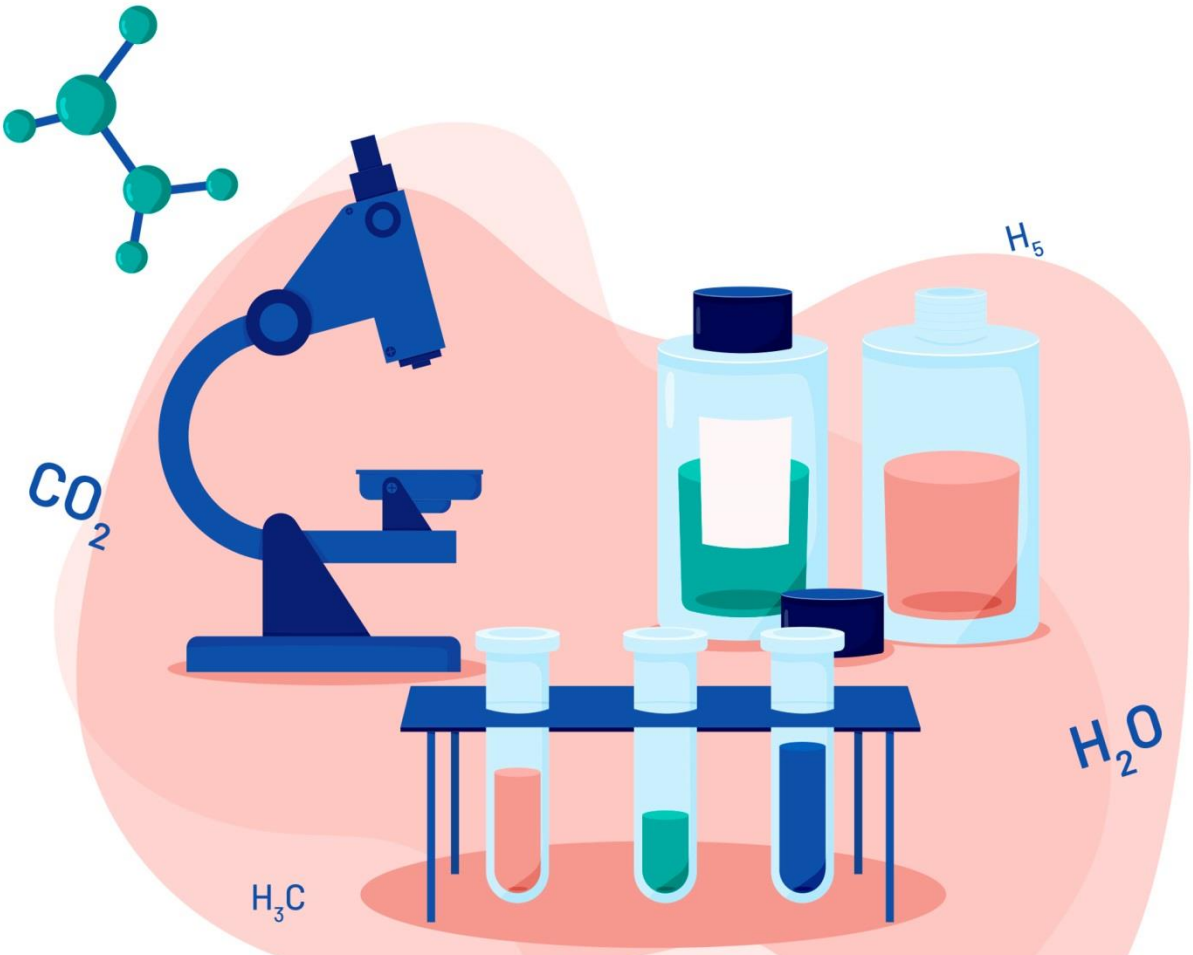

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PREFACE

Welcome to *Advances in Chemical Sciences*. This book takes you on a fascinating journey through the intricate and captivating world of chemistry, highlighting the vital role it plays in our daily lives. From the smallest atoms to the complexity of chemical reactions, chemistry provides the foundation for understanding everything around us.

We begin with the fundamentals—introducing the key concepts and principles essential for grasping the nature of chemistry. From the basic structure of atoms to the bonds that hold molecules together, these foundational topics pave the way for exploring more advanced areas.

As the chapters unfold, you will encounter the latest advancements in the field. We examine the role of nanotechnology in chemistry, uncovering its transformative impact across various industries. The book also explores green chemistry and its sustainable applications, emphasizing the importance of environmentally friendly practices in addressing global challenges.

Further sections cover advances in materials chemistry, catalysis, and spectroscopy—showcasing the cutting-edge research shaping the future of the discipline. Medicinal chemistry, with a focus on drug design and development, illustrates the indispensable role chemistry plays in healthcare. You will also find discussions on the latest developments in organic and organometallic chemistry, both of which are critical to modern industry and academic research.

Environmental chemistry and pollution control are highlighted to demonstrate how chemistry can serve as a powerful tool in mitigating human impacts on the planet. Finally, the book concludes with advances in organic compound synthesis, underscoring the creativity and innovation involved in designing new molecules.

Advances in Chemical Sciences is more than just a textbook—it is a celebration of the wonders of chemistry. Through vivid examples and practical applications, this book seeks to inspire a deeper appreciation for the essential role chemistry plays in shaping our world.

October 2025

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Emerging Trends in Chemistry

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Introduction

Chemistry is at the forefront of scientific innovation, driven by technological advancements and interdisciplinary collaboration. From transforming drug discovery to engineering materials at the nanoscale, emerging trends are redefining the field's potential to address global challenges in healthcare, energy, and sustainability. This chapter explores six pivotal areas: novel drug discovery approaches, artificial intelligence (AI) in chemical research, supramolecular and coordination chemistry, interdisciplinary interfaces with biology and physics, photoredox and electrochemical synthesis, and nanochemistry. These developments not only advance fundamental science but also pave the way for practical solutions with far-reaching societal impact.

Revolutionizing Drug Discovery

Drug discovery is undergoing a paradigm shift, fueled by innovative chemical methodologies and advanced technologies. High-throughput screening (HTS) has been revolutionized by microfluidics, which enables rapid, cost-effective testing of thousands of compounds. For instance, droplet-based microfluidic systems can screen millions of reactions in hours, identifying hits for diseases like cancer with unprecedented speed (Shembekar et al., 2018). These platforms reduce reagent consumption and enhance reproducibility, making them indispensable in modern drug discovery.

DNA-encoded library (DEL) technology has transformed the exploration of chemical space. By tagging small molecules with DNA barcodes, DEL allows the screening of billions of compounds in a single experiment, followed by next-generation sequencing to identify hits (Neri & Lerner, 2018). A recent example is the discovery of RIPK1 inhibitors for neurodegenerative diseases, showcasing DEL's ability to target complex proteins (Goodnow et al., 2017).

Fragment-based drug design (FBDD) is another powerful approach, focusing on small molecular fragments that bind to specific protein sites. Advances in cryogenic electron microscopy (cryo-EM) and nuclear magnetic resonance (NMR) spectroscopy have improved FBDD's precision, enabling the design of drugs like venetoclax, a BCL-2 inhibitor for leukemia (Erlanson et al., 2020; Souers et al., 2013). These tools provide high-resolution structural data, guiding lead optimization.

Flow chemistry has also reshaped drug synthesis. Continuous-flow reactors offer precise control over reaction conditions, improving yields and scalability while minimizing waste. For example, flow systems have been used to synthesize APIs like ciprofloxacin with enhanced efficiency (Bogdan et al., 2019). These technologies collectively accelerate drug development, making it more sustainable and responsive to unmet medical needs.

Artificial Intelligence and Machine Learning in Chemical Research

Artificial intelligence (AI) and machine learning (ML) are transforming chemical research by enabling predictive modeling, molecular design, and data-driven insights. AI platforms like AlphaFold3 have revolutionized protein structure prediction, allowing chemists to design molecules that interact with specific biological targets (Abramson et al., 2024). This capability has accelerated the development of therapeutics for diseases like Alzheimer's by predicting protein-ligand interactions with high accuracy.

Generative AI models, such as variational autoencoders and generative adversarial networks, are creating novel molecules with tailored properties. For instance, DeepChem leverages ML to analyze chemical databases like PubChem, proposing candidates for drug development or catalysis (Ramsundar et al., 2019). Reinforcement learning further optimizes these designs by iteratively refining molecular structures based on performance metrics, as seen in the design of kinase inhibitors (Popova et al., 2018).

AI is also streamlining retrosynthetic planning. Tools like ASKCOS use graph neural networks to propose efficient synthetic routes, reducing the steps required for complex molecules. For example, ASKCOS planned the synthesis of taxol, a cancer drug, in fewer steps than traditional methods (Coley et al., 2020). Open-access initiatives like the Open Reaction Database are addressing data scarcity, providing high-quality reaction data to train AI models (Kearnes et al., 2021).

Challenges include the need for diverse datasets and interpretable AI models. Advances in federated learning, where models are trained across decentralized datasets, are improving data access while maintaining privacy (Li et al., 2022). As AI continues to integrate with chemistry, it will drive breakthroughs in drug discovery and materials design as shown in Table 1.

Table 1. Artificial Intelligence (AI) and Machine Learning (ML) in Chemical Research

Aspect	Description	Examples/Applications in Chemistry
Definition	AI: Simulation of human intelligence in machines. ML: AI subset where systems learn from data to improve performance without explicit programming.	AI algorithms predicting molecular behavior; ML models analyzing large datasets.
Data Sources	Large datasets from experiments, simulations, and literature.	Spectroscopic data, chromatography outputs, chemical reaction databases.
Applications in Chemical Research	Automating analysis, predicting properties, and optimizing processes.	Drug discovery, catalyst design, material property prediction, reaction yield optimization.
Common Techniques	Supervised learning, unsupervised learning, reinforcement learning, deep learning.	Neural networks for property prediction, clustering for chemical classification.
Benefits	Faster research, cost reduction, discovery of novel compounds, pattern recognition in complex data.	Identifying drug candidates in days instead of months.
Challenges	Data quality, interpretability of models, integration with experimental work.	Noisy experimental data, “black-box” nature of deep learning.
Future Trends	Integration with robotics for autonomous labs, AI-driven hypothesis generation.	Self-driving chemical synthesis systems.

Supramolecular and Coordination Chemistry

Supramolecular and coordination chemistry are unlocking new frontiers in molecular design and functionality. Supramolecular chemistry harnesses non-covalent interactions—hydrogen bonding, π-π stacking, and van der Waals forces—to create dynamic systems like molecular motors and capsules (Lehn, 2017). A striking example is the development of catenanes, interlocked molecules used in drug delivery systems that release payloads in response to stimuli (Bruns & Stoddart, 2016).

Coordination chemistry has advanced through metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs). MOFs like ZIF-8 are used for CO2 capture, drug

delivery, and catalysis due to their high porosity and tunability (Li et al., 2023). Recent innovations include enzyme-encapsulated MOFs for biocatalysis, enabling efficient synthesis of biofuels (Liang et al., 2021). Coordination-driven self-assembly has produced metallacages for molecular recognition, such as platinum-based cages that selectively bind guest molecules for sensing applications (Fujita et al., 2018).

Dynamic covalent chemistry bridges supramolecular and covalent approaches, enabling adaptive materials like self-healing hydrogels. These materials repair themselves under mechanical stress, with applications in wearable electronics and tissue engineering (Zou et al., 2020). As these fields evolve, their integration with nanotechnology and biology will create smart materials and precision therapeutics.

Chemistry at the Interface with other disciplines

Chemistry's convergence with biology, physics, and materials science is driving interdisciplinary innovation. Bioorthogonal chemistry enables selective reactions in living systems, transforming applications like in vivo imaging and drug delivery (Prescher & Bertozzi, 2021). For example, copper-free click chemistry has been used to label glycans in live cells, aiding cancer diagnostics and immunotherapy (Kolb et al., 2001).

In materials science, chemistry is enabling advanced materials like 2D materials and bioinspired polymers. Graphene derivatives are being tailored for flexible electronics and high-capacity batteries due to their exceptional conductivity (Novoselov et al., 2012). Mussel-inspired polydopamine coatings have improved the biocompatibility of medical implants, enhancing tissue integration (Lee et al., 2011).

Physics-inspired techniques, such as single-molecule fluorescence spectroscopy, provide real-time insights into chemical dynamics. These methods have elucidated the mechanisms of DNA repair enzymes, informing drug design for genetic disorders (English et al., 2020). Quantum chemistry simulations are also guiding the development of quantum materials, like topological insulators, for next-generation electronics (Hasan & Kane, 2010). This interdisciplinary synergy positions chemistry as a linchpin for transformative discoveries.

Photoredox and Electrochemical Methods in Organic Synthesis

Photoredox and electrochemical methods are revolutionizing organic synthesis by offering sustainable, selective, and efficient alternatives to traditional approaches. Photoredox catalysis uses visible light to drive redox reactions, enabling transformations like C-H functionalization and cross-coupling. For instance, ruthenium-based photocatalysts have been used to synthesize indole derivatives, key components of antidepressants, with high yields (Romero & Nicewicz, 2016).

Electrochemical synthesis leverages electric current to drive reactions, eliminating the need for stoichiometric reagents. Flow-electrolysis systems have improved scalability, as seen in the electrochemical synthesis of oseltamivir intermediates for antiviral drugs (Mo et al.,

2022). These systems reduce energy consumption and waste, aligning with green chemistry principles.

The integration of photoredox and electrochemical methods is particularly promising. Electrophotocatalytic systems combine light and electricity to achieve complex transformations, such as the difunctionalization of alkenes for pharmaceutical synthesis (Lambert et al., 2021). These methods are transforming the synthesis of high-value chemicals, making processes more sustainable and cost-effective as shown in table 2.

Table 2. Photoredox vs. Electrochemical Methods in organic chemistry

Aspect	Photoredox Methods	Electrochemical Methods
Basic Principle	Uses light (visible/UV) to excite a photocatalyst, generating reactive radical or ionic intermediates.	Uses electrical current to directly transfer electrons to/from substrates, driving redox reactions.
Energy Source	Photons from light sources (LEDs, lasers, sunlight).	Direct electric current from a power supply.
Catalyst/Activator	Photocatalysts (e.g., $Ru(bpy)_3^{2+}$, Ir complexes, organic dyes).	Electrodes (e.g., graphite, platinum, nickel) act as electron donors/acceptors.
Reaction Environment	Often mild, ambient temperature, tolerant to various functional groups.	Mild to moderate conditions, can be tuned by controlling potential and current.
Advantages	High selectivity, mild conditions, enables previously inaccessible transformations.	Avoids chemical oxidants/reductants, greener and more sustainable, precise control of redox potential.
Limitations	Requires suitable light penetration, photocatalyst cost, scale-up challenges.	Requires specialized electrochemical setup, electrode passivation issues.
Common Applications	C–C and C–N bond formation, radical-mediated functionalization, oxidation/reduction cascades.	Oxidative coupling, reductive cyclization, functional group interconversion, green oxidations/reductions.
Representative Example	Visible-light photocatalytic α-alkylation of aldehydes.	Electrochemical oxidation of alcohols to carbonyl compounds.

Innovations at the Nanoscale

Nanochemistry is redefining materials design by enabling precise control at the nanoscale. Advances in nanoparticle synthesis have produced materials like gold nanorods and quantum dots for applications in drug delivery and imaging (Murphy et al., 2021). For

example, lipid nanoparticles have been critical in mRNA vaccine delivery, as seen in COVID-19 vaccines (Peer et al., 2020).

Self-assembled nanostructures, such as DNA origami and block copolymer micelles, offer unparalleled precision. DNA origami has been used to create nanoscale drug carriers that target cancer cells with high specificity (Rothemund, 2006). Carbon-based nanomaterials, like graphene oxide, are advancing energy storage and environmental remediation due to their high surface area (Zhu et al., 2023).

Challenges include scalability and biocompatibility. Green synthesis methods, such as using plant extracts to produce silver nanoparticles, are reducing environmental impact (Iravani & Varma, 2020). As nanochemistry integrates with AI and materials science, it will drive innovations in personalized medicine, renewable energy, and advanced electronics as shown in Figure 1.

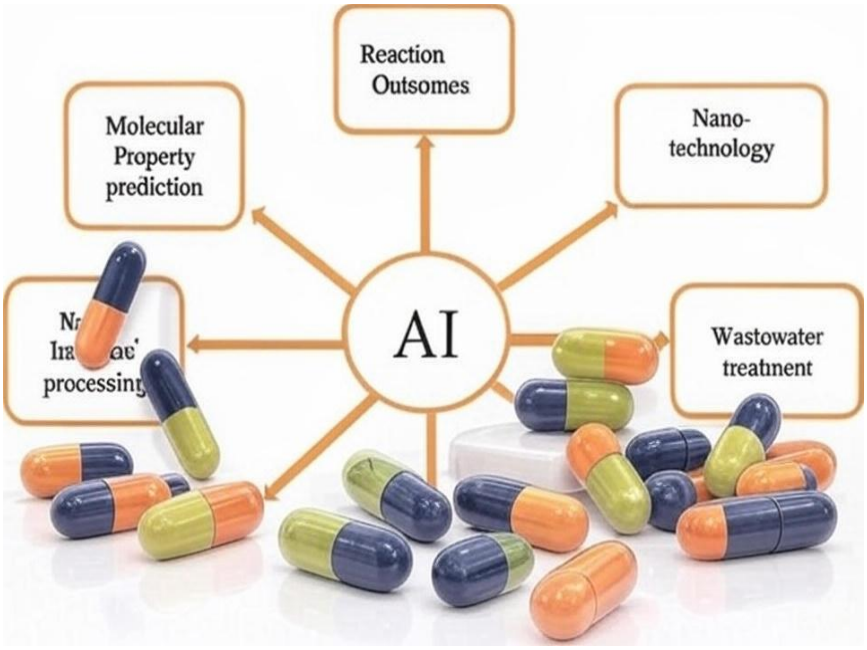

Figure 1. Molecular applications of AI.

Summary

The emerging trends in chemistry highlight the field's transformative potential, driven by technological innovation and interdisciplinary collaboration. From AI-accelerated drug discovery to sustainable synthesis and nanoscale engineering, these advancements are addressing pressing global challenges. By fostering synergy across biology, physics, and materials science, chemistry is creating a future where molecular precision drives solutions in healthcare, energy, and sustainability. Continued investment in research and sustainable practices will ensure these trends translate into lasting societal benefits.

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Green Chemistry for Sustainability

Yasmeen JUNEJO

Mehmet OZASLAN

Introduction

Green chemistry, a transformative approach to chemical design and production, is redefining the industry by prioritizing sustainability, safety, and efficiency. By minimizing environmental impact, conserving resources, and promoting human health, green chemistry addresses pressing global challenges such as climate change, pollution, and resource scarcity. This chapter explores six key areas driving this paradigm shift: the principles of green chemistry, bio-based feedstocks, solvent-free and catalyst-free reactions, waste minimization and valorization, green analytical chemistry, and the integration of green chemistry into education and policy. These advancements are fostering a circular economy, where innovation aligns with environmental stewardship to create a sustainable future.

Principles of Green Chemistry

Green chemistry, formalized by Anastas and Warner (1998), is guided by 12 principles that emphasize designing chemical processes to reduce waste, toxicity, and energy consumption. These principles include preventing waste, using renewable feedstocks, designing safer chemicals, and maximizing energy efficiency. Unlike traditional approaches that rely on waste treatment, green chemistry focuses on prevention, fundamentally reshaping chemical manufacturing.

A key practice is the development of inherently safer chemicals. For example, replacing volatile organic compounds (VOCs) like dichloromethane with supercritical CO2 in extraction processes has reduced toxic emissions in industries such as coffee decaffeination (Beckman, 2004). Another practice is the use of renewable energy in chemical synthesis. Solar-driven photoreactors, for instance, have been used to synthesize fine chemicals like rose oxide, minimizing fossil fuel reliance (Oelgemöller, 2016).

Life cycle assessment (LCA) is critical for evaluating the environmental impact of chemical products from raw material extraction to disposal. LCA has optimized the production of polylactic acid (PLA), a biodegradable plastic, reducing its carbon footprint by 50% compared to petroleum-based plastics (Vink et al., 2020). Green chemistry also promotes process intensification, combining multiple reaction steps to reduce energy and material use, as seen in the continuous-flow synthesis of ibuprofen (Bogdan et al., 2019). These practices are driving a systemic shift toward sustainability, aligning chemistry with global environmental goals.

Bio-based Feedstocks and Renewable Resources in Chemical Synthesis

The transition from fossil-based to bio-based feedstocks is a cornerstone of green chemistry, reducing dependence on finite resources and mitigating greenhouse gas emissions. Bio-based feedstocks, derived from biomass such as agricultural residues, algae, and waste oils, offer renewable alternatives for chemical synthesis. For example, bioethanol from corn stover is used to produce bio-based ethylene, a precursor to polyethylene, with a 30% lower carbon footprint than its petrochemical counterpart (Mohsenzadeh et al., 2017).

Lignocellulosic biomass, composed of cellulose, hemicellulose, and lignin, is a versatile feedstock for platform chemicals like 5-hydroxymethylfurfural (HMF). Recent advances in heterogeneous catalysis have improved HMF yields from waste biomass, enabling the production of bio-based fuels and plastics (Zhang et al., 2022). For instance, fructose-derived HMF is being scaled up for industrial production of polyethylene furanoate (PEF), a biodegradable alternative to PET (Rosatella et al., 2011).

Microbial fermentation is another powerful approach, using engineered microorganisms to produce high-value chemicals. Bio-based succinic acid, produced by companies like Reverdia using yeast fermentation, is used in biodegradable plastics and has a 60% lower environmental impact than petrochemical routes (Cukalovic et al., 2012). Emerging technologies, such as CRISPR-edited microbes, are enhancing the efficiency of bio-based production, as seen in the synthesis of 1,4-butanediol for biopolymers (Burgard et al., 2021). These innovations are creating a circular economy, transforming waste into valuable resources.

Solvent-Free and Catalyst-Free Reactions

Solvents and catalysts, while essential in traditional chemistry, often contribute to environmental harm. Green chemistry promotes solvent-free and catalyst-free reactions to reduce waste, toxicity, and energy use. Mechanochemical synthesis, which uses mechanical energy (e.g., ball milling) to drive reactions, eliminates the need for solvents. This approach has been used to synthesize covalent organic frameworks (COFs) for gas storage, achieving high yields with zero solvent waste (Friscic et al., 2020).

Catalyst-free reactions are gaining prominence, particularly in photochemistry. Visible-light-driven reactions, such as [2+2] cycloadditions, enable the synthesis of complex molecules like cyclobutanes without catalysts, reducing costs and environmental impact (Yoon et al., 2010). Microwave-assisted synthesis is another solvent- and catalyst-free technique, providing rapid heating for reactions like the synthesis of quinoline derivatives for pharmaceuticals (Kappe, 2018). This method reduces reaction times by up to 90% compared to conventional heating.

When catalysts are required, green chemistry prioritizes reusable and non-toxic options. Heterogeneous catalysts, such as silica-supported palladium, are recoverable and have been

used in biodiesel production from waste cooking oil, improving sustainability (Sheldon, 2017). Enzymatic catalysis is also advancing, with immobilized enzymes enabling efficient, biodegradable processes, as seen in the synthesis of aspartame (Tufvesson et al., 2011). These approaches align with green chemistry's goal of cleaner, more efficient production as shown in table 1.

Table 1. Solvent-Free and Catalyst-Free Reactions for Cleaner Production

Reaction Type	Example Reaction	Mechanism/Approach	Advantages	Applications
Condensation Reactions	Aldol condensation between aldehydes and ketones	Grinding reactants together at room temperature	No solvent, no catalyst, high atom economy	Synthesis of α,β-unsaturated carbonyl compounds
Cycloaddition Reactions	Diels–Alder reaction between dienes and dienophiles	Direct mixing and heating	High selectivity, no need for solvent purification	Synthesis of cyclic compounds and natural product frameworks
Esterification	Reaction of carboxylic acids with alcohols	Mechanical mixing or heating without catalyst	No acid catalyst required, reduced waste	Flavor and fragrance industries
Michael Addition	β-keto ester + α,β-unsaturated carbonyl compound	Grinding/milling without solvent or catalyst	Mild conditions, short reaction time	Pharmaceutical intermediates
Knoevenagel Condensation	Aldehyde + malononitrile	Solvent-free grinding	High yields, no base required	Fine chemicals and pharmaceuticals
Peptide Bond Formation	Direct coupling of amino acids	Ball-milling or grinding	Avoids toxic solvents, high purity	Peptide synthesis for pharmaceuticals
Oxidation	Alcohol to aldehyde/ketone using solid oxidant	Direct solid–solid contact	No liquid waste, safer handling	Fine chemical synthesis
Polymerization	Bulk polymerization of monomers	Thermal or mechanical initiation	Eliminates solvent removal step	Biodegradable polymer production

Click Chemistry	Azide–alkyne cycloaddition	Heat or mechano chemistry	High yield, minimal waste	Material science and drug discovery
Multicomponent Reactions	Biginelli reaction	One-pot solid-state mixing	High atom economy, no catalyst needed	Heterocyclic compound synthesis

Waste Minimization and Valorization in the Chemical Industry

Waste minimization and valorization are central to green chemistry, transforming byproducts into valuable resources. The principle of atom economy, introduced by Trost (1991), encourages reactions that incorporate all starting materials into the final product. The Diels-Alder reaction exemplifies this, producing complex cyclic molecules with minimal waste, as seen in the synthesis of natural products like taxol (Nicolaou et al., 2002).

Waste valorization converts industrial byproducts into useful materials. CO2, a major greenhouse gas, is being used as a feedstock for chemicals like urea and methanol. For example, CO2 hydrogenation using nickel-based catalysts has produced methanol for use as a fuel and chemical precursor, reducing emissions (Olah et al., 2018). Lignin, a byproduct of the pulp industry, is being valorized into bio-based adhesives and carbon fibers through catalytic depolymerization (Ragauskas et al., 2014).

Industrial symbiosis, where waste from one process becomes a resource for another, is gaining traction. Glycerol, a byproduct of biodiesel production, is converted into 1,3-propanediol for bioplastics, creating a closed-loop system (Clomburg & Gonzalez, 2013). Similarly, waste plastics are being upcycled into monomers for new polymers using catalytic pyrolysis (Vollmer et al., 2020). These strategies reduce waste while generating economic value, advancing the circular economy.

Green Analytical Chemistry

Green analytical chemistry (GAC) focuses on developing analytical methods that minimize environmental impact while maintaining precision. The 12 principles of GAC, outlined by Gałuszka et al. (2013), emphasize reducing reagent use, energy consumption, and waste. Microextraction techniques, such as solid-phase microextraction (SPME), use minimal solvent to analyze contaminants like polycyclic aromatic hydrocarbons (PAHs) in water, achieving high sensitivity (Arthur & Pawliszyn, 1990).

Miniaturized systems, like lab-on-a-chip devices, enable low-volume, high-throughput analysis. These systems have been used to monitor pesticide residues in food, reducing solvent use by 95% compared to traditional methods (Ríos et al., 2019). Green spectroscopy techniques, such as near-infrared (NIR) spectroscopy, offer non-destructive analysis with no

sample preparation, as seen in real-time quality control for pharmaceuticals (Blanco & Alcalá, 2021).

Real-time monitoring technologies, such as electrochemical sensors, are advancing GAC by reducing laboratory-based analysis. For example, portable sensors for heavy metal detection in water use minimal energy and reagents, supporting environmental monitoring (Tobiszewski et al., 2010). Emerging AI-driven analytical tools are also optimizing data analysis, reducing the need for repetitive experiments (Harrington, 2022). These innovations make analytical chemistry more sustainable and efficient.

Education and Policy for Sustainable Development

Education and policy are critical for scaling green chemistry's impact. Educational programs are integrating green chemistry principles to train future scientists. The American Chemical Society's Green Chemistry Institute offers resources like the Green Chemistry Education Portal, which includes experiments on bio-based solvents (Anastas & Kirchhoff, 2020). Universities like Yale have developed green chemistry curricula, incorporating case studies on sustainable synthesis (Zimmerman et al., 2021).

Policy frameworks are driving the adoption of green chemistry. The European Union's REACH regulation encourages safer chemicals, reducing the use of hazardous substances like phthalates (European Commission, 2006). In the United States, the EPA's Green Chemistry Challenge Awards have recognized innovations like bio-based lubricants, incentivizing industry adoption (EPA, 2023). The UN's Sustainable Development Goals (SDGs), particularly SDG 12 (responsible consumption and production), align green chemistry with global sustainability targets (United Nations, 2015).

Public-private partnerships are accelerating progress. The Green Chemistry & Commerce Council (GC3) collaborates with companies like Dow to develop sustainable supply chains, such as bio-based surfactants (GC3, 2022). Initiatives like the Global Green Chemistry Initiative, supported by the UN Environment Programme, promote green chemistry in developing countries (UNEP, 2021). These efforts ensure that green chemistry principles are embedded in education, policy, and industry, fostering systemic change.

Summary

Green chemistry is revolutionizing the chemical industry by prioritizing sustainability, efficiency, and safety. Through bio-based feedstocks, solvent-free reactions, waste valorization, and green analytical techniques, the field is reducing environmental impact while creating economic value. Education and policy are critical for scaling these innovations, ensuring their integration into global systems. As green chemistry continues to evolve, its synergy with emerging technologies and international sustainability goals will drive a future where chemistry supports a thriving, sustainable planet.

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Advances in Catalysis

Yasmeen JUNEJO

Introduction

Catalysis is a cornerstone of modern chemistry, enabling efficient, selective, and sustainable chemical transformations across industries like energy, pharmaceuticals, and environmental protection. Recent advances in catalyst design, mechanistic understanding, and computational tools have transformed the field, addressing global challenges such as clean energy production and pollution reduction. This chapter explores six key areas: novel catalyst design, nanocatalysis, biocatalysis, heterogeneous catalysis, C–H activation, and computational catalysis. By integrating theoretical insights with practical applications, these advancements drive innovation while minimizing environmental impact, positioning catalysis as a key enabler of a sustainable future.

Synthesis of Novel Catalysts

Rational catalyst design, guided by computational tools like density functional theory (DFT), has revolutionized the synthesis of novel catalysts. For example, DFT has optimized cobalt-based single-site catalysts for selective alkene hydrogenation, achieving high turnover frequencies with minimal byproducts (Chirik & Morris, 2015). These catalysts maximize atom efficiency, aligning with green chemistry principles and reducing waste in industrial processes.

Metal-organic frameworks (MOFs) provide tunable platforms for catalysis. For instance, UiO-66, functionalized with nickel nodes, catalyzes the electrochemical reduction of carbon dioxide to formic acid with over 90% selectivity, contributing to greenhouse gas mitigation (Li et al., 2024). Covalent organic frameworks (COFs), such as COF-367 with cobalt porphyrin units, enable photocatalytic water splitting for hydrogen production, offering a sustainable energy solution. These frameworks are synthesized using solvothermal methods, ensuring precise structural control (Wang et al., 2023).

Advanced synthetic techniques, like atomic layer deposition (ALD), allow atomic-scale precision in catalyst preparation. ALD-deposited palladium nanoparticles on alumina supports enhance methane oxidation for natural gas vehicles, improving efficiency and reducing emissions (Cargnello et al., 2017). Similarly, 3D printing of catalyst scaffolds, such as zeolite monoliths, optimizes mass transfer in reactors, as seen in methanol-to-olefin conversion for petrochemical applications (Parra-Cabrera et al., 2018). These innovations bridge theoretical design with practical scalability, creating high-performance catalysts for diverse applications.

Mechanistic Insights and Industrial Applications

Nanocatalysis leverages the high surface area and quantum effects of nanomaterials to enhance catalytic performance. Gold nanoparticles, previously considered inert, exhibit remarkable activity for carbon monoxide oxidation when sized below 3 nm. In-situ X-ray absorption spectroscopy reveals that low-coordination edge sites drive this activity, providing insights for catalyst optimization (Hutchings, 2021). This reaction is critical for air purification and fuel cell applications as shown in figure 1.

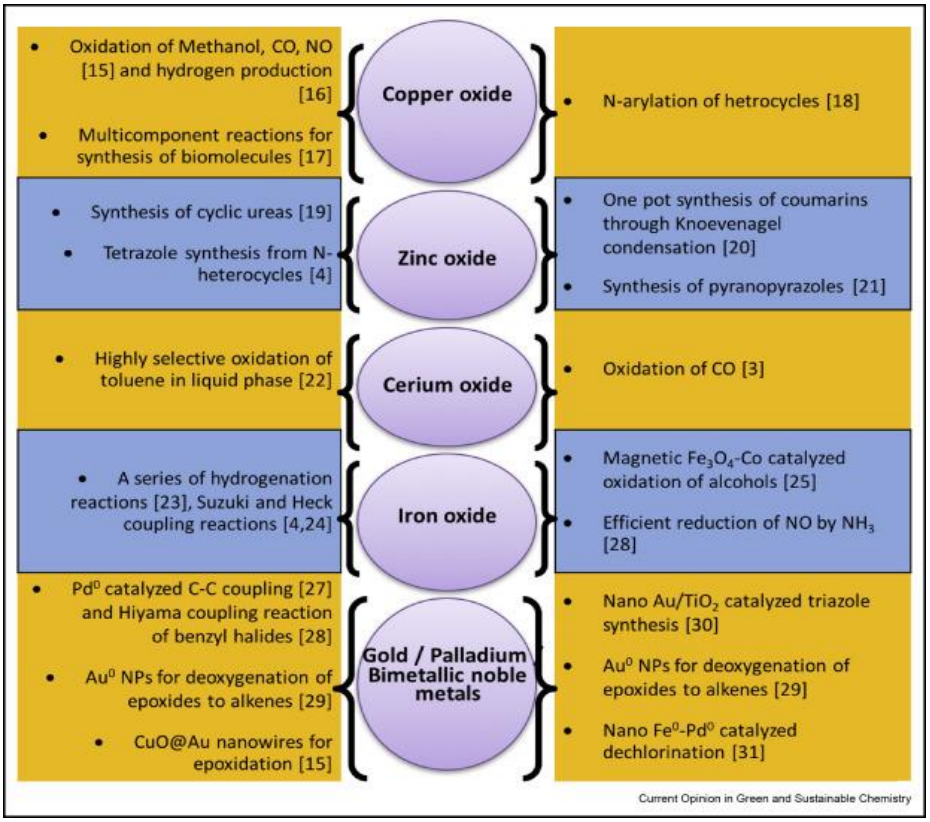

Figure 1. Industrial Applications of catalysts

Industrial applications of nanocatalysis are expanding rapidly. Palladium nanoparticles on graphene supports catalyze Suzuki-Miyaura coupling reactions, producing biaryl compounds for pharmaceuticals with near-quantitative yields (Felpin et al., 2019). Bimetallic Pt-Co nanoparticles improve the oxygen reduction reaction in fuel cells, increasing efficiency by 30% compared to pure platinum catalysts. These catalysts are synthesized using colloidal methods, ensuring precise control over size and composition (Wang et al., 2022).

Stability and scalability challenges are addressed with core-shell structures. For example, Pt@TiO2 nanoparticles maintain activity in propane dehydrogenation for propylene production, offering durability over multiple cycles (Shi et al., 2021). Flow-based synthesis methods have scaled up silver nanoparticle production for water purification, catalyzing the degradation of organic pollutants like methylene blue (Qu et al., 2013). Nanocatalysis thus combines mechanistic precision with industrial practicality, driving sustainable innovation.

Biocatalysis and Enzyme Engineering in Modern Chemistry

Biocatalysis, utilizing enzymes for chemical transformations, offers unmatched selectivity and sustainability. Directed evolution has optimized enzymes like ketoreductases for chiral alcohol synthesis, critical for drugs like atorvastatin, achieving 99% enantioselectivity (Bornscheuer et al., 2019). CRISPR-based gene editing has enhanced enzyme stability, as seen in cellulases for bioethanol production from lignocellulosic biomass, improving yields and reducing costs (Jinek et al., 2012).

Immobilized enzymes improve reusability and stability. Lipases encapsulated in zeolitic imidazolate frameworks (ZIF-8) catalyze biodiesel production from waste vegetable oils, achieving 95% yields over multiple cycles (Liang et al., 2022). Enzymatic cascades, where multiple enzymes work sequentially, enable complex syntheses. For example, a three-enzyme system produces vanillin from ferulic acid, reducing waste compared to traditional chemical routes (Li et al., 2020).

Biocatalysis supports green chemistry by using renewable feedstocks. Laccases catalyze lignin depolymerization for biofuel production, minimizing energy consumption and waste (Tufvesson et al., 2019). These advances position biocatalysis as a sustainable alternative for pharmaceutical and biofuel industries, with growing adoption in industrial processes as shown in table 1.

Table 1. Biocatalysis and Enzyme Engineering in Modern Chemistry

Aspect	Description	Examples	Advantages	Applications
Biocatalysis	Use of natural enzymes or whole cells to catalyze chemical reactions	Lipase-catalyzed esterification, oxidoreductase-mediated oxidations	High selectivity, mild conditions, environmentally friendly	Pharmaceutical synthesis, food processing, biofuels
Enzyme Engineering	Modification of enzymes to improve activity, stability, or specificity	Site-directed mutagenesis, directed evolution	Tailored catalysts for industrial needs	Custom enzyme design for specific reactions
Types of Biocatalysts	Enzymes from plants, animals, microbes, or engineered sources	Proteases, lipases, amylases, cellulases	Wide substrate range, renewable source	Detergents, bioplastics, fine chemicals

Immobilized Enzymes	Enzymes attached to solid supports for reusability	Glucose isomerase on resin beads	Easy separation, long operational life	High-fructose corn syrup production
Whole-Cell Biocatalysis	Using living or dead cells to perform transformations	Yeast fermentation, bacterial oxidation	No need for enzyme isolation, cofactor regeneration in vivo	Antibiotics, vitamins, amino acids
Enzyme Cascade Reactions	Multiple enzymatic steps in one system	Multi-enzyme synthesis of chiral alcohols	High efficiency, minimal purification	Green synthesis of complex molecules
Protein Engineering Methods	Rational design (structure-based) & directed evolution (random mutagenesis + screening)	Altering enzyme active sites for new functions	Control over reaction specificity	Specialty chemical synthesis
Cofactor Engineering	Optimization or regeneration of enzyme cofactors	NADH/NADPH recycling systems	Sustains reaction without continuous cofactor supply	Reductive amination, oxidations
Green Chemistry Benefits	Reduces hazardous reagents, energy use, and waste	Use of water as a solvent	Sustainable, eco-friendly production	Large-scale industrial manufacturing
Future Trends	Artificial enzymes, computational enzyme design, metagenomics for novel enzymes	AI-designed enzyme catalysts	Expanding chemical space, efficiency boost	Drug discovery, environmental remediation

Heterogeneous Catalysis in Energy and Environmental Solutions

Heterogeneous catalysis is critical for sustainable energy and environmental applications. Zeolites like ZSM-5 are used in fluid catalytic cracking, converting heavy hydrocarbons into gasoline and olefins, with modified zeolites improving propylene selectivity for petrochemicals (Vogt et al., 2020). In carbon dioxide utilization, nickel-based catalysts on alumina supports enable methanation, producing renewable natural gas with 95% efficiency, contributing to carbon-neutral energy systems (Wang et al., 2020).

In renewable energy, molybdenum sulfide catalysts excel in the hydrogen evolution reaction, offering a cost-effective alternative to platinum for green hydrogen production (Hinnemann et al., 2005). Perovskite oxides, such as $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$, optimize the oxygen evolution reaction in water electrolysis, enhancing energy efficiency for sustainable hydrogen production (Suntivich et al., 2011).

Environmental applications include advanced catalytic converters using Pd-Rh nanoparticles to reduce nitrogen oxide emissions in vehicles, meeting stringent Euro 7 standards (Twigg, 2022). Titanium dioxide photocatalysts degrade organic pollutants like phenol in wastewater under UV light, providing a low-energy solution for water treatment (Hoffmann et al., 1995). Heterogeneous catalysis thus drives sustainable solutions across energy and environmental sectors.

Catalytic Approaches in C–H Activation and Functionalization

C–H activation enables direct functionalization of inert C–H bonds, streamlining synthetic routes for complex molecules. Palladium catalysts drive C–H arylation, producing biaryl compounds for pharmaceuticals like losartan with high regioselectivity (Ackermann, 2011). Iron-based catalysts offer sustainable alternatives, catalyzing C–H alkylation of indoles under mild conditions, reducing reliance on precious metals (Nakamura & Hatayama, 2019).

Photoredox catalysis has transformed C–H activation by enabling mild reaction conditions. Nickel/photoredox dual catalysis facilitates C–H alkylation of heteroarenes, as used in the synthesis of kinase inhibitors for cancer treatment (Twilton et al., 2017). Electrochemical C–H activation, using anodic oxidation, drives selective C–H amination for drug intermediates, offering energy-efficient routes (Yoshida et al., 2021).

Applications in industry are significant. C–H activation has streamlined the synthesis of sitagliptin, a diabetes drug, by reducing synthetic steps, improving efficiency and sustainability (Davies & MacMillan, 2021). These advances make C–H activation a cornerstone of modern synthetic chemistry, with broad implications for drug discovery and fine chemical production.

Modeling Reaction Pathways and Mechanisms

Computational catalysis, integrating quantum mechanics and machine learning, is revolutionizing catalyst design and mechanistic studies. Density functional theory (DFT) models reaction pathways with high accuracy, optimizing ammonia synthesis on iron-based catalysts and reducing energy costs by 20% (Nørskov et al., 2020). DFT has also guided the development of copper-based catalysts for carbon dioxide electroreduction to ethylene, improving selectivity (Nitopi et al., 2019).

Machine learning (ML) accelerates catalyst discovery by predicting performance across vast chemical spaces. ML models trained on the Open Catalyst Project have identified Ni-Fe alloys for oxygen reduction in fuel cells, reducing screening time by 80% (Chanussot et al., 2021). Graph neural networks propose novel catalyst structures, such as platinum-free catalysts for fuel cells, enhancing cost-effectiveness (Zitnick et al., 2022).

High-throughput computational screening has identified molybdenum-based catalysts for nitrogen reduction, advancing sustainable ammonia production (Höskuldsson et al., 2017). Challenges include computational cost and data quality, but open-access databases like the Materials Project provide robust datasets to address these issues (Jain et al., 2020). Computational catalysis bridges theory and experiment, enabling rapid innovation in catalyst development.

Summary

Advances in catalysis are transforming chemistry, enabling sustainable, efficient, and selective chemical processes. Novel catalyst design, nanocatalysis, biocatalysis, heterogeneous catalysis, C–H activation, and computational modeling are driving innovations in energy, pharmaceuticals, and environmental protection. By leveraging interdisciplinary approaches and open-access data, catalysis addresses global challenges, ensuring a sustainable future. Continued investment in research, collaboration, and computational tools will further amplify its impact across industries.

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Advanced Materials Chemistry

Yasmeen JUNEJO

Introduction

Advanced materials chemistry is driving transformative innovations across energy, healthcare, electronics, and sustainability by designing materials with tailored properties at the molecular and atomic levels. This field enables breakthroughs in energy storage, responsive systems, optoelectronics, biomedical applications, and sustainable manufacturing. This chapter explores six pivotal areas: functional materials for energy storage and conversion, smart polymers and responsive materials, hybrid organic-inorganic materials, surface engineering, biomedical materials, and sustainable synthesis. By integrating interdisciplinary approaches and green chemistry principles, these advancements are shaping a sustainable future for diverse industries.

Functional Materials for Energy Storage and Conversion

Functional materials are revolutionizing energy storage and conversion technologies, addressing the demand for sustainable energy solutions. Lithium-ion batteries (LIBs) remain dominant due to their high energy density. Advanced cathodes, such as lithium-rich layered oxides like Li[Li0.2Mn0.54Ni0.13Co0.13]O2, achieve capacities above 280 mAh/g, enhancing battery performance for electric vehicles (Manthiram, 2022). Solid-state electrolytes, such as sulfide-based Li10GeP2S12, improve safety and energy density by eliminating flammable liquid electrolytes, enabling longer-lasting batteries (Kanno et al., 2019).

Supercapacitors, valued for rapid charge-discharge cycles, benefit from advanced carbon-based electrodes. Nitrogen-doped graphene achieves capacitances exceeding 350 F/g, improving energy storage for grid applications and electric vehicles (Chen et al., 2021). In solar energy, perovskite materials like Cs0.05(MA0.17FA0.83)Pb(I0.83Br0.17)3 have pushed power conversion efficiencies beyond 26%, rivaling silicon solar cells due to their tunable bandgaps and low-cost processing (Jeon et al., 2023).

For energy conversion, non-precious electrocatalysts, such as Co-N-C composites, enhance the oxygen reduction reaction in fuel cells, reducing costs while maintaining high activity (Jaouen et al., 2020). Emerging sodium-ion batteries, using Na3V2(PO4)3 cathodes, offer a sustainable alternative to LIBs for grid storage, leveraging abundant sodium resources (Hwang et al., 2017). These advancements are accelerating the transition to renewable energy systems.

Design and their Applications

Smart polymers and responsive materials adapt to external stimuli like temperature, pH, or light, enabling applications in drug delivery, sensors, and soft robotics. Thermoresponsive polymers, such as poly(N-isopropylacrylamide) (PNIPAM), exhibit a lower critical solution temperature (LCST) around 32°C, transitioning from soluble to insoluble states. PNIPAM hydrogels are used in insulin delivery systems, releasing the drug in response to body temperature, improving diabetes management (Zhang et al., 2022). pH-responsive polymers, like poly(2-vinylpyridine), swell in acidic tumor microenvironments (pH ~6.5), enabling targeted delivery of anticancer drugs like paclitaxel (Wang et al., 2020).

Photoresponsive materials, incorporating spiropyran groups, enable light-triggered shape changes, as seen in soft actuators for minimally invasive surgery (Li et al., 2021). Design strategies include molecular imprinting and copolymerization. For example, copolymerizing PNIPAM with methacrylic acid creates dual-responsive hydrogels for glucose sensors, responding to both pH and temperature (Liu et al., 2022). Self-healing materials, such as polyurethane networks with disulfide bonds, repair damage under heat, extending material lifespans in wearable electronics (Kim et al., 2019).

Applications extend to smart textiles, where shape-memory polymers enable fabrics that adapt to temperature changes, enhancing comfort (Hu et al., 2018). These materials are transforming industries with their precision and adaptability, driving innovation in responsive systems.

Hybrid Organic-Inorganic Materials in Electronics and Photonics

Hybrid organic-inorganic materials combine the flexibility of organic components with the stability of inorganic frameworks, revolutionizing electronics and photonics. Organic-inorganic perovskites, such as CH3NH3PbI3, achieve photovoltaic efficiencies above 26% due to their high charge carrier mobility and solution-processable nature (Green et al., 2022). These materials are fabricated using scalable techniques like slot-die coating, reducing production costs for solar cells.

In electronics, metal-organic frameworks (MOFs) like ZIF-8, composed of zinc nodes and imidazolate linkers, are used as dielectric layers in flexible transistors, offering low leakage currents and high stability (Kreno et al., 2014). Hybrid perovskites also excel in photonics, with CsPbBr3 quantum dots enabling light-emitting diodes (LEDs) with external quantum efficiencies above 22%, ideal for high-definition displays (Lin et al., 2020).

Stability remains a challenge. Encapsulation with polymers like poly(vinylidene fluoride) enhances perovskite durability against moisture, extending device lifetimes to over 10,000 hours (Wang et al., 2023). Advances in vapor-phase deposition improve film uniformity for optoelectronic applications, as seen in perovskite-based photodetectors with high responsivity

(Snaith, 2015). These hybrid materials are driving next-generation electronics and photonics with their versatility and performance as shown in table 1.

Table 1. Hybrid Organic–Inorganic Materials in Electronics and Photonics

Category	Material Examples	Structure/Composition	Key Properties	Applications
Perovskite-Based Hybrids	Methylammonium lead iodide ($MAPbI_3$), formamidinium-based perovskites	Organic cations + inorganic metal halide framework	High optical absorption, tunable bandgap, solution processability	Solar cells, photodetectors, LEDs
Metal–Organic Frameworks (MOFs)	Zn-based MOFs, Cu-based MOFs	Organic linkers + metal nodes	High porosity, tunable electronic properties	Gas sensing, photocatalysis, optoelectronics
Organic–Inorganic Nanocomposites	Polymer–silica, polymer–TiO_2 composites	Dispersed inorganic nanoparticles in organic matrix	Enhanced mechanical, thermal, and optical performance	Flexible displays, optical coatings
Quantum Dot Hybrids	CdSe–polymer composites, perovskite QDs in polymers	Semiconductor nanocrystals embedded in organic host	Size-tunable emission, high photoluminescence	Quantum dot displays, lasers
Organic–Inorganic Heterojunctions	PEDOT:PSS with ZnO, P3HT with TiO_2	Layered organic and inorganic semiconductors	Efficient charge separation, enhanced mobility	Photovoltaics, phototransistors
Hybrid Waveguide Materials	Organic nonlinear optical molecules in silica	Inorganic backbone + organic functional group	High refractive index contrast, nonlinear optical effects	Optical modulators, integrated photonics

Hybrid Light-Emitting Materials	Inorganic phosphors in polymer matrices	Rare-earth doped oxides with polymer host	Strong luminescence, stability	OLEDs, lighting
Organic–Inorganic Ferroelectric Hybrids	PVDF–$BaTiO_3$ composites	Ferroelectric ceramic nanoparticles in polymer	High dielectric constant, flexibility	Sensors, memory devices
2D Layered Hybrids	MoS_2–organic dye composites, graphene–polymer hybrids	2D inorganic nanosheets functionalized with organic molecules	High conductivity, tunable surface chemistry	Transparent electrodes, flexible electronics
Self-Assembled Hybrids	Block copolymer–nanoparticle systems	Spontaneous organization of organic and inorganic components	Ordered nanostructures, enhanced device performance	Nanophotonics, plasmonics

Surface Engineering and Interface Chemistry of Advanced Materials

Surface engineering and interface chemistry tailor material properties like wettability, adhesion, and catalytic activity. Plasma treatment enhances the hydrophilicity of polymer surfaces like polyetheretherketone (PEEK), improving biocompatibility for orthopedic implants (Yoshida et al., 2015). Self-assembled monolayers (SAMs), such as thiol-based coatings on gold, control surface energy, enabling antifouling coatings for biomedical devices and marine applications (Love et al., 2005).

In composites, interface chemistry is critical. Functionalizing carbon nanotubes with epoxy groups improves adhesion in polymer composites, increasing tensile strength by 35% for aerospace components (Ma et al., 2020). Atomic layer deposition (ALD) enables precise surface coatings, such as TiO2 on lithium-ion battery anodes, reducing capacity fade and extending cycle life by 50% (Jung et al., 2012).

In catalysis, surface engineering optimizes active sites. For example, Ni nanoparticles on Al2O3 supports, modified with sulfur, enhance methane reforming activity for hydrogen production (Cargnello et al., 2014). Advanced characterization, like scanning tunneling microscopy, provides atomic-scale insights into surface interactions, enabling precise control over material performance across applications.

Materials Chemistry for Biomedical Applications

Materials chemistry is transforming biomedical applications, from drug delivery to regenerative medicine. Biocompatible polymers like poly(lactic-co-glycolic acid) (PLGA) are used in nanoparticles for controlled drug release. PLGA nanoparticles encapsulating cisplatin achieve sustained release over months, improving chemotherapy efficacy (Danhier et al., 2014). Hydrogels, such as polyethylene glycol (PEG)-based systems, mimic extracellular matrices, supporting stem cell differentiation for cartilage repair (Khademhosseini & Langer, 2010).

Bioactive ceramics, like hydroxyapatite (Ca10(PO4)6(OH)2), promote bone regeneration in dental implants due to their osteoinductive properties (Hench, 2018). Surface functionalization with RGD peptides enhances cell adhesion, improving implant integration (Shin et al., 2005). In diagnostics, magnetic nanoparticles, such as Fe3O4 coated with silica, enable sensitive detection of cancer biomarkers like HER2, achieving detection limits below 0.1 ng/mL (Liu et al., 2021).

Bioresorbable electronics, using magnesium alloys, degrade safely in the body, enabling temporary implants for monitoring wound healing (Kang et al., 2018). These advancements highlight materials chemistry's role in improving healthcare through tailored biomaterials.

Sustainable Synthesis and Processing of Advanced Materials

Sustainable synthesis is critical for minimizing the environmental impact of advanced materials. Green chemistry principles guide eco-friendly processes. For example, bio-based polymers like polyhydroxyalkanoates (PHA) are produced from microbial fermentation of agricultural waste, reducing carbon emissions by 60% compared to petroleum-based plastics (Vink et al., 2022). Solvent-free synthesis, such as ball milling, produces covalent organic frameworks (COFs) for gas storage, eliminating toxic solvents and reducing waste (Friscic et al., 2021).

Additive manufacturing, or 3D printing, minimizes material waste. For instance, 3D-printed nickel alloys for turbine blades reduce material use by 45% compared to traditional casting (Frazier, 2016). Chemical recycling of polystyrene into monomers achieves 95% recovery rates, supporting a circular economy (Rahimi & García, 2019).

Energy-efficient processing, like ultrasound-assisted synthesis, reduces energy consumption in nanomaterial production by 65% (Clark & Sutton, 1998). Life cycle assessments (LCAs) optimize processes, as seen in the sustainable production of carbon nanotubes, lowering environmental impact by 40% (Arvidsson et al., 2016). These approaches ensure advanced materials are produced sustainably, aligning with global environmental goals.

Summary

Advanced materials chemistry is driving innovation across energy, healthcare, electronics, and sustainability. Functional materials enhance energy storage and conversion, while smart polymers enable responsive systems for drug delivery and robotics. Hybrid organic-inorganic materials advance optoelectronics, and surface engineering optimizes material performance. Biomedical applications benefit from biocompatible materials, and sustainable synthesis ensures minimal environmental impact. By integrating interdisciplinary approaches and sustainable practices, this field is shaping a future where materials meet global challenges. Continued research and collaboration will further amplify its impact across industries.

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Chemical profile, analysis and extraction methods of olive leaf

Ali CAPAN

1. Introduction

In recent years, the use of natural raw materials in the food, pharmaceutical, and cosmetic industries has been increasing. Especially medicinal and aromatic plants stand out in these sectors due to their functional components (Khalil et al., 2024). Among these plants, the olive tree (Olea europaea L.), whose true origin is unknown, has been a part of the Mediterranean landscape since prehistoric times (Ronca, Marques, et al., 2024). This plant thrives in hot and dry summers; traditionally, it represents nobility, wisdom, health, peace, and victory (de Oliveira et al., 2024). The olive tree is a long-lived plant that can remain green in all seasons. It has narrow, long leaves. The olive tree, an evergreen species, covers a total area of 10.8 million hectares and is cultivated in 67 countries, particularly in the Mediterranean basin (Selim et al., 2022). The olive tree has attracted attention for centuries due to its cultural and economic value; today, it stands out for its antioxidant properties thanks to its rich phenolic content (Pasković et al., 2020; Zakraoui et al., 2023).

Olive leaves are one of the most important byproducts of olive cultivation, second only to olive oil in nutritional value (Mir-Cerdà et al., 2024) . Olive leaves are one of the most nutritious parts of the olive tree, second only to the fruit and oil production. These leaves make up 4-7% of olive processing residues, approximately 25% of pruning residues, up to 10% of the total weight of harvested olives, and 5% of olive oil byproducts (Mushtaq et al., 2025). It is estimated that the total amount of olive leaves that can be collected in Spain alone is approximately 750,000 tons per year (Espeso et al., 2021). The amount of accumulated olive leaves can exceed one million tons annually worldwide (Khelouf et al., 2023).

Oleuropein, the dominant phenolic compound in olive leaves, typically constitutes 70-97% of total phenolics; its concentration varies from 2,000 to 8,000 mg/100 g dry matter depending on the variety and extraction method (Ramírez et al., 2022; Zhang et al., 2022). Other important phenolic compounds include hydroxytyrosol, verbascoside, tyrosol, and various phenolic acids (e.g., gallic, ferulic, caffeic, syringic, coumaric) (Borghini et al., 2024; Chaji et al., 2023).

Triterpenic acids, particularly oleanolic and maslinic acids, are present in significant amounts (up to 35 mg/g dry weight), and their levels vary depending on the variety and extraction method (Baccouri et al., 2022; Kabbash et al., 2023). Mannitol, the main sugar with concentrations ranging from 4 to 22 g/kg, is particularly high in some varieties (Kokkotos et al., 2024; Lama-Muñoz et al., 2020). Olive leaves also contain iridoids, secoiridoids, coumarins, and lignans, which contribute to their diverse bioactive profiles (Ilgaz et al., 2024; Zhang et al., 2022). The lignocellulosic part of olive leaves contains cellulose, hemicellulose,

and lignin (lignin content is approximately 15%), making them suitable for biorefining and industrial applications (Lama-Muñoz et al., 2020). Mineral elements such as potassium, calcium, magnesium, phosphorus, iron, and zinc are present, and their content is influenced by genotype, environment, and agricultural practices (López-Salas et al., 2024; Ronca, Duque-Soto, et al., 2024). The mineral content contributes to the nutritional and therapeutic value of olive leaves, supporting their use as a dietary supplement and functional ingredient (Chaji et al., 2023; Zakraoui et al., 2023). Volatile compounds (e.g., β-caryophyllene, α-humulene, myristicin, oleic acid) and amino acids, which contribute to the nutritional and sensory properties of olive leaves, have also been detected (Fayek et al., 2024; Grubić Kezele & Ćurko-Cofek, 2022; Jurišić Grubešić et al., 2021).

The chemical composition of olive leaves is highly variable depending on the variety, geographical origin, season, environmental stress, and processing or extraction method (Contreras et al., 2020; Martín-García et al., 2020). For example, wild varieties often have higher phenolic and flavonoid content, while commercial varieties may contain more mannitol (Razola-Díaz et al., 2025). Drying techniques (e.g., freeze-drying, oven-drying, air-drying) significantly impact the yield and profile of bioactive compounds (Šimat et al., 2022; Wang et al., 2021). Extraction techniques are critical for maximizing the yield and purity of these bioactives. While traditional methods such as maceration and Soxhlet extraction are still in use, modern technologies—including UAE, MAE, PLE, SFE, and DES/NADES—offer improved efficiency, reduced solvent use, and enhanced selectivity (Contreras et al., 2020; Mir-Cerdà et al., 2024; Sánchez-Gutiérrez et al., 2021). Advanced analytical techniques such as HPLC, LC-MS/MS, GC-MS, and multivariate statistical analyses allow for detailed chemical profiling and differentiation of olive leaf varieties and origins (Guetat et al., 2025). Olive leaf powders and extracts are incorporated into edible films, food packaging, and encapsulated products to enhance antioxidant capacity, stability, and functional properties (Gerasopoulos et al., 2025; Ronca, Duque-Soto, et al., 2024). These applications evaluate the physicochemical properties of olive leaves for food, nutraceutical, and cosmetic purposes.

The purpose of this section is to provide a reference source for industry professionals and policy applications, summarizing the extensive bioactive compounds found in olives, discussing current advancements in their extraction and characterization, and highlighting the potential role of olives in applications.

2. Olive Leaf

The olive tree (Olea europaea L.) is one of the oldest and most important agricultural plants in the Mediterranean basin. The olive tree, which has large growers both economically and culturally, is the basis for olive oil and table olive production (Çapan et al., 2025; Evon et al., 2025). The olive tree is known for its drought tolerance and longevity, which is why it is also called the "immortal tree" (Rotondi et al., 2025; Zhang et al., 2022). The olive tree is cultivated in approximately 10.8 million hectares across 67 countries worldwide. Intensive production occurs in the Mediterranean basin, where the olive tree has both economic and

growth characteristics (Ronca, Duque-Soto, et al., 2024). There are over 2600 varieties of olives worldwide. This diversity arises from both natural selection and human-created breeding efforts (Marchioni et al., 2024).

Olive leaves, olive oil, and table olive industries are a significant byproduct, produced in large quantities annually. Millions of tons of olive leaf waste are generated globally each year, leading to significant environmental and economic consequences (Mir-Cerdà et al., 2024; Selim et al., 2022). Olive oil production is concentrated in Mediterranean countries, which account for approximately 98% of global production. Olive cultivation and processing generate a vast amount of byproducts, including olive leaves (Selim et al., 2022). Olive leaves make up approximately 10% of the total weight of olives brought to the mill (Şahin & Bilgin, 2018). For example, Spain: Spain alone produces approximately 1.25 million tons of olive leaf waste annually, which accounts for about 50% of the total global production (Espeso et al., 2021).

Olive leaves are generally lance-shaped, have a tough, leathery texture, and a thick cuticle (Figure 1). While there are few trichomes on the upper (adaxial) surface, the lower (abaxial) surface is densely covered with trichomes, which contribute to water retention and protection against environmental stress (Gholami et al., 2022). Leaf area varies significantly among cultivars (2.9–9.5 cm^2), and structural features such as petiole flexibility, leaf thickness, and cuticle wax content are linked to drought resistance (Kassout et al., 2025; Marchioni et al., 2024). For example, leaves collected from home gardens often have a larger surface area and higher dry matter and ash content, while those collected from public spaces are smaller and thinner (Ibrahim et al., 2024) stomatal density and size of olive leaves also vary, affecting gas exchange and water use efficiency (Razouk et al., 2022; Tunç et al., 2023).

Şekil 1. Olive (*Olea europaea* L.) leaves (Borjan et al., 2020)

Olive leaf is a plant resource that stands out for its physical parameters such as structural durability, high lignin and cellulose content, dense trichome structure, and surface wettability (Gerasopoulos et al., 2025). The interaction between physical structure and chemical composition not only supports the plant's resilience but also increases the value of olive leaves as a byproduct for nutraceutical, food, and industrial applications (Cardoni et al., 2022; Grabska-Zielińska et al., 2025).

3. Chemical profile of olive leaf

Olive leaf is one of the plant materials that stands out for its wide range of chemical components (Table 1). Olive leaf has a rich phytochemical profile containing over 150 bioactive compounds (Ramírez et al., 2022). Phenolic compounds make up a significant portion of the chemical profile, including oleuropein, hydroxy-oleuropein, secoiridoid derivatives, flavonoids (luteolin, apigenin, quercetin, kaempferol), phenylethanoids (verbascoside), and phenolic acids (ferulic, caffeic, gallic, syringic, coumaric) (Razola-Díaz et al., 2025). Additionally, triterpenic acids such as oleanolic and maslinic acid are also found in significant quantities and contribute to the plant's pharmacological potential (Khelouf et al., 2023; Zhang et al., 2022).

Olive leaves are rich in lignocellulosic components such as cellulose, hemicellulose, and lignin, as well as sugars (mannitol, glucose, fructose, sucrose), fatty acids, essential oils, vitamins (tocopherols, carotenoids, chlorophylls), and minerals (potassium, calcium, magnesium, phosphorus, iron, zinc) (Lama-Muñoz et al., 2020). This diversity supports the use of olive leaves in food, nutraceutical, and industrial applications.

Table 1. Phytochemical composition of olive leaves: principal compound groups, representative constituents, and approximate concentrations

Compound Class	**Representative Compounds**	**Approx. Concentration Range**	**Selected References**
Secoiridoids	Oleuropein, oleuropein aglycone, hydroxyoleuropein, ligstroside, oleacein	Dominant group; oleuropein reaching several g/100 g DW	(Contreras et al., 2020; Gagour et al., 2024; Palmeri et al., 2022)
Phenolic Alcohols	Hydroxytyrosol, tyrosol, glucosides	Few hundreds mg/100 g	(Mir-Cerdà et al., 2024; Ramírez et al., 2022; Romani et al., 2019)
Phenolic Acids	Caffeic, ferulic, gallic, syringic acids	Trace – tens of mg/100 g	(Dobrinčić et al., 2020; Esther et al., 2021; Martín-García et al., 2020)
Phenylethanoids	Verbascoside, isoverbascoside	Few hundreds mg/100 g	(Mir-Cerdà et al., 2024)
Flavonoids	Luteolin, apigenin, diosmetin, quercetin, rutin, kaempferol	Several mg/g; glycosides often higher than aglycones	(Borghini et al., 2024; Magyari-Pavel et al., 2024; Wang et al., 2021)
Triterpenic Acids	Oleanolic, maslinic, ursolic acids	Tens of mg/g DW; oleanolic acid most abundant	(Cláudio et al., 2018; Palmeri et al., 2022)

Triterpenic Alcohols	Erythrodiol, uvaol, lupeol isomers	Trace – few mg/g	(Mushtaq et al., 2025; Olmo-García et al., 2018; Ramírez et al., 2022)
Sugars (Major)	Mannitol, glucose, fructose, sucrose	Several g/kg; mannitol a dominant sugar	(Ramírez et al., 2022; Razouk et al., 2022)
Sugars (Minor)	Galactose, myo-inositol, raffinose, stachyose	Trace – few %	(Gagour et al., 2024; Sánchez-Gutiérrez et al., 2025; Zouari et al., 2020)
Lipids (Crude)	Total lipid fraction	Around 1–10% DW	(Guetat et al., 2025; Panou & Karabagias, 2025; Rahmanian et al., 2015)
Fatty Acids	α-Linolenic, oleic, linoleic, palmitic acids	α-Linolenic predominant	(de Oliveira et al., 2024; Ferreira et al., 2023; López-Salas et al., 2024)
Volatiles	(E)-2-hexenal, benzaldehyde, β-caryophyllene, α-humulene	Variable; (E)-2-hexenal often dominant	(Grubić Kezele & Ćurko-Cofek, 2022; Ilgaz et al., 2024; Jurišić Grubešić et al., 2021)
Vitamins (Tocopherols)	α-, β-, γ-tocopherol, α-tocotrienol	Few tens mg/100 g	(Baccouri et al., 2022; de Oliveira et al., 2024)
Other Vitamins	Vitamin A, Vitamin C	Low mg/100 g range	(de Oliveira et al., 2024; Panou & Karabagias, 2025)
Pigments	β-Carotene, lutein, chlorophylls	Carotenoids in tens µg/g; chlorophylls several hundred µg/g	(Franić et al., 2024; Pasković et al., 2020; Zakraoui et al., 2023)
Minerals	K, Ca, Mg, Fe, Zn, Cu, Mn	Highly variable; %–mg/g levels depending on soil	(Chaji et al., 2023; López-Salas et al., 2024; Magyari-Pavel et al., 2024)
Proteins & AAs	Glutamic acid, aspartic acid	Around 5–10% DW	(Evon et al., 2025; Panou & Karabagias, 2025; Zandona et al., 2025)
Sterols	β-Sitosterol, campesterol, stigmasterol	Trace	(Gagour et al., 2024; Panou & Karabagias, 2025)
Hydrocarbons	Heneicosane, tetratriacontane, squalene	Trace	(Olmo-García et al., 2018; Razola-Díaz et al., 2025)
Ash & Organic Matter	Inorganic residue, organic fraction	Ash ≈ few %; organic matter >70%	(Evon et al., 2025; Ferreira et al., 2023; Rahmanian et al., 2015)

Abbreviations: DW: Dry Weight; FA(s): Fatty Acid(s); mg/g: milligrams per gram; mg/100 g: milligrams per 100 grams; g/kg: grams per kilogram; µg/g: micrograms per gram; mg/kg: milligrams per kilogram; OM: Organic Matter.

3.1. Phenolic Compounds in Olive Leaves

Studies on olive leaves have identified over 65 phenolic compounds (Kabbash et al., 2023; Martín-García et al., 2020; Martínez-Navarro et al., 2023). The total phenolic content of olive leaves can reach up to 75.58 g/kg on a fresh weight basis (Mir-Cerdà et al., 2024; Palmeri et al., 2022). Secoiridoids are the main phenolic group, accounting for approximately 70% of the analyzed phenolic compounds (Razola-Díaz et al., 2025). The most dominant phenolic compound found in olive leaves is oleuropein, which accounts for approximately 74–97% of total phenols and has been reported at concentrations ranging from 2,000 to 8,000 mg/100g dry matter, depending on the variety and extraction method (Zandona et al., 2025). Oleuropein is found in high amounts in olive fruit during early developmental stages and decreases as the fruit ripens due to enzymatic processes. In contrast, the amount of oleuropein in olive oil is negligible (Koutra et al., 2025). According to some sources, the amount of oleuropein in olive oil ranges from 0.005% to 2%, in the production by-product called alperujo it is 0.87%, and in olive leaves it ranges from 1% to 14% (Yıldız et al., 2011). Some studies have reported that these values are even higher (Khalil et al., 2024). Although oleuropein is also found in the pulp, pits, and skin of olive fruit, the highest concentration has been detected in olive leaves. Oleuropein, hydroxyoleuropein, oleuropein aglycone, 2″-methoxyoleuropein isomers, demethyloleuropein, and oleuropein diglucoside isomers are present (Razola-Díaz et al., 2025). Ligstroside, Ligstroside aglycone, oleoside, secologanoside, oleacein elenolic acid hexosides, lucidumoside, and *p*-coumaroyl secologanic acid are other important secoiridoids found in olive leaves (Deng et al., 2025; Palmeri et al., 2022).

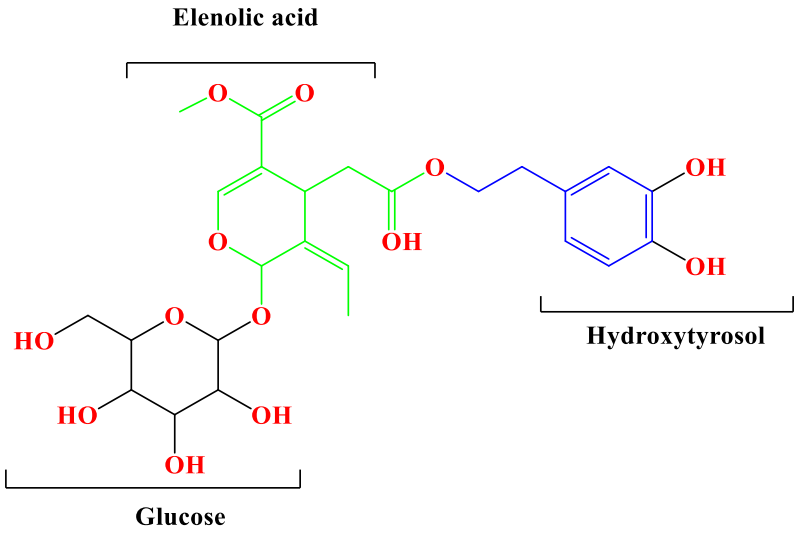

Figure 2. Proposed structure of oleuropein

Other important phenolic compounds include hydroxytyrosol (250–700 mg/100g DM), and oleuropein (Figure 2) and verbascoside (Figüre 3), which are major phenolic metabolites (Tarchi et al., 2025). Various phenolic alcohols such as 3-hydroxytyrosol and tyrosol have a high capacity to neutralize free radicals and are effective in reducing cellular oxidative stress (Romani et al., 2019). It is known for its anti-inflammatory, anti-tumor, antiviral, and antibacterial effects, and is an approved phenolic compound in the EU. Hydroxytryrosol 1-glucoside and 4-glucoside forms are also present in olive leaves (Ramírez et al., 2022). Verbascoside (216–673 mg/100g DM) is a significant phenylpropanoid glycoside (Dobrinčić et al., 2020; Khelouf et al., 2023; Mir-Cerdà et al., 2024). Among the main metabolites of verbaskosit are hydroxytyrosol and hydroxycinnamic acids such as caffeic acid, ferulic acid, coumaric acid, and sinapic acid, which, although present in low amounts, exhibit high antioxidant properties (Palmeri et al., 2022; Zhang et al., 2022). Additionally, olive leaves contain benzoic acid derivatives such as 3,4-dihydroxybenzoic acid and 4-hydroxybenzoic acid (Esther et al., 2021; Martín-García et al., 2020). These simple phenolic compounds have been detected in significant quantities in olive leaves (Dobrinčić et al., 2020; Mushtaq et al., 2025).

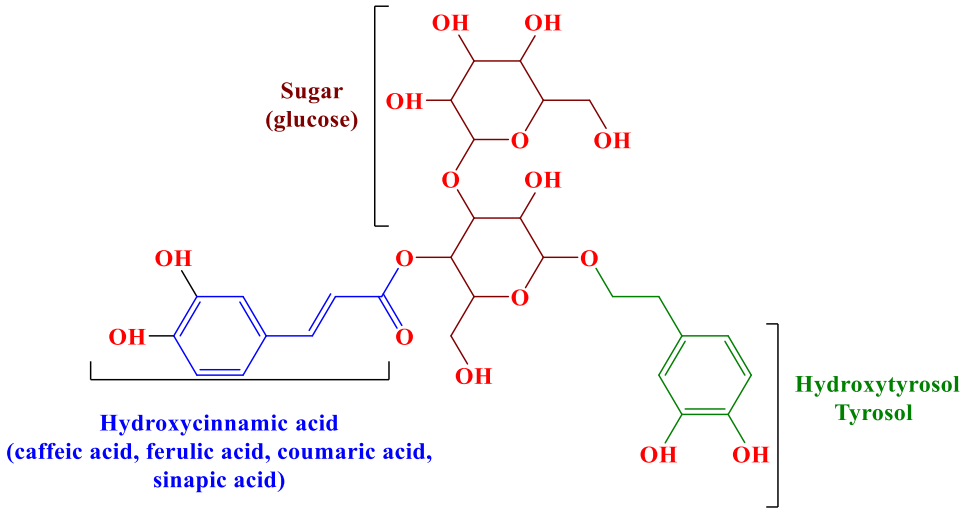

Figure 3. Proposed structure of verbascoside

Olive leaves contain various flavonoid compounds, including flavones such as luteolin, apigenin, diosmetin (Kabbash et al., 2023), luteolin-7-O-glucoside (Zakraoui et al., 2023), luteolin-3',7-di-O-glucoside, luteolin-4',7-di-O-glucoside, apigenin-rutinoside, apigenin-glucoside (Difonzo et al., 2021), luteolin-rutinoside, and diosmin (Ciriminna et al., 2025). Additionally, they include flavanones like hesperidin (Ciriminna et al., 2025) and dihydroflavonols such as. Also present are flavonols, including quercetin, rutin, kaempferol, and galangin, along with quercetin-3-O-glucoside, quercetin-rhamnoside, and the isomer of quercetin-3-O-glucoside (either quercetin-3-O-galactoside or quercetin-4’-O-glucoside) (Borghini et al., 2024; Magyari-Pavel et al., 2024). Glycosylated flavonoids are approximately 10 times more abundant than their aglycone forms. Olive leaves Luteolin-7-O-glucoside, kaempferol-7-O-glucoside and quercetin are the most abundant flavonoids (Figure 4) (Zhang et al., 2022).

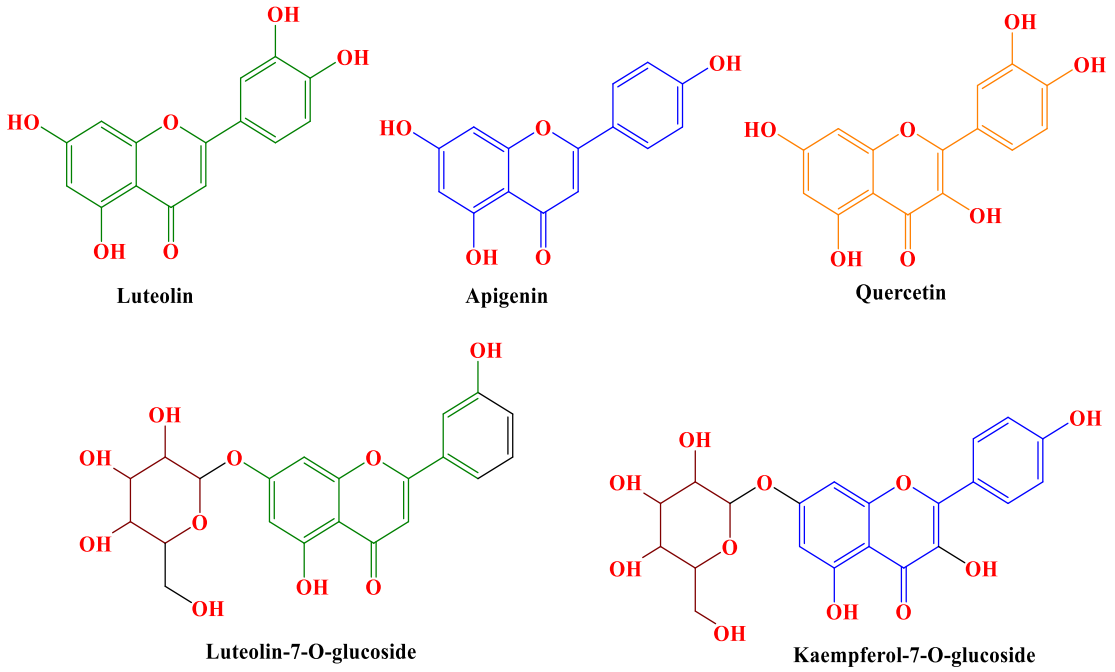

Figure 4. Chemical structure of some important flavonoids in olive leaves

Phenolic compounds in olive leaves are found in both free (FP) and bound (BP) forms. The free phenolic fraction is rich in flavonoids, triterpenic acids, and iridoids, while the bound phenolics primarily contain phenolic acids (e.g., caffeic, ferulic, sinapic, and *p*-coumaric acids) and hydroxytyrosol (Li et al., 2023). Studies have shown that the free phenolic fraction has higher values than bound phenolics in terms of total phenolic and flavonoid content and antioxidant capacity(Mir-Cerdà et al., 2024). While these compounds show supportive effects on the immune system, they also play a role in anti-inflammatory processes (Talhaoui et al., 2015).

3.2. Triterpenic acids found in olive leaves

Olive leaves contain a significant amount of triterpenic acid and alcohol. Triterpenes are found in high concentrations, especially in the waxy outer surface of olive leaves. In addition to playing a role in the plant's defense mechanisms, these compounds exhibit various bioactive effects on human health (Olmo-García et al., 2018; Ramírez et al., 2022). The most common triterpenic acids found in olive leaves are oleanolic acid (Figure 5), maslinic acid, and ursolic acid (up to 35 mg/g dry weight) (Ramírez et al., 2022). Betulinic acid, corosolic acid, dihydroxy oleanolic acid isomers, and hydroxy-oxo-oleanenoic acids have been identified in olive leaves, with oleanolic acid being the primary triterpenic acid present (averaging 15.83 g/kg). It is a component with high commercial value, reaching up to €1200 per gram depending on its purity (Cláudio et al., 2018; Palmeri et al., 2022; Pyrka et al., 2023).

Additionally, compounds such as erythrodiol and uvaol, which are triterpenic diols, have also been found(Magyari-Pavel et al., 2024; Ramírez et al., 2022). For example, Urs-12-en-28-ol and Lupeol isomers have been detected in olive leaves. Erythrodiol has been detected in olive leaves and is associated with neuroprotection (Grubić Kezele & Ćurko-Cofek, 2022; Mushtaq et al., 2025). Triterpenic acid and Triterpen Alcohol levels are influenced by factors such as olive variety and harvest time. It has been reported that the concentration of these compounds is higher in leaves collected, especially during the summer months (Martín-García et al., 2020). Although processing conditions like drying temperature can affect phenolic compounds, triterpenic acids are generally less influenced by these variables (Pyrka et al., 2023). Additionally, studies have shown that the triterpenic acid content is higher in varieties with a particularly high fat content (Zhang et al., 2022). Other structures commonly found in these compounds include erythrodiol and uvaol (Olmo-García et al., 2018)

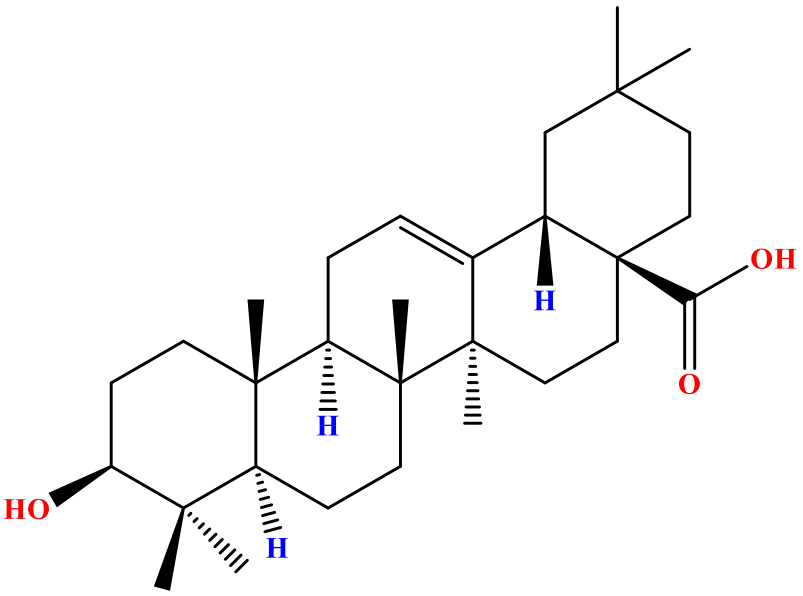

Figure 5. Possible structure of oleanolic acid

3.3 Sugars found in olive leaves

Olive leaf is a notable plant source due to its diverse carbohydrate content. Among the most common sugars found in leaves are glucose, fructose, mannitol, and sucrose (3% dry weight); other carbohydrates such as hexose, hexitol, dihexose, galactose, myo-inositol, galactinol, raffinose, and stachyose were detected in lower proportions (Evon et al., 2025; Razouk et al., 2022; Sánchez-Gutiérrez et al., 2025). Glucose, sucrose, fructose, and mannitol make up approximately 90% of the total soluble carbohydrates. The total carbohydrate content varies from 8.7% to 32.6% depending on the variety (Kokkotos et al., 2024). These rates can vary depending on environmental conditions, season, irrigation status, and fertilization practices (Gagour et al., 2024). Specifically, carbohydrate accumulation increases during the flowering period, while a decrease is observed in these reserves during fruit development (Zouari et al., 2020).

Innovative methods such as steam explosion and ultrasound-assisted extraction are used to efficiently extract sugars from olive leaves. Under suitable conditions, sugar recovery of up to 18% per dry leaf can be achieved (Sánchez-Gutiérrez et al., 2025). Additionally, studies have shown that glucose, fructose, and sucrose increase during the oral and gastric phases of digestion and decrease during the intestinal phase; however, they exhibit high bioavailability (Sánchez-Gutiérrez et al., 2025).

The carbohydrate profile in olive leaves is an important indicator not only in terms of energy storage but also for stress tolerance and metabolic adaptation mechanisms (Zouari et al., 2020). These sugars, primarily mannitol (4 to 22 g/kg) (Figure 6), contribute to the functional properties of olive leaves and are potentially valuable for industrial use as a functional food ingredient or natural sweetener (Bilalov et al., 2025; Ibrahim et al., 2024).

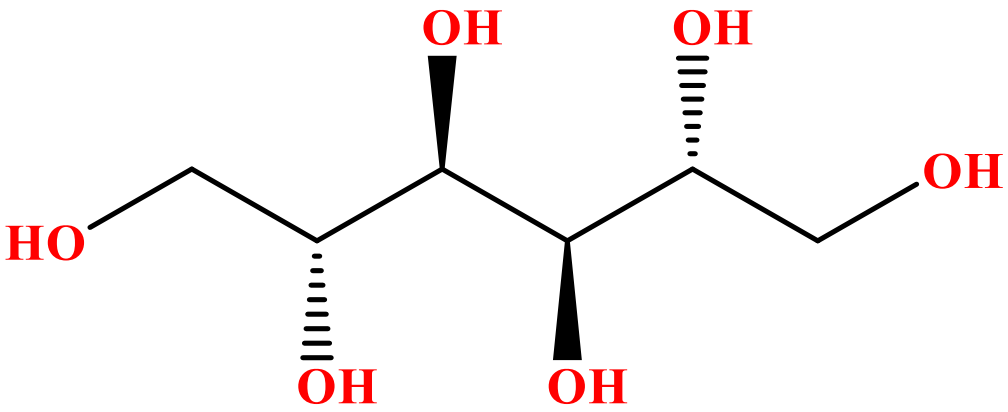

Figure 6. Possible structure of mannitol

3.4. Fatty acids and other bioactive compounds found in olive leaves

Olive leaf has a rich lipid profile containing both saturated and unsaturated fatty acids. In addition to the high proportions of important fatty acids such as linolenic, oleic, and palmitic acids, oxidized fatty acids like 9-Oxooctadeca-10,12-dienoic acid and Hydroxyoctadecadienoic acid have also been identified (Mushtaq et al., 2025). However, the high linolenic acid content in all varieties makes olive leaf a particularly noteworthy plant source, especially for n-3 PUFAs (Ferreira et al., 2023). These polyunsaturated fatty acids are known for their positive effects on cardiovascular health (Gagour et al., 2024; López-Salas et al., 2024). A total of 23 volatile compounds have been identified in olive leaves, including mainly aldehydes and alcohols (Ilgaz et al., 2024). A total of 23 volatile compounds were detected, with aldehydes and alcohols being the most dominant groups. (E)-2-hexenal was found to be the most concentrated compound among the total volatile compounds (22694.5 µg/L), followed by 2-decenal-(E) (20.43%), benzaldehyde (4.00%), and 2-undecanal (3.71%). Acetic acid, 1-methyl-4-(1-methylpropyl)-benzene, and benzyl alcohol are other important volatile compounds (Ilgaz et al., 2024; Jurišić Grubešić et al., 2021; Rahmanian et al., 2015). It has been detected in volatile compounds such as β-caryophyllene, α-humulene,

and myristicin. These fatty acids are critically important for cell membrane integrity and the regulation of inflammatory processes (Bilalov et al., 2025; Chaji et al., 2023). Additionally, Heneicosane, tetratriacontane, and docosane-like n-alkanes; octadecadienal-like fatty aldehydes; quinic acid and 12-hydroxyjasmonate sulfate; and amino acids such as glutamic acid and aspartic acid have been detected in olive leaves (Bilalov et al., 2025; Razola-Díaz et al., 2025). sterols like β-sitosterol are found in olive leaves and possess skin-protective properties (Mushtaq et al., 2025; Panou & Karabagias, 2025).

3.5. Vitamins and Minerals Found in Olive Leaves

Olive leaf stands out for its rich profile, particularly in terms of vitamin E and certain provitamin compounds. In addition to α-tocopherol, other tocopherol derivatives such as β-tocopherol, γ-tocopherol, and α-tocotrienol have also been detected in small amounts in olive leaves (Ferreira et al., 2023). Additionally, it has been reported that olive leaves contain 5.10 mg of vitamin A and 36.64 mg of vitamin C per 100 g of dry matter (de Oliveira et al., 2024; Panou & Karabagias, 2025). These vitamins are important for immune system functions and antioxidant defense mechanisms (Ferreira et al., 2023). Olive leaf is rich in carotenoids and chlorophylls in addition to vitamin E. Among carotenoids, β-carotene and lutein are particularly prominent. Lutein is defined as an effective provitamin in the prevention of eye diseases such as age-related macular degeneration (Franić et al., 2024). According to the study by Tarchoune et al. (2019), the total carotenoid content in the leaves of the Neb Jmel and Oueslati varieties was determined to be 26.90 and 44.33 μg/g, respectively. In the same study, the total chlorophyll amounts were reported as 506.08 μg/g and 829.29 μg/g, respectively (Tarchoune et al., 2019). The natural source of vitamin E and carotenoids in olive leaves makes it a valuable botanical ingredient that can be utilized in various industrial fields such as food supplements, cosmetic products, and animal feed (Şahin & Bilgin, 2018; Tarchoune et al., 2019). In olive leaf extracts, in addition to mineral elements such as potassium, calcium, magnesium, and phosphorus, metals like Cd, Ni, Mn, Zn, Cu, Cr, Fe, and Al have been detected. Additionally, Pb, As, and Co were found to be below the detection limit (López-Salas et al., 2024; Magyari-Pavel et al., 2024). These contents are influenced by genotype, environment, and agricultural practices (Chaji et al., 2023; Franić et al., 2024).

3.6. Lignocellulosic compounds found in olive leaves

The lignocellulosic part of olive leaves contains cellulose, hemicellulose, and lignin (with a lignin content of approximately 15%), making them suitable for biorefining and industrial applications (Chaji et al., 2023). For example, olive leaves offer many possibilities for the biorefinery sector as lignocellulosic biomass. Fermentable sugars (glucose and xylose) obtained from cellulose and hemicellulose can be used for the production of ethanol and xylitol (Guetat et al., 2025) (a high-value product used as a sweetener in the food industry), respectively. Mannitol can be used for various applications in the food and pharmaceutical industries (Figure 5). Lignins, on the other hand, can be used in the manufacture of resins, composites, polymers, aromatic compounds, carbon fiber, etc. (Ibrahim et al., 2024; Lama-Muñoz et al., 2020).

Additionally, olive leaves also show variability in terms of their overall organic matter (76.4–92.7% dry matter), crude protein (6.31–10.9% dry matter), and crude fat (2.28–9.57% dry matter) content (Cardoni et al., 2022; Evon et al., 2025; Rahmanian et al., 2015; Sarı et al., 2017). The moisture content of olive leaves was determined to be 1.64%; volatile matter 78.64%; ash 3.66%; fixed carbon 16.06%; and the higher heating value was determined to be 5.08 kcal/g. The high fixed carbon content and low ash ratio make olive leaf a suitable material for pore formation during the carbonization process (Sarı et al., 2017).

4. Factors Affecting the Chemical Profile of Olive Leaves

The chemical composition of olive leaves is highly variable depending on the variety, geographical origin, seasonal variation, agricultural practices and processing or extraction method (Franić et al., 2024; Zakraoui et al., 2023) (Figure 7). A more detailed examination of the biological effects of these components could further optimize the industrial use of olive leaves.

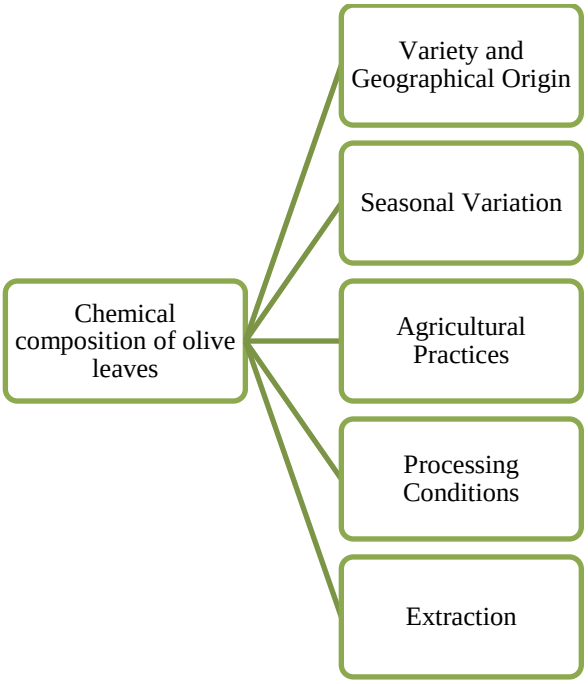

Figure 7. Factors affecting the chemical composition of olive leaves

The phenolic acid profile and amounts vary significantly between different olive varieties and seasons. Especially oleuropein and its derivatives stand out as inter-varietal distinguishing markers (Orak et al., 2019; Palmeri et al., 2022). For example, Deng et al. (2025) stated that among three olive varieties grown in China (Arbosana, Arbequina, and Picholine), young Picholine leaves exhibited the highest content (Deng et al., 2025). Similarly, wild varieties often have higher phenolic and flavonoid content, while commercial varieties may contain more mannitol (Bilalov et al., 2025; Chaji et al., 2023). Environmental factors such as altitude and soil composition also affect phenolic synthesis (Zakraoui et al., 2023).

The seasonal variation in phenolic compounds showed the most pronounced fluctuation during the summer and autumn months. The optimal sampling time is during the spring and winter months (Wang et al., 2021). Tanrısever (2024) reported that in a study of 8 local varieties specific to the Mardin region, the phenolic content of the leaves reached its highest level in November and March (Tanrisever et al., 2024). Olive leaves are harvested in the early morning in modern systems for higher phenolic compound content (Ezzarrouqy et al., 2024).

Foliar fertilization has significant effects on the mineral and carbohydrate metabolism of both the leaves and roots of olive trees. Fertilization leads to both qualitative and quantitative changes in the nutrient profile (Zouari et al., 2020). The use of nitrogenous fertilizers and biostimulants in particular helps the tree meet its seasonal needs by promoting the accumulation of primary metabolites (carbohydrates) in the leaves. It is important for developing fertilization strategies for olive cultivation under rainfall-dependent conditions (Zouari et al., 2020).

Drying temperature and grinding degree directly affect the extraction yield of phenolic compounds (El Adnany et al., 2024). Cör et al. (2022) found that drying at room temperature is the most suitable method for oleuropein yield in the Istrska Belica and Leccino varieties, while freeze-drying is not suitable (Cör Andrejč et al., 2022). Zhang ve meslektaşları, farklı kurutma tekniklerinin aroma profili ve biyoaktivite üzerindeki etkilerini incelemiş ve sıcak hava kurutmasının fenolik bileşikleri geri kazanmada etkinliğini vurgulamıştır.(Zhang et al., 2022). Sueishi & Nii (2020) stated that drying converts some phenols into less oxidatively active forms. A decrease in phenolic compounds is observed when the drying temperature exceeds 50°C [83]. Adnany et al. (2024) stated that the highest yield of polyphenols and pigments was obtained from olive leaves dried at 80°C and ground to a size of <25 µm (El Adnany et al., 2024).

4.1 Methods used in olive leaf extraction

Extraction techniques significantly affect the yield, composition, and bioactivity of olive leaf extracts (Ronca, Duque-Soto, et al., 2024). The non-structural components of olive leaves include phenolic compounds, mannitol, peptides, proteins, and soluble sugars (Kokkotos et al., 2024). These compounds are generally obtained in the form of aqueous and ethanolic extracts. Aqueous extracts are particularly rich in glucose and mannitol, while smaller amounts of xylose, galactose, arabinose, and xylitol are also detected. Notably, hot water extraction is preferred for recovering high amounts of oleuropein and total phenolics without the use of organic solvents (Esther et al., 2021; Monteleone et al., 2021). In contrast, ethanolic extracts contain pigments and bioactive phenolic compounds, and solvent mixtures with 50–80% ethanol/water have been reported to provide higher yields (Li et al., 2023; Şahin & Bilgin, 2018). Thus, solvent composition and extraction conditions directly influence the chemical profile of olive leaf extracts.

Conventional methods, such as maceration and Soxhlet extraction, are simple and widely used but present notable drawbacks, including long extraction times, low efficiency, and high solvent/energy consumption (Contreras et al., 2020; da Rosa et al., 2019; Şahin & Bilgin, 2018). In contrast, modern extraction techniques provide superior performance in terms of efficiency, selectivity, and sustainability.

Although maceration and Soxhlet methods are simple and low-cost, they have limited effectiveness due to their long processing time, high solvent consumption, and low efficiency (Table 2) (da Rosa et al., 2019; Sánchez-Gutiérrez et al., 2021). To address these shortcomings, Difference in Pressure Extraction (DPE) was developed, offering an environmentally friendly option by providing higher phenolic yield (273.5 mg GAE/g) in a short time (Khizrieva et al., 2022) Solar Heating Extraction, on the other hand, creates a low-cost and green alternative using only water and solar energy, achieving a higher total phenolic content compared to conventional methods; however, its dependence on weather conditions is a significant limitation (Carlucci et al., 2024)

Table 2. Traditional methods used in olive leaf extraction

Extraction Method	**Solvents Used**	**Extracted Bioactives and Reported Yields**	**Sustainability, Advantages, and Limitations**	**Key References**
Conventional Maceration / Soxhlet	Water, ethanol, methanol	Oleuropein, total phenolics; generally lower yield, lengthy process	Simple, low-cost, easy to scale; but solvent-intensive, less sustainable, time-consuming	(da Rosa et al., 2019; Sánchez-Gutiérrez et al., 2021)
Difference in Pressure Extraction (DPE)	Ethanol (reduced pressure)	Polyphenols, antioxidants; TPC up to 273.5 mg GAE/g	Greener than maceration; shorter time, higher efficiency	(El-Hadary et al., 2025; Khizrieva et al., 2022)
Solar Heating Extraction	Water (solar-assisted)	Polyphenols, flavonoids, antioxidants; TPC up to 189.6 mg GAE/g	Very green, low cost; higher yield than decoction/maceration; weather-dependent	(Carlucci et al., 2024; Ezzarrouqy et al., 2024)

Green extraction techniques stand out compared to conventional methods by offering higher yields, the use of environmentally friendly solvents, and shorter processing times (Table 3**)**. Ultrasound-assisted extraction (UAE) enhances the recovery of oleuropein, hydroxytyrosol, and flavonoids by 30–47% while preserving thermolabile compounds (Dobrinčić et al., 2020; Lama-Muñoz et al., 2020). Microwave-assisted extraction (MAE) increases phenolic yields by up to 82% and provides rapid results, although the risk of compound degradation at high power remains a limitation (Şahin & Bilgin, 2018). Pressurized liquid extraction (PLE) demonstrates high selectivity, particularly for secoiridoids and flavonoids, with yields reaching up to 158 mg/g DW; however, equipment costs are considerable (Huamán-Castilla,

Mamani Apaza, et al., 2024). Supercritical fluid extraction (SFE) is selective for triterpenes and lipophilic phenolic compounds, producing solvent-free extracts highly valued in the food and pharmaceutical industries, yet its large-scale application is restricted by high investment requirements (Kyriakoudi et al., 2024)

Table 3. Modern and green technologies used in olive leaf extraction

Extraction Method	**Solvents Used**	**Extracted Bioactives and Reported Yields**	**Sustainability, Advantages, and Limitations**	**Key References**
Ultrasound-Assisted Extraction (UAE)	Water, ethanol, NADES, DES	Oleuropein, hydroxytyrosol, flavonoids, proteins; up to 30–47% higher than conventional; TPC up to 80 mg/g; oleuropein up to 42.6 mg/g	Green, energy-efficient, scalable; preserves thermolabile compounds; requires optimization	(Dobrinčić et al., 2020; Ilgaz et al., 2024; Lama-Muñoz et al., 2020)
Microwave-Assisted Extraction (MAE)	Water, ethanol, DES/NADES	Oleuropein, total phenolics, quercetin; up to 82% higher than maceration; TPC up to 169 mg GAE/g DW; oleuropein 12.99 mg/mL	Green and scalable; high yield in short time; efficient for heat-stable compounds; risk of degradation at high power	(da Rosa et al., 2019; Karaogul & Nedjip, 2025; Şahin et al., 2017)
Pressurized Liquid Extraction (PLE)	Water, ethanol, glycerol	Secoiridoids, flavonoids, phenolics; very high yield up to 158 mg/g DW	Green and industrially suitable; high selectivity, short extraction time; higher equipment cost	(Huamán-Castilla, Mamani Apaza, et al., 2024; Lama-Muñoz et al., 2020)
Supercritical Fluid Extraction (SFE)	CO_2 + ethanol/ methanol /water	Triterpenes, fatty acids, oleuropein; moderate yield, oleuropein up to 1.9 mg/g	Green and scalable; solvent-free extracts; selective for non-polar compounds; requires high-cost equipment	(Debs et al., 2023; Kyriakoudi et al., 2024)

DES/NADES Extraction	Choline chloride + organic acids/sugars	Polyphenols, hydroxytyrosol, rutin, luteolin-7-O-glucoside; comparable or higher than ethanol, up to 15% more; TPC up to 55 mg GAE/g DW	Highly green and safe; scalable; tunable selectivity; viscosity can hinder mass transfer	(Alañón et al., 2020; Mir-Cerdà et al., 2024; Siamandoura & Tzia, 2023)
Magnetic Stirrer with Green Solvents	PPG, lactic acid, water	Oleuropein, verbascoside; extracts with high phenolic content and bioactivity	Green and energy-efficient; direct use in cosmetics without solvent evaporation; limited applications	(Huamán-Castilla, Díaz Huamaní, et al., 2024; Marijan et al., n.d.)
Organosolv Extraction (Glycerol/DES)	Glycerol, glycerol-based DES; 110 °C+	Polyphenols, hydroxytyrosol, luteolin; TPC up to 69.4 mg GAE/g	Greener than ethanol; effective under milder conditions; differentiated phenolic profile	(Khelouf et al., 2023; Tapia-Quirós et al., 2025)

In recent years, deep eutectic solvents (DES/NADES) have emerged as eco-friendly and tunable alternatives, achieving comparable or even 15% higher recovery of polyphenols and hydroxytyrosol than ethanol (Siamandoura & Tzia, 2023). Additionally, the use of magnetic stirring with green solvents has been reported to yield phenolic-rich extracts that can be directly applied in cosmetics (Marijan et al., n.d.). Organosolv extraction, employing glycerol and DES-based solvents, enables the recovery of differentiated phenolic profiles (Khelouf et al., 2023). Moreover, natural deep eutectic solvents (NaDES) have been proposed as sustainable tools aligned with circular economy principles, combining high selectivity with reduced environmental impact (Alañón et al., 2020; Mir-Cerdà et al., 2024)

Novel green extraction approaches provide promising alternatives for the efficient and sustainable recovery of bioactive compounds from olive leaves (*Table 4)*. Pulsed electric field (PEF) treatment enhances cell permeability, leading to a 15–38% increase in phenolic recovery, with the advantages of low energy consumption and scalability; however, the requirement for specialized equipment remains a limitation (Pappas et al., n.d.; Razola-Díaz et al., 2025). Ball milling-assisted extraction (BMAE) improves mass transfer via particle size reduction and achieves recovery rates of up to 79% for oleuropein and hydroxytyrosol, though additional purification of the extracts may be necessary (Xiang et al., 2024). Infrared-assisted extraction (IR) has been reported to provide yields over 30% higher than conventional water bath heating, offering a rapid and energy-efficient method, albeit still requiring further validation (Abi-Khattar et al., 2019).

Enzyme-assisted extraction (EAE), employing enzymes such as pectinase, cellulase, and viscozyme, enables remarkably high phenolic yields (up to 605.6 mg GAE/L) under mild conditions; nevertheless, enzyme cost and limited reusability restrict large-scale applications (Ramírez et al., 2022). Membrane-assisted extraction allows for selective concentration of oleuropein and phenolics, producing extracts with strong antioxidant capacity and demonstrating industrial potential (Castillo-Luna et al., 2023). Wall-breaking extraction (WBE) combined with deep eutectic solvents (DES) has achieved high yields of oleuropein (up to 88.9 mg/g DM) while also exhibiting strong antioxidant and antitumor potential, highlighting its applicability in functional product development (Pedrosa et al., 2022). Finally, freeze-drying (FD) has been shown to promote the in situ biotransformation of oleuropein into oleacein, resulting in enriched extracts through a cost-*effective and environmentally friendly method (ÜNVER & ÇELİK, 2022)*

Table 4. Supported Techniques Used in Olive Leaf Extraction

Extraction Method	**Solvents Used**	**Extracted Bioactives and Reported Yields**	**Sustainability, Advantages, and Limitations**	**Key References**
Pulsed Electric Field (PEF)	Water, ethanol	Hydroxytyrosol, oleuropein, phenolics; 15–38% higher than untreated	Green, low-energy, scalable; enhances cell disruption; requires specialized equipment	(da Rosa et al., 2019; Pappas et al., n.d.)
Ball Milling-Assisted Extraction (BMAE)	Water, ethanol, NADES	Oleuropein, luteoloside, hydroxytyrosol; recovery up to 79%	Green and scalable; enhances mass transfer via particle size reduction; extracts may require purification	(Cubero-Cardoso et al., n.d.; Xiang et al., 2024)
Infrared-Assisted Extraction (IR)	Water, ethanol	Oleuropein, hydroxytyrosol; yield >30% higher than water bath	Green and energy-saving; rapid; requires further validation	(Abi-Khattar et al., 2019; Debs et al., 2023)

Enzyme-Assisted Extraction (EAE)	Water + enzymes (pectinase, cellulase, viscozyme)	Polyphenols; TPC up to 605.6 mg GAE/L	Green and mild process; very high yield; enzyme cost and reusability may limit industrial application	(Ramírez et al., 2022; Vardakas et al., 2024)
Membrane-Assisted Extraction	Ethanol:Water (75:25), 50 °C, 90 min + UF/NF	Oleuropein, phenolics, flavonoids; oleuropein up to 119 mg/g	Green and scalable; efficient concentration; high antioxidant capacity	(Castillo-Luna et al., 2023; Magyari-Pavel et al., 2024)
Wall-Breaking Extraction (WBE) + DES	Choline chloride:ethylene glycol (1:2), 30% moisture, 140 s	Oleuropein, luteolin-7-O-glucoside, flavonoids; oleuropein up to 88.9 mg/g DM	Green and scalable; high yield; strong antioxidant and antitumor potential	(Papageorgiou et al., 2022; Pedrosa et al., 2022)
Freeze-Drying (FD) for Oleacein	N/A (drying method)	Oleacein (from oleuropein); significantly enriched	Green and scalable; promotes in situ biotransformation; cost-effective	(Evon et al., 2025; ÜNVER & ÇELİK, 2022)

The choice of extraction method should ultimately be guided by the target compounds, intended application, and sustainability considerations. For example, MAE, UAE, and PLE are particularly suitable for the recovery of total phenolics and antioxidants (da Rosa et al., 2019; Giacometti et al., 2021; Martín-García et al., 2020), PLE provides higher yields for secoiridoids and flavonoids (Martín-García et al., 2020; Mushtaq et al., 2025), while SFE is preferred for triterpenes and fatty acids (Mushtaq et al., 2025).

In conclusion, the extraction of olive leaves represents a dynamic and continuously evolving field that integrates both traditional and advanced methodologies with the aim of maximizing the yield, purity, and bioactivity of target compounds. Ongoing research combining different extraction techniques with drying strategies and green alternatives will further enhance the health-promoting potential of olive leaves while promoting sustainable practices in the food, nutraceutical, and pharmaceutical industries. Nevertheless, for long-term sustainability, there is a clear need for a transition toward greener extraction technologies(Contreras et al., 2020; Lama-Muñoz et al., 2020).

6. Analytical techniques used to determine the chemical profile of olive leaves

The characterization of bioactive compounds in olive leaves has advanced significantly, driven by the growing interest in valorizing this agricultural byproduct for food, nutraceutical, and pharmaceutical applications. A wide range of analytical techniques has been employed, spanning from classical chromatographic and spectrophotometric assays to advanced mass spectrometry, vibrational spectroscopy, and chemometric tools (Table 5). Among these, high-performance liquid chromatography (HPLC) coupled with different detectors (UV, DAD, MS) remains the reference method for qualitative and quantitative profiling of phenolics, flavonoids, and secoiridoids (Karaogul & Nedjip, 2025; Mir-Cerdà et al., 2024). Recent progress in liquid chromatography–mass spectrometry (LC-MS/MS, QTOF, Orbitrap HRMS) has enabled high-resolution identification of a broad spectrum of compounds, including minor metabolites present at trace levels (Beteinakis et al., 2024). Gas chromatography–mass spectrometry (GC-MS) provides complementary information for volatile constituents, triterpenoids, and fatty acids (Jurišić Grubešić et al., 2021; Mir Najibullah et al., 2023).

Spectrophotometric assays such as Folin–Ciocalteu, DPPH, ABTS, and CUPRAC continue to be widely applied for assessing total phenolic content and antioxidant activity (Difonzo et al., 2022; Khelouf et al., 2023). In parallel, vibrational spectroscopy (FTIR, ATR-FTIR) and nuclear magnetic resonance (NMR) offer rapid fingerprinting and structural elucidation, while elemental spectroscopic methods (ICP-MS, ICP-AES, LPAS) are particularly valuable for authentication and traceability of geographical origin (Pucci et al., n.d.; Ronca, Duque-Soto, et al., 2024).

Recent methodological innovations have emphasized the use of natural deep eutectic solvents (NADES), resin adsorption/desorption, counter-current chromatography, and membrane-based fractionation to improve extraction efficiency and compound enrichment (Bilalov et al., 2025) Sun et al., 2024). In addition, chemometric and metabolomic strategies have become essential for data interpretation, enabling cultivar discrimination, process optimization, and untargeted metabolite discovery, with studies reporting over 100 metabolites including novel phenolic derivatives and triterpenoids (Fayek et al., 2024; Kabbash et al., 2023).

Table 2. Analytical methods used in the chemical profiling of olive leaf extracts

Analytical Method / Platform	**Target Compounds**	**Purpose / Key Features**	**Representative Studies**
HPLC-DAD / HPLC-UV	Oleuropein,hydroxytyrosol, quercetin, verbascoside, total phenolics	Quantitative & qualitative analysis; routine validation; cultivar comparison	(Karaogul & Nedjip, 2025; Martínez-Navarro et al., 2023)
HPLC-MS / LC-MS/MS / Orbitrap-MS / QTOF-MS	Comprehensive phenolic profiling, secoiridoids, flavonoids, triterpenoids	High sensitivity; >60 phenolics; targeted & untargeted metabolomics	(Baccouri et al., 2022; Mir-Cerdà et al., 2024; Pucci et al., n.d.)
UHPLC / UPLC-QTOF-MS	Oleuropein, iridoids, coumarins, flavonoids	Rapid, high-resolution separation; cross-validation	(Carrara et al., 2024; Mushtaq et al., 2025)
GC-MS	Volatiles, triterpenoids, fatty acids	Essential oils, hydrosols, lipophilic fractions; seasonal effects	(Fayek et al., 2024; Jurišić Grubešić et al., 2021)
FTIR / ATR-FTIR / DRIFT	Polyphenols, flavonoids, triterpenoids	Fingerprinting; authentication; fermentation effects	(Agatonovic-Kustrin et al., 2021; Leonova & Kuregyan, 2024)
NMR (^{1}H, ^{13}C, ^{2}D)	Structural elucidation, triterpenoids	Compound identification; quantification; metabolomics workflows	(Beteinakis et al., 2024; Tarchi et al., 2025)
ICP-MS / ICP-AES / LPAS	Multi-elemental profiling	Authentication; cultivar & geographic origin discrimination	(Martín-García et al., 2020; Ronca, Duque-Soto, et al., 2024)
HPTLC / TLC	Polyphenols, oleuropein, hydroxycinnamic acids	Rapid screening; effect-directed detection	(Agatonovic-Kustrin et al., 2021)

Spectrophotometric Assays (TPC, DPPH, ABTS, FRAP, CUPRAC)	Total phenolics, antioxidant activity	Routine quantification; correlation with bioactivity	(Difonzo et al., 2022; Khelouf et al., 2023)
Electrochemical Sensors (CV, SWV, TiOx-RGO@GCE)	Oleuropein, trace phenolics	Sensitive, rapid detection; green extraction compatible	(Kurtulbaş et al., 2020)
Chemometric Analysis (PCA, PLS-DA, Cluster Analysis)	Multivariate datasets (chromatography, spectroscopy, elemental)	Data interpretation; cultivar discrimination; process optimization	(Fayek et al., 2024; Lo Scalzo et al., 2025)
Resin Adsorption / Membrane Techniques (UF, NF, RO)	Phenolic enrichment, fractionation	Selective isolation; process optimization; kinetic modeling	(Liu et al., 2020)
Counter-Current Chromatography (HPCCC)	High-purity polyphenols (e.g., luteolin-4′-O-β-D-glucoside, oleuropein)	Efficient isolation of target compounds	(Sun et al., 2025)

Abbreviations; HPLC: High-Performance Liquid Chromatography; DAD: Diode Array Detector; UV: Ultraviolet Detector; LC-MS/MS: Liquid Chromatography–Tandem Mass Spectrometry; QTOF-MS: Quadrupole Time-of-Flight Mass Spectrometry; Orbitrap-MS: Orbitrap Mass Spectrometry; UHPLC/UPLC: Ultra-High-Performance/Ultra-Performance Liquid Chromatography; GC-MS: Gas Chromatography–Mass Spectrometry; FTIR: Fourier Transform Infrared Spectroscopy; ATR-FTIR: Attenuated Total Reflectance–FTIR; DRIFT: Diffuse Reflectance Infrared Fourier Transform; NMR: Nuclear Magnetic Resonance; ICP-MS/ICP-AES: Inductively Coupled Plasma–Mass Spectrometry/Atomic Emission Spectroscopy; LPAS: Laser Photoacoustic Spectroscopy; HPTLC/TLC: High-Performance Thin Layer Chromatography/Thin Layer Chromatography; TPC: Total Phenolic Content; DPPH/ABTS/FRAP/CUPRAC: Radical scavenging and antioxidant capacity assays; CV/SWV: Cyclic Voltammetry/Square Wave Voltammetry; TiOx-RGO@GCE: Titanium Oxide–Reduced Graphene Oxide Modified Glassy Carbon Electrode; PCA/PLS-DA: Principal Component Analysis/Partial Least Squares Discriminant Analysis; UF/NF/RO: Ultrafiltration/Nanofiltration/Reverse Osmosis; HPCCC: High-Performance Countercurrent Chromatography.

Recent advances in analytical methods have greatly expanded the ability to characterize the complex phytochemical profile of olive leaves. Chromatographic techniques, particularly HPLC and LC-MS/MS, remain the cornerstone for both targeted and untargeted analyses, offering high sensitivity and specificity for a wide range of phenolic and triterpenoid compounds (Esther et al., 2021; Karaogul & Nedjip, 2025; Mir-Cerdà et al., 2024). The integration of high-resolution mass spectrometry platforms such as QTOF and Orbitrap, combined with innovative sample preparation strategies including natural deep eutectic solvents (NADES), resin adsorption, and counter-current chromatography, has enabled the identification of novel compounds and improved quantification even in complex matrices (Fayek et al., 2024). Spectrophotometric and electrochemical methods continue to provide rapid and cost-effective screening tools, while vibrational and elemental spectroscopies (FTIR, NMR, ICP-MS) offer complementary information for authentication and quality control (Agatonovic-Kustrin et al., 2021; Kurtulbaş et al., 2020; Pucci et al., n.d.). In parallel, chemometric and metabolomic approaches have become increasingly essential for data interpretation, cultivar discrimination, and process optimization, with recent studies reporting the detection of more than 100 metabolites including novel secoiridoids and triterpenoids (Difonzo et al., 2022; Fayek et al., 2024; Kabbash et al., 2023).

7. Conclusion

Olive leaves are a chemically rich matrix dominated by phenolic compounds, particularly oleuropein, together with flavonoids, phenolic alcohols, and phenolic acids that contribute to their bioactivity. Triterpenic acids such as oleanolic and maslinic acid provide additional pharmacological potential, while sugars like mannitol highlight nutritional and industrial value. Fatty acids, volatiles, vitamins, pigments, minerals, proteins, and lignocellulosic fractions further enhance their functional profile, emphasizing their importance both as a nutraceutical source and as a raw material for biorefinery and agricultural applications. This chemical diversity explains the increasing interest in olive leaves across food, health, cosmetic, and sustainable industries.

Extraction methods have progressed from conventional solvent-based techniques to advanced and sustainable technologies. Traditional approaches are simple and low-cost but limited in efficiency, whereas innovative methods such as UAE, MAE, PLE, and SFE achieve higher yields, better selectivity, and shorter processing times, making them suitable for industrial applications. Newer techniques, including PEF, ball milling, and infrared-assisted extraction, show promise for improving efficiency and preserving bioactivity. The adoption of green solvents such as DES and NADES further supports sustainability by reducing environmental impact without loss of performance. Future research will likely focus on combining extraction strategies and optimizing greener solvents to fully exploit the bioactive potential of olive leaves.

Analytical methods each provide distinct advantages depending on the target compounds. HPLC and its variants remain the primary tools for phenolics and triterpenes, while GC-MS is essential for volatiles and fatty acids. UV-Vis spectroscopy offers a cost-effective solution

for routine screening, and complementary techniques such as FTIR, HPTLC, chemometric tools, and ICP-MS/AES add value for fingerprinting, authenticity, and mineral analysis. Recent advances, particularly NaDES combined with LC-UV-MS and UHPLC-HR-MS/MS, indicate a move toward greener and more comprehensive practices. Rather than relying on a single approach, integrated analytical strategies provide the most complete characterization and should balance sensitivity, cost, and environmental sustainability.

In conclusion, the integration of optimized cultivation practices, advanced extraction methods, and comprehensive analytical techniques provides a clear framework for maximizing the value of olive leaves. Continued research in this area will support the sustainable utilization of this abundant resource, foster innovation in food, nutraceutical, pharmaceutical, and cosmetic applications, and contribute to reducing agricultural waste.

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Nanotechnology and its chemical applications

Shamsa SHABBIR

Tatheer FATIMA

Introduction

Nanotechnology is defined as any technology that operates at the nanoscale and has practical uses, such as using individual atoms and molecules to create useful structures.(Kaehler, 1994)Nanotechnology is derived from the Greek word nano, which means dwarf. The term "nanoparticles" refers to a distinct entity with dimensions of 100 nm or less. (Ahmida & Ahmeida, 2017).

A core principle in nanotechnology is the importance of nanoscale. At this scale, the chemical behavior of materials such as reactivity, solubility, optical and electrical properties can deviate from their bulk equivalents, presenting unparalleled prospects for innovation in chemistry, materials science, and engineering.(Whitesides, 2005)

The properties of matter are different at the nanoscale. The increased surface-to-volume ratio leads to enhanced catalytic activity, modified thermodynamic stability and quantum confinement effects that alter optical and electronic properties. These phenomena serve as the basis for advancements in targeted medicine delivery, environmental cleanup,nanocatalysis, and nanosensors.This was the nanoworld to which Nobel Prize winner in physics Richard Feynman referred in the title of a 1959 talk on nanoscience: Plenty of space is available at the bottom.

Norio Taniguchi originally used the word "nanotechnology" in 1974 to refer to precise machining at the nanoscale. Gerd Binnig and Heinrich Rohrer's development of the Scanning Tunnelling Microscope (STM) in the 1980s gave the field a major boost by enabling researchers to view and work with individual atoms. Research was further accelerated by the creation of nanomaterials like fullerenes, carbon nanotubes, and quantum dots, which resulted in ground-breaking scientific and engineering applications.

Nanotechnology plays a crucial role in enhancing chemical processes through the development of advanced nanocatalysts and functional nanomaterials. Because of their vast surface area, nano catalysts such as metal nanoparticles (including platinum, gold, and silver) display much increased catalytic activity. Nanocatalysts, for example, are used in environmental applications to break down pollutants and hazardous substances in air and water purification systems. (Beni & Jabbari, 2022)

Nanostructured materials are used as carriers in the pharmaceutical industry to enhance medication solubility and targeted delivery, enabling controlled release and mitigating adverse effects. Furthermore, to improve chemical resistance or facilitate particular reactant

interactions, nanoscale coatings and films are applied to surfaces, boosting the effectiveness of procedures like chemical sensing and extraction. (Emma)

This chapter aims to provide a comprehensive overview of nanotechnology within the chemical sciences its foundations, applications, challenges, and prospects. This overview explains how these principles affect the reactivity and behaviour of nanomaterials as well as their synthesis, characterisation, and use in chemical environments. This covers a broad range of chemical applications, such as drug delivery, chemical sensing, environmental cleanup, and catalysis. The interdisciplinary character of nanotechnology and its increasing integration with engineering, and biology are also discussed in this chapter. Lastly, it discusses significant issues including sustainability, safety, and ethical issues and provides information on new developments that could influence the direction of nanotechnology in chemical research and industry.

Fundamental Concepts of Nanotechnology:

Nanotechnology focuses on the manipulation of materials at extremely small dimensions, generally within the range of 1 to 100 nanometers. When matter is scale down to these dimensions, it displays distinctive chemical, physical and biological behaviours driven by changes in atomic arrangements and energy dynamics. These behaviours are governed by several core principles: size dependent phenomena, quantum effects and surface related interactions. An in-depth understanding of these mechanisms is crucial for advancing chemical innovations at the nanoscale.

Classification of Nanomaterials:

Nanomaterials can be categorized on the basis of

Structural dimensions

Chemical composition

Dimensional classification

Zero-Dimensional nanomaterials:

These materials includes nanostructures where all the external dimensions measured in nanoscale. Examples:. Quantum dots, e.g., CdSe, are semiconductor nanocrystals ranging from 2 to 10 nanometers in diameter.

One-dimensional nanomaterials:

These nanomaterials are characterized by having two dimension at the nanoscale with extended surface in the other dimension.

Examples: nanowires, nanosheets, nanotubes, nanorods, and nanofibers. They have a high aspect ratio, which provides excellent charge transport and mechanical strength, used in sensors and electronic devices.

Two- dimensional nanomaterials:

One dimension is at the nanoscale, with extended surface in the other two dimensions. Examples: Graphene, MXenes, MoS2 nanosheets.

They have unique surface related properties, high surface area for catalysis, energy storage and membrane separation.

Three-dimensional nanomaterials:

Three-dimensional nanomaterials are characterized by having nanostructures with nanoscale dimensions in complex 3D architectures. For example; nanocomposites. Nanomaterials classification by type on the basis of their chemical composition:

Carbon-based nanomaterials:

These include diverse forms such as fullerenes (e.g., C60), carbon nanotubes, nanowires, carbon black and graphene. They are characterized by their unique carbon structures and are produced through methods like laser ablation, arc discharge and chemical vapor deposition.

Inorganic-based nanomaterials:

They comprise particles made from metals or metal oxides, each measuring less than 100 nanometers. These comprise particles made from metals and metal oxides such as gold and silver nanoparticles, titanium dioxide, zinc oxide, and semiconductors like silicon. They find application in catalysis, electronics, and biomedical fields.

Organic-based nanomaterials:

Organic-based nanomaterials composed of organic substances. Dendrimers, micelles, liposomes, and polymers can be generated by non-covalent interactions, or self-assembly properties.

Composite nanomaterials:

These are made by combining different nanomaterials or integrating NMs into bulk materials such as metals, ceramics, and polymers. These composites have tailored properties and applications across electronics, materials science, and medicine.

Hybrid nanomaterials:

These include the integration of organic and inorganic components at the nanoscale. Examples include Core–shell nanoparticles (like Au@SiO_2), metal organic frameworks (MOFs). Their characteristics include synergistic properties that combine flexibility and functionality, enabling advanced catalysis, targeted drug delivery, and multifunctional devices.(Khan et al., 2022)

The physicochemical properties of nanomaterials are characterized by their unique behaviours from their nanoscale dimensions which differ significantly from bulk materials. Key properties include:

1. High surface area to volume ratio: Due to their small size, nanomaterials have a dramatically increased surface area compared to their volume, enhancing surface related phenomena such as catalytic activity, reactivity and interaction with biological systems.

2. Quantum Effects: Quantum effects become prominent at the nanoscale, leading to size-dependent optical, electronic, and magnetic properties. These effects enable tunable photoluminescence and electrical conductivity.

3. Optical properties: Nanomaterials can exhibit unique optical behaviors such as localized surface plasmon resonance in metal nanoparticles, which makes them highly sensitive for detection applications such as pesticides, heavy metals, and other hazardous chemicals with high sensitivity.

4. Electrical Conductivity: Many nanomaterials especially carbon and metal based nanoparticles display exceptional electrical properties such as high conductivity and electron mobility.

5. Mechanical Properties: Nanomaterials demonstrate enhanced strength, flexibility and resilience attributed to their nanostructure making them suitable for advanced composite materials.

6. Chemical Reactivity: The increased surface area and exposed active sites lead to elevated chemical reactivity useful in catalysis and sensing applications.

7. Magnetic Properties: Some nanomaterials exhibit super-paramagnetism or other size-dependent magnetic behaviours critical for biomedical imaging and data storage.

These properties are highly tunable based on size, shape, composition, and surface chemistry, allowing precise control for specific nanotechnology applications.(Pleus& Murashov, 2018)

Techniques for the synthesis and characterization of nanoparticles:

Bottom up approach:

In the bottom up approach, nanoparticles are synthesized by assembling atoms, molecules, ions into larger structures. This method includes sol-gel synthesis, chemical vapor deposition, and biological synthesis using microorganisms or plant extracts.

Top Down approach:

The top-down approach starts with bulk material, which is broken down into nanoscale structures using physical or mechanical methods. Common techniques include mechanical milling, laser ablation, and lithography.

Chemical Applications of Nanotechnology:

Nanotechnology significantly advances chemical applications by improving reaction efficiency, material performance, and precision. Nanocatalysts boost industrial and green processes, while nanosensors enhance analytical detection. In environmental chemistry, nanoparticles aid in pollutant removal and purification. They also enable targeted drug delivery and enhance energy and material technologies, supporting sustainable innovation.

Catalysis and reaction enhancement:

Due to their high surface area and unique surface energies, nanocatalysts greatly enhance chemical reaction efficiency, rate, and selectivity. They are widely used in industrial synthesis, environmental remediation, and energy conversion.(Hemalatha et al., 2013). Gold nanoparticles supported on metal oxides (like Au/TiO_2) are used in automotive catalytic converters to efficiently convert toxic carbon monoxide (CO) into carbon dioxide (CO_2) at lower temperatures. In the petroleum industry, zeolite-based Nano catalysts play a vital role in fluid catalytic cracking processes, enhancing fuel yield while minimizing sulfur emissions, making refining processes cleaner and more energy-efficient.(Walton, 2016)Recent innovations focus on single-atom catalysis, defect engineering, and bimetallic nanostructures to optimize activity while reducing material costs. Emerging concepts like programmable nanocatalysts and dynamic in situ tuning are revolutionizing how reactions are controlled at the nanoscale, offering greater precision and energy efficiency.(Li, Chen, Jiang, Jiang, & Zhang, 2022)

Analytical chemistry and nanosensors:

Nanotechnology has significantly advanced analytical chemistry by enabling the creation of highly sensitive and selective nanosensors using materials like carbon nanotubes, quantum dots, graphene, and metal nanoparticles. These sensors are widely used in environmental monitoring, medical diagnostics and food safety allowing rapid detection of pollutants, toxins and biomarkers even in trace amounts. Recent trends focus on integrating machine learning for smarter sensing, developing wearable and flexible sensors for continuous monitoring and creating self powered and eco-friendly nanosystems that enhance portability and sustainability for real world applications.Nanotechnology has enabled highly sensitive and reliable sensors, such as glucose monitors like FreeStyleLibre for diabetes care and graphene-based sensors for detecting trace levels of heavy metals in water, enhancing both healthcare and environmental monitoring. (Ghosh & Verma, 2024)

Environmental chemistry and remediation:

Nanotechnology offers powerful tool for environmental chemistry by enabling efficient detection and removal of pollutant from air, water and soil. Sunlight activated photocatalysts like TiO2 nanoparticles are employed in wastewater treatment plants to breakdown dyes, pharmaceuticals and organic pollutants . Magnetic nanoparticles such as Fe3O4 are used in removing heavy metals from industrial effluents and can be easily recovered with magnets reducing waste. Bio-nano hybrids are applied in bioremediation of oil spills and pesticide

degradation, offering eco-friendly alternatives by enhancing the natural breakdown processes through microbial nanoparticle synergy (Guerra, Attia, Whitehead, & Alexis, 2018)Carbon nanotube filters like LifeStraw purify drinking water by removing heavy metals and microbes. (Ghosh & Verma, 2024)

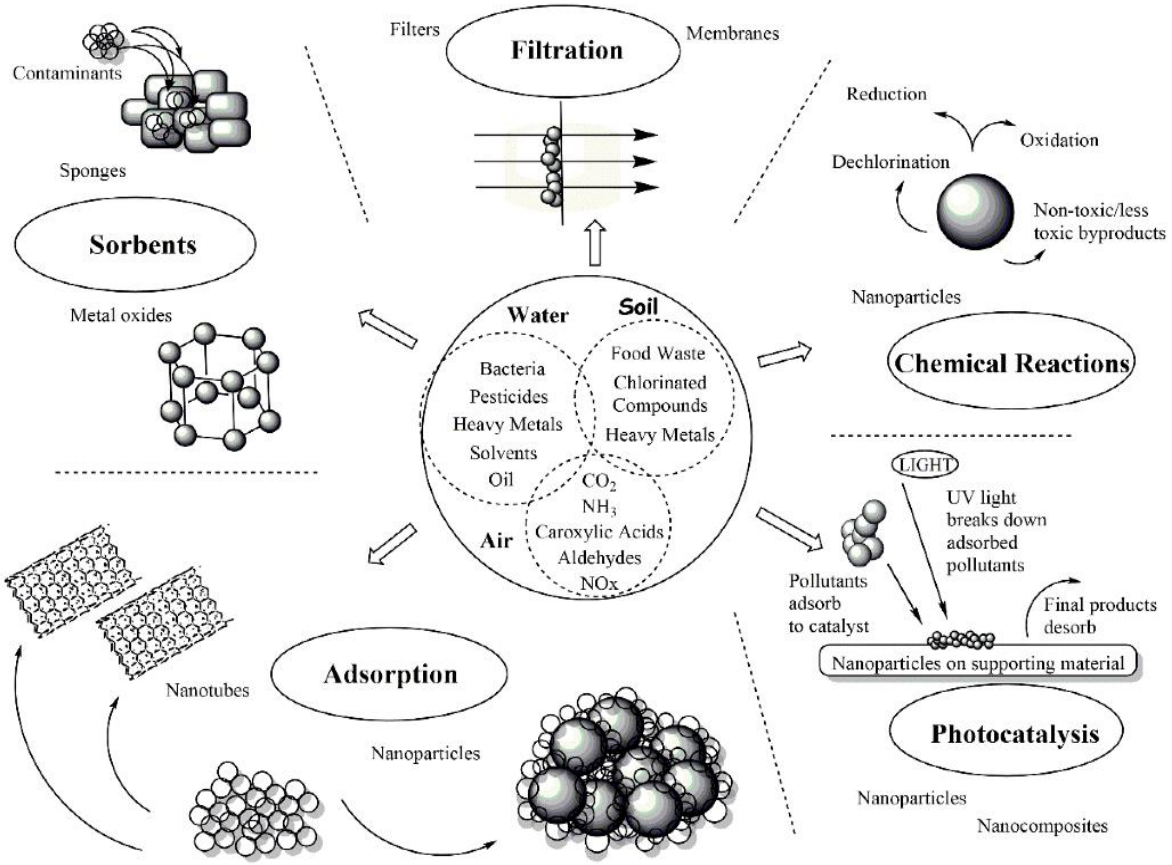

Figure 1: Nanotechnology in environmental chemistry and remediation

Drug Delivery and Nanocarriers:

Nanotechnology has significantly enhanced drug delivery by enabling targeted, controlled, and efficient treatments across multiple medical domains. Liposomal formulations like Doxil® have improved cancer therapy by reducing toxicity and enhancing drug accumulation at tumor sites, while lipid nanoparticles have become the backbone of mRNA vaccine delivery systems, such as those used in COVID-19 immunization. In chronic diseases like diabetes, nanocarriers allow non-invasive insulin administration, and nanoparticles have also been used to deliver drugs across the blood–brain barrier for treating neurological disorders. A major recent innovation involves the integration of DNA-based artificial nanomembranes into lipid bilayers, creating highly programmable and biocompatible delivery systems that mimic natural transport mechanisms offering precise control over drug release and cellular targeting.(Park, 2007)

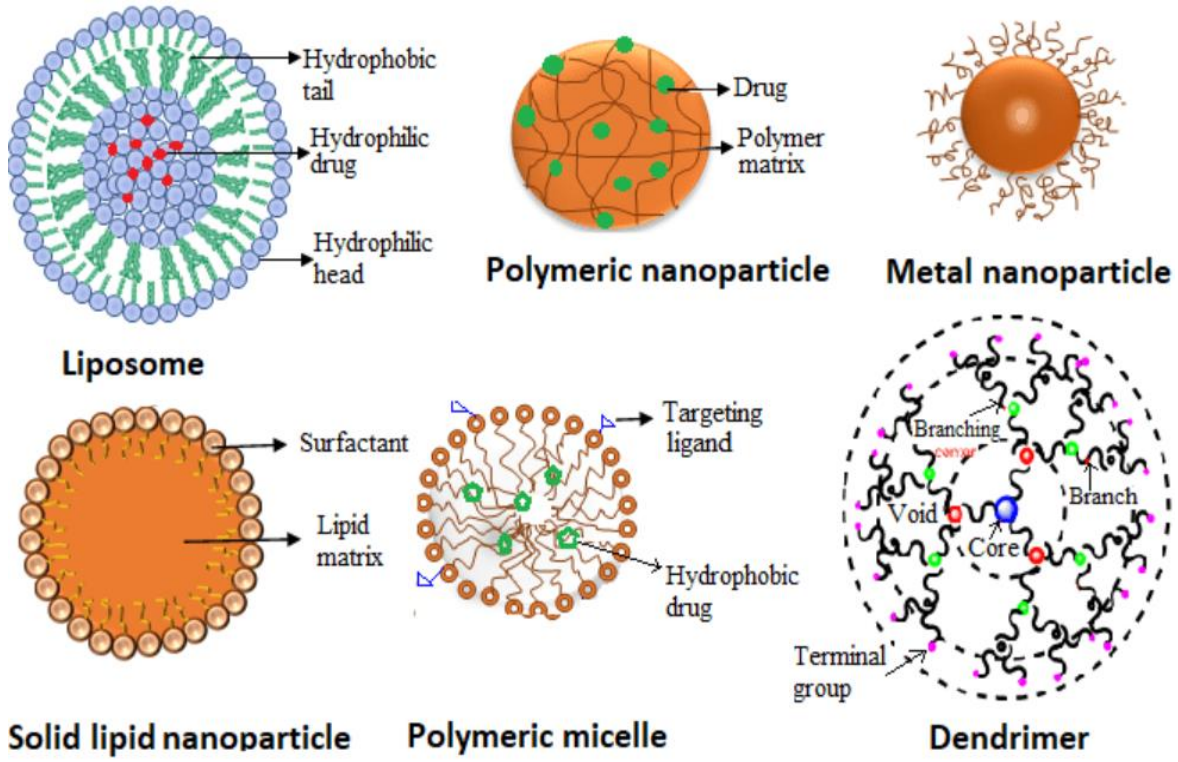

Figure 2: Nanocarriers in drug delivery

Energy Systems

Nanotechnology is reshaping energy chemistry by enabling high-performance materials for batteries, fuel cells, and supercapacitors. For lithium-ion and sodium-ion batteries, nanostructured anode materials like silicon nanoparticles and metal oxides (e.g., TiO_2, Fe_3O_4) accommodate volume expansion and shorten ion diffusion paths, leading to higher capacity and longer cycle life. In proton-exchange membrane (PEM) fuel cells, platinum-based nanocatalysts on carbon supports enhance reaction kinetics while reducing precious metal use. Supercapacitors leverage nanomaterials such as graphene, carbon nanotubes (CNTs), and metal–organic frameworks to deliver high power density and ultrafast charge/discharge rates. Looking forward, nanotechnology is key to developing flexible, solid-state, and eco-friendly energy devices for next-generation wearables, electric vehicles, and smart grids(Mohammed, Mia, Wiggins, &Desai, 2025)

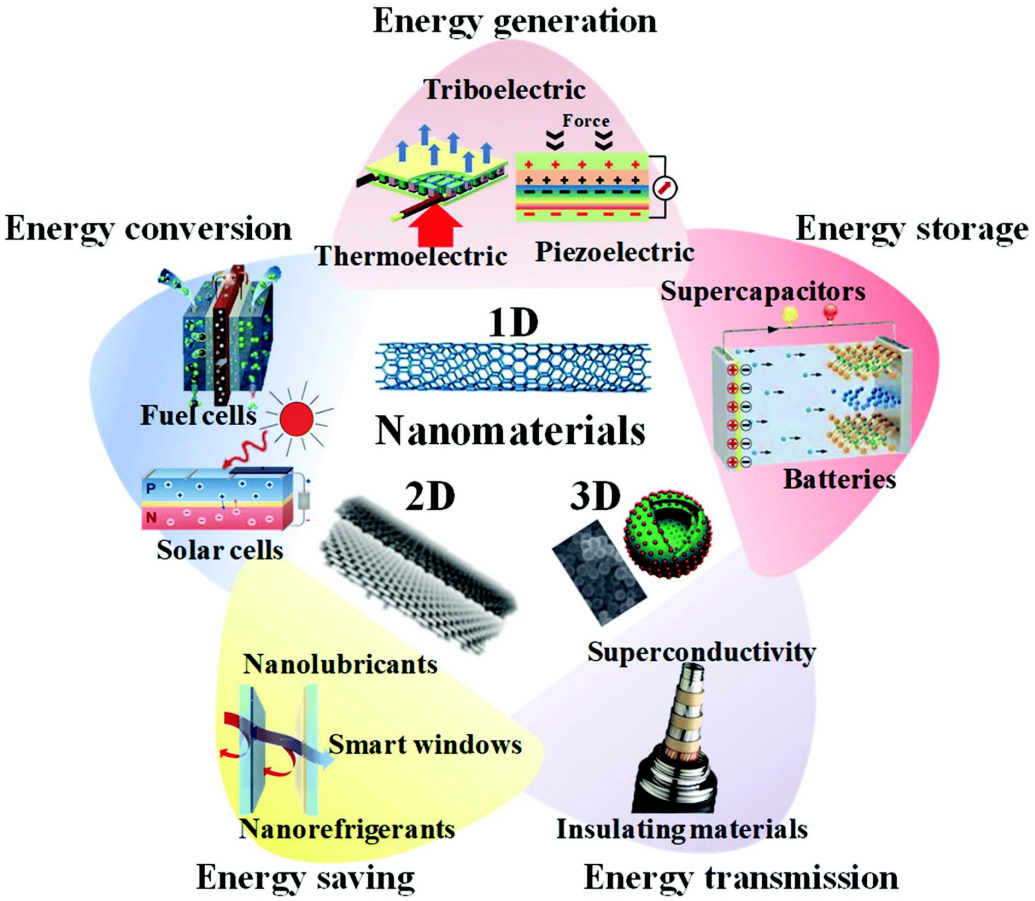

Figure 3: Nano materials in energy systems

Agriculture and Food Chemistry:

Nanotechnology in agriculture and food chemistry is paving the way for smarter, more sustainable solutions. Innovations such as nano-fertilizers and nano-pesticides enhance nutrient delivery and pest control with minimal environmental harm. Nanosensors support precision farming by enabling real-time monitoring of soil and crop conditions. In food technology, nanomaterials improve packaging by extending shelf life and preventing spoilage. Nano-enabled seed technology, particularly nanopriming, is a cutting-edge innovation in agriculture that involves coating seeds with nanoparticles like ZnO or SiO_2 to boost germination, stress resistance, and early growth. This method has shown increased biomass in crops such as wheat and maize, and holds promise for long-term improvements in crop yield, reduced chemical input, and greater food security over the next two decades

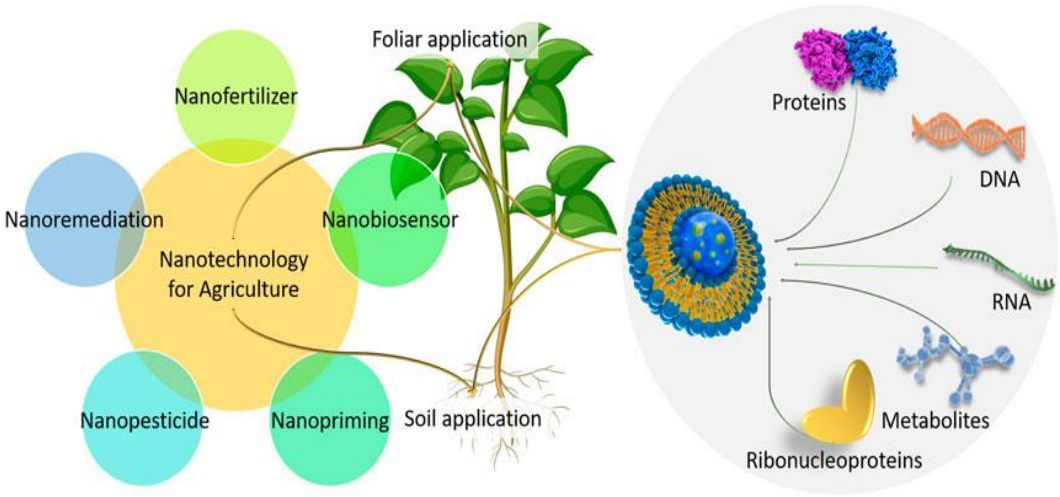

Figure 4: Nanotechnology for agriculture

Safety, Ethics, and Governance of Nanomaterials:

The increasing use of nanomaterials raises concerns about their long-term health and environmental effects. Their small size allows them to interact deeply with biological systems, potentially leading to toxicity, bioaccumulation, or ecological disruption. Global regulations, like those by the EU and U.S. agencies, aim to ensure ethical deployment through precautionary principles, but regulatory gaps still exist. As nanotechnology evolves rapidly, adaptive governance based on real-time risk assessment and flexible policy is essential to manageemerging risks and innovations responsibly.(Kaur, Singh, & Khatri, 2020)

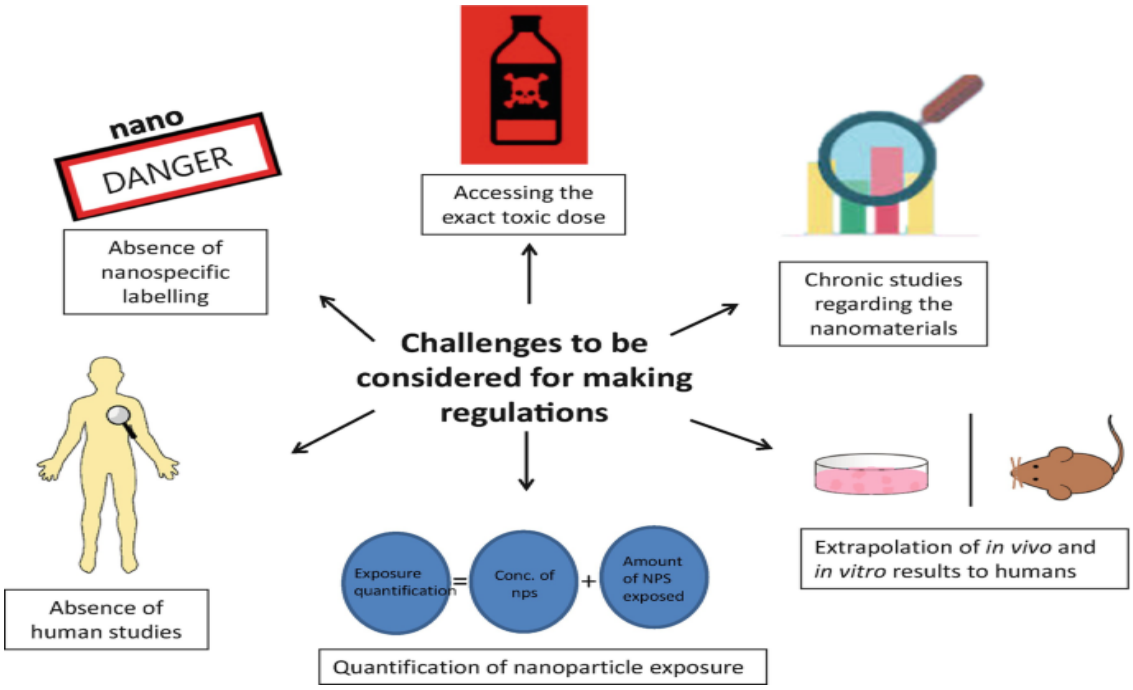

Figure 5: Possible challenges encountered with nanoparticles

Future Prospects and Research Directions in Nanotechnology:

Nanotechnology is poised to revolutionize various sectors through several emerging innovations:

Nanozymes: These are nanomaterials with enzyme-like activities, offering enhanced stability and cost-effectiveness over natural enzymes. They hold promise in diagnostics, environmental remediation, and therapeutic applications.

Lab-on-a-Chip Systems: Integrating nanotechnology with microfluidics, these devices enable rapid, on-site chemical and biological analyses, reducing sample volumes and enhancing diagnostic capabilities. (Gorjikhah et al., 2016)

Integration with Artificial Intelligence (AI):AI algorithms are being employed to design and optimize nanomaterials, predict their interactions, and accelerate research in drug discovery and materials science. (Behgounia& Zohuri, 2020)

Synthetic Biology: Combining nanotechnology with synthetic biology allows for the creation of programmable biological systems, leading to advancements in targeted drug delivery and the development of artificial cells. (Jewett & Patolsky, 2013)

These interdisciplinary approaches are expected to drive sustainable innovations, addressing challenges in healthcare, environmental protection, and industrial processes.

Conclusion:

In conclusion, nanotechnology has profoundly impacted chemical sciences by enabling the design and manipulation of materials at the nanoscale, leading to unprecedented control over chemical reactivity, selectivity, and functionality. Its applications span a wide range of sectors, including catalysis, drug delivery, environmental remediation, energy storage, and analytical sensing, benefiting from nanomaterials' enhanced surface area, reactivity, and unique physicochemical behavior. Breakthroughs such as DNA-based artificial nano membranes and nano-enabled seed technologies are paving the way for precision medicine, sustainable agriculture, and clean energy solutions expected to remain impactful for decades.

As this technology continues to evolve, the importance of addressing its safety, ethical deployment, and regulatory oversight becomes more critical. Ensuring responsible innovation through global frameworks and adaptive policy making will safeguard public health and the environment while fostering continued progress. Overall, nanotechnology represents a transformative force in modern chemistry, one that not only enhances current practices but also opens doors to novel, future-ready applications that align with global sustainability and technological advancement goals.

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Biomolecular Chemistry Breakthroughs

Tatheer FATIMA

Adnan NOOR SHAH

1. The Interdisciplinary Nature of Modern Biomolecular Research

Contemporary biomolecular chemistry is inherently interdisciplinary, integrating principles from organic chemistry, molecular biology, physics, computational modeling, and systems biology. Researchers now employ a wide array of techniques—from quantum chemistry simulations and bioinformatics to high-throughput screening and machine learning algorithms—to investigate complex biological systems. This collaborative approach has accelerated the pace of discovery and enhanced our ability to translate molecular insights into real-world applications, including novel therapeutics, diagnostics, and engineered biosystems (Alberts, 2015).

2. Advances in Nucleic Acid Chemistry

2.1 Structural Features and Biological Roles of DNA and RNA

Deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) are essential macromolecules responsible for storing, transmitting, and executing genetic instructions. DNA is characterized by its stable double-helix structure formed by complementary base pairing, whereas RNA typically exists as a single strand, allowing it to adopt diverse three-dimensional shapes and perform a wider array of biological functions. In addition to their primary roles in inheritance (DNA) and protein synthesis (RNA), both molecules are now known to contribute to gene regulation and enzymatic activity. The identification of functional non-coding RNAs, ribozymes, and riboswitches has significantly broadened the functional landscape of nucleic acids, highlighting their involvement in cellular communication, regulation of gene expression, and metabolic pathways.

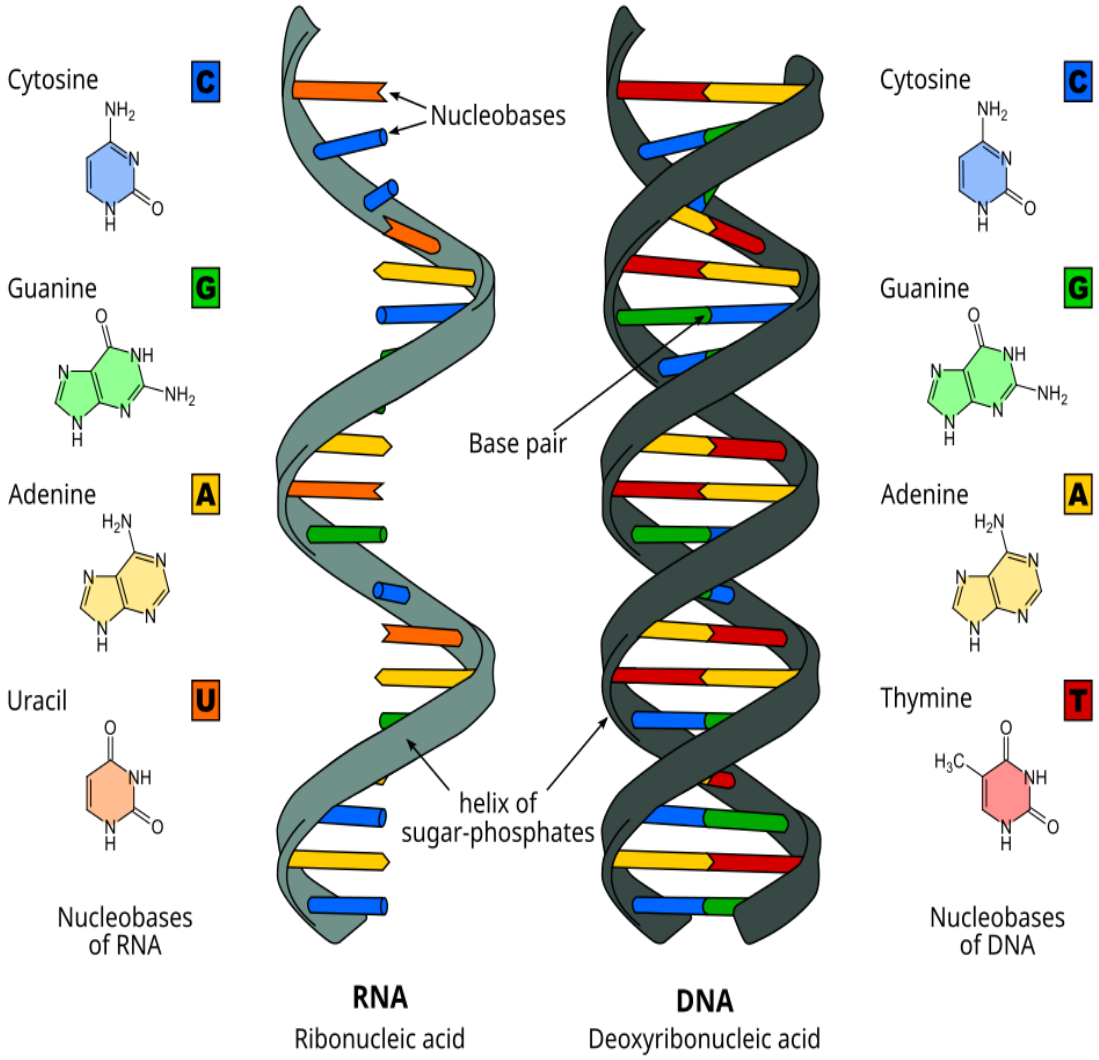

Figure 1. Difference Between RNA and DNA

2.2 Advances in Modified and Synthetic Nucleic Acids

Recent progress in nucleic acid research has focused on the creation of chemically altered nucleotides and synthetic nucleic acid mimics, offering enhanced stability and functionality. These engineered molecules, such as locked nucleic acids (LNAs), peptide nucleic acids (PNAs), and morpholino oligonucleotides, exhibit superior binding characteristics and resistance to degradation, making them valuable tools in gene silencing and diagnostic applications. Additionally, modifications like base methylation play a central role in epigenetic regulation, influencing gene activity without changing the DNA sequence itself. Such advances not only deepen our insight into molecular biology but also enable the custom design of nucleic acids for therapeutic and research purposes (Nelson, 2021).

2.3 CRISPR-Cas Systems and Genome Editing

One of the most groundbreaking innovations in nucleic acid research is the introduction of CRISPR-Cas technology for genome modification. Originally derived from the adaptive immune systems of bacteria, this method enables highly specific and programmable alterations of DNA within living organisms. The Cas9 protein, a commonly used nuclease in this system, is directed by a guide RNA to introduce precise double-stranded breaks at chosen genomic sites, thereby allowing the deletion, insertion, or correction of genes. More advanced forms of this technology—such as base editors and prime editors—allow for subtle changes to the genome without creating double-strand breaks. This versatile tool has dramatically advanced genetic engineering and shows great potential for applications in disease therapy, agricultural enhancement, and the control of disease-transmitting organisms (Judson, 1996).

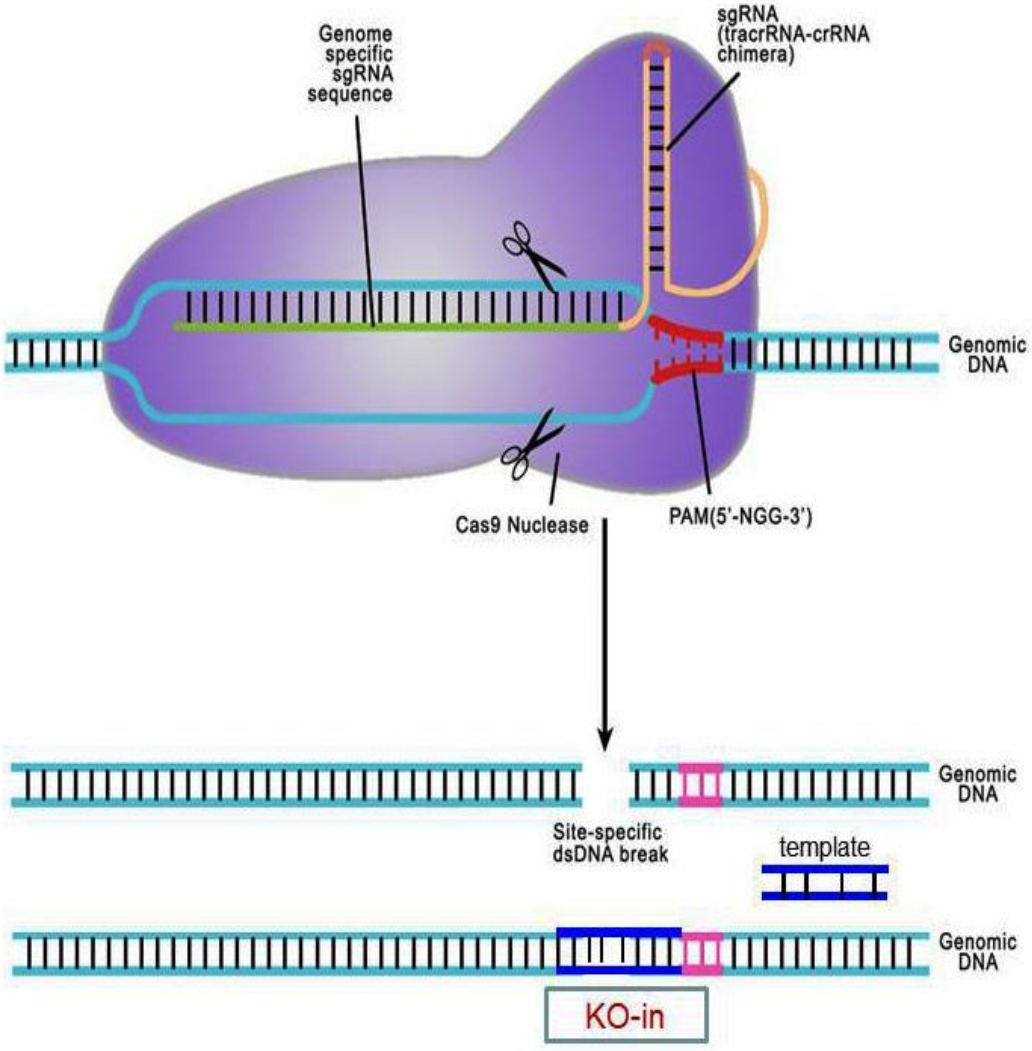

Figure 2. CRISPR/ CAS 9 System Background

2.4 RNA Therapeutics: siRNA, mRNA Vaccines, and Beyond

RNA-based therapeutics have emerged as a powerful class of medicines, offering specificity, flexibility, and rapid development timelines. Small interfering RNAs (siRNAs) and microRNAs (miRNAs) can silence disease-associated genes post-transcriptionally, providing targeted approaches for cancer, viral infections, and genetic disorders. The success of mRNA vaccines against COVID-19 has validated the therapeutic potential of synthetic mRNA platforms. These vaccines leverage lipid nanoparticles to deliver mRNA encoding viral antigens, stimulating robust immune responses. Looking ahead, self-amplifying RNA, circular RNA, and RNA aptamers represent the next frontier, promising novel treatments for a broad range of diseases (Alberts, 2015).

3. Breakthroughs in Protein Chemistry

Protein chemistry has undergone transformative advances that have deepened our understanding of biological function and enabled revolutionary applications in medicine, biotechnology, and industry. Central to this field is the study of how proteins fold into their functional three-dimensional structures, a process governed by complex intra- and intermolecular forces. Misfolding, however, can lead to aggregation and is implicated in numerous diseases, including Alzheimer's, Parkinson's, and prion disorders, making protein folding a critical target for therapeutic intervention.

Protein engineering has made it possible to tailor proteins with enhanced stability, specificity, or novel functionalities for use in diverse sectors. From the development of insulin analogs for diabetes management to thermostable enzymes in biofuel production, engineered proteins have shown immense practical value. This progress is largely driven by enzyme design and directed evolution, techniques that mimic natural selection in the lab to evolve proteins with improved or entirely new capabilities, dramatically accelerating biocatalyst development.

Furthermore, breakthroughs in structural biology—especially cryo-EM and NMR spectroscopy—have allowed researchers to visualize proteins at near-atomic resolution in their native states. These tools have unveiled dynamic conformational changes and complex molecular interactions, providing insight into mechanisms of action and informing rational drug design. Together, these advancements in protein chemistry are redefining the possibilities in molecular medicine and synthetic biology (Petsko, 2004).

Figure 3. Nuclear Magnetic Resonance (NMR) and Cryo-Electron Microscope (cryo-EM)

4. Biomolecular Interactions and Dynamics

Understanding biomolecular interactions and their dynamic behaviors is fundamental to deciphering how biological systems function at the molecular level. These interactions govern processes such as enzyme catalysis, signal transduction, immune recognition, and drug-target binding. Advances in both experimental and computational approaches have significantly enhanced our ability to probe these complex systems with increasing precision and predictive power.

4.1 Protein-Ligand and Protein-Protein Interactions

Protein-ligand and protein-protein interactions (PPIs) form the basis of nearly all cellular activities. Ligand binding to proteins can regulate enzymatic activity, trigger conformational changes, or modulate signaling cascades. PPIs, on the other hand, facilitate the assembly of multiprotein complexes and molecular networks. Targeting these interactions is a major focus in drug discovery, especially for conditions like cancer and autoimmune diseases. Structural and thermodynamic insights into binding interfaces have enabled the design of inhibitors, stabilizers, or mimetics that can modulate these interactions with high specificity.

4.2 Computational Chemistry and Molecular Docking

Computational tools, including molecular docking, molecular dynamics simulations, and quantum mechanical calculations, have revolutionized the prediction and analysis of biomolecular interactions. sMolecular docking algorithms explain that how small molecules fit into protein binding sites, aiding virtual screening and drug design. Meanwhile, MD simulations allow the visualization of atomic movements over time, offering insight into conformational flexibility, stability, and reaction mechanisms. Integration with machine learning further enhances accuracy, speed, and the ability to model large, complex systems (Berg, 2019).

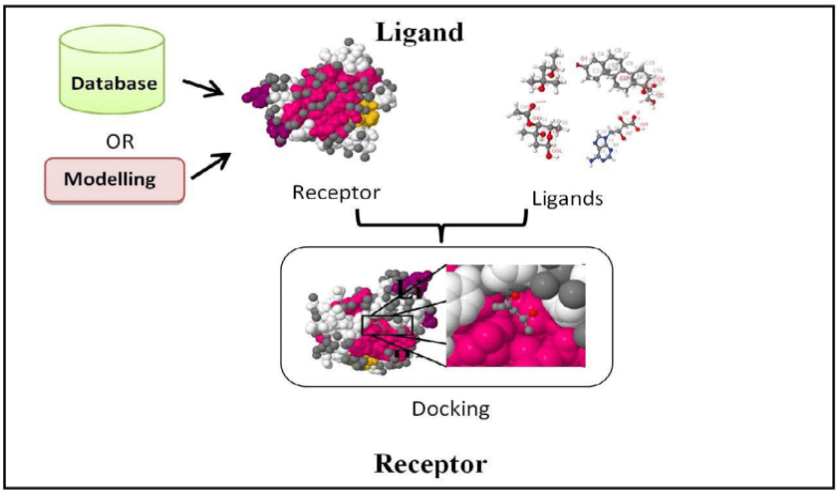

Figure 4: Molecular Docking Flow Chart

4.3 Kinetics and Thermodynamics in Biomolecular Systems

Kinetics and thermodynamics provide a quantitative understanding of how and why biomolecular interactions occur. Binding affinity, reaction rates, activation energies, and equilibrium constants are essential parameters that define the behavior of molecular interactions under physiological conditions. Techniques like isothermal titration calorimetry (ITC), surface plasmon resonance (SPR), and fluorescence resonance energy transfer (FRET) are commonly used to measure these parameters. Such data are critical for optimizing drug candidates, predicting biological outcomes, and elucidating energy landscapes of biomolecular folding and binding.

4.4 Biosensors and Real-Time Monitoring Tools

Modern biosensors enable the detection and quantification of biomolecular interactions in real time with high sensitivity and specificity. These tools combine molecular recognition elements—such as antibodies, aptamers, or enzymes—with signal transduction systems to produce measurable outputs. Applications range from point-of-care diagnostics and environmental monitoring to drug screening and intracellular signaling studies. Advances in nanotechnology and microfluidics have further improved biosensor capabilities, allowing integration into lab-on-a-chip platforms for high-throughput, multiplexed analysis (Garcia,2021).

5. Biomolecular Chemistry in Drug Discovery

Biomolecular chemistry plays an important role in modern drug discovery, enables the precise identification of disease targets, rational drug design, and the improvement of innovative delivery systems. The integration of structural biology, computational tools, and chemical biology has transformed the traditional trial-and-error approach into a more strategic, efficient, and predictive process.

5.1 Target Identification and Validation

The first step in drug discovery involves identifying biomolecular targets—often proteins, enzymes, or nucleic acids—that play a critical role in disease progression. Target validation ensures that modulating the target produces the desired therapeutic effect. Techniques such as high-throughput screening, CRISPR-Cas9 gene editing, RNA interference (RNAi), and proteomics are employed to discover and validate potential drug targets. The success of this phase is fundamental to the downstream stages of drug development.

5.2 AI and Machine Learning in Medicinal Chemistry

Artificial intelligence (AI) and machine learning (ML) are revolutionizing medicinal chemistry by accelerating hit discovery, optimizing lead compounds, and predicting pharmacokinetic and toxicological properties. Deep learning models can analyze massive chemical datasets, predict drug-target interactions, and design novel molecules with desired properties. AI-driven platforms are also used to repurpose existing drugs and identify synergistic combinations, significantly reducing development timelines and costs (Vamathevan, 2019).

6. Case Studies of Recent Breakthroughs

6.1 Development of COVID-19 mRNA Vaccines

It is a historic milestone in biomolecular chemistry in the production of mRNA vaccines during the COVID-19 pandemic. Using an artificial messenger RNA encoding the SARS-CoV-2 spike protein, these vaccines leveraged the cellular machinery of the host to produce viral antigens and elicit robust immune responses. Different vaccines like, Pfizer-BioN Tech and Moderna vaccines demonstrated high efficacy and were developed in record time, thanks to decades of prior research in RNA stabilization, lipid nanoparticle delivery systems, and innate immune modulation. This breakthrough validated the mRNA platform as a flexible and rapidly deployable tool against emerging infectious diseases.

6.2 Discovery of RNA-targeted Small Molecules

Traditionally, drug development has focused on targeting proteins; however, recent advances have enabled the design of small molecules that selectively bind RNA. These compounds can modulate RNA structure and function, offering new therapeutic strategies for diseases driven by aberrant RNA behavior, such as certain cancers and neurodegenerative disorders. One notable example is the development of small molecules targeting the expanded RNA repeats in myotonic dystrophy, which disrupt pathogenic RNA-protein interactions. These discoveries mark a paradigm shift, opening new possibilities for targeting previously “undruggable” biomolecular structures.

6.3 CRISPR Therapies for Genetic Disorders

CRISPR-Cas systems have progressed from laboratory tools to clinical therapies with unprecedented speed. In recent years, clinical trials have shown promising results in treating inherited conditions such as sickle cell disease and β-thalassemia using ex vivo edited hematopoietic stem cells. Moreover, in vivo editing approaches—such as those targeting the liver or retina—are emerging, with trials addressing conditions like Leber congenital amaurosis and transthyretin amyloidosis. These therapies illustrate the power of precision gene editing and the potential of CRISPR to correct the root causes of genetic diseases.

6.4 De Novo Protein Design and Therapeutic Applications

De novo protein design, enabled by computational algorithms and AI-based models like AlphaFold, has opened new horizons in synthetic biology. Scientists can now design proteins with entirely novel sequences and functions not found in nature. For instance, newly designed protein nanocages and binders have been developed to neutralize viruses, regulate immune responses, or deliver drugs with high specificity. One breakthrough includes the creation of synthetic enzymes for therapeutic detoxification or metabolic intervention. These advances highlight the potential of rational protein design in creating bespoke biological tools and therapeutics (Kirkpatrick, 2021).

7. Challenges and Future Prospects

Despite the remarkable advancements in biomolecular chemistry, various prospects are still to be unveiled to understand its potential in different fields, such as healthcare, industry, and environmental applications. Due to continuous progress in this filed, careful consideration of ethical, economic, and technological factors is essential for sustainable and responsible innovation.

7.1 Ethical and Safety Considerations

The rapid development of technologies such as CRISPR gene editing, synthetic biology, and AI-guided drug design raises critical ethical and safety concerns. Issues such as off-target genetic modifications, germline editing, and data privacy in genomics must be carefully regulated. Furthermore, the deployment of novel therapies requires thorough clinical validation to ensure patient safety. Ethical frameworks and public engagement are crucial to guide research and policy, particularly when manipulating the molecular fabric of life.

7.2 Scalability and Cost-Efficiency

Translating laboratory breakthroughs into real-world applications often encounters barriers related to scalability and cost. Many biomolecular innovations, such as personalized therapies or advanced biosensors, are expensive and require complex infrastructure for mass production. Developing cost-effective, robust manufacturing processes—particularly for

biologics and nanomedicines—is vital to ensure equitable access and commercial viability. Bridging the gap between academic research and industrial implementation remains a persistent challenge.

7.3 Integration of Omics Data and Systems Biology

The integration of genomics, proteomics, metabolomics, and transcriptomics—collectively known as omics—offers a holistic view of cellular function and disease mechanisms. However, managing and interpreting these massive datasets require sophisticated computational tools and interdisciplinary collaboration. Systems biology approaches aim to model complex biological networks, predict cellular responses, and identify novel therapeutic targets. The successful integration of omics data into drug discovery and diagnostics will pave the way for more informed, data-driven decision-making in biomolecular research.

7.4 The Future of Personalized and Precision Medicine

Personalized and precision medicine represent the frontier of biomolecular chemistry's impact on healthcare. By tailoring treatments based on individual genetic, molecular, and environmental profiles, these approaches promise increased efficacy and reduced adverse effects. Advances in biomarker discovery, companion diagnostics, and genome sequencing are already enabling more targeted therapies in oncology, rare diseases, and chronic conditions. In the future, wearable biosensors, real-time molecular monitoring, and AI-powered diagnostics will further refine personalized treatment strategies, bringing us closer to truly individualized medicine (Collins, 2015).

8. The Role of Biomolecular Chemistry in Aging and Age-Related Diseases

Aging is a biological process in which continuous cellular and molecular dysfunctions occur. Biomolecular chemistry plays an important role to understand such mechanism and also the diseases which are related to cancer like heart and brain diseases. Recent advancements in this field are providing new insights into aging pathways and offering potential targets for therapeutic interventions to delay or prevent the onset of these diseases.

8.1 Aging Biomarkers: Tools for Prevention and Intervention

Biomarkers of aging are essential for diagnosing age-related diseases early, assessing the efficacy of interventions, and understanding the molecular basis of aging. Several types of biomarkers are emerging as potential tools for aging research and clinical application:

- **Genetic Biomarkers**: Variations in genes related to longevity, such as those in the FOXO, APOE, and IGF1 pathways, are being studied as genetic biomarkers of aging. These genetic markers could be used to identify individuals at greater risk of age-related diseases, allowing for personalized prevention strategies.

- **Metabolic Biomarkers**: Changes in metabolites, such as those related to mitochondrial function, NAD+ levels, and lipid metabolism, are being used as biomarkers to monitor aging and disease progression. Technologies like MS and NMR spectroscopy are helping to identify these metabolic changes in aging individuals.

- **Epigenetic Biomarkers**: Epigenetic clocks, which measure DNA methylation patterns, have shown great promise as indicators of biological age, independent of chronological age. These clocks can provide insight into the aging process and help predict the onset of age-related diseases, offering potential for early diagnosis and intervention.

- **Proteomic and Lipidomic Biomarkers**: Proteomics and lipidomics, which analyze the protein and lipid profiles of cells and tissues, offer a wealth of information about aging. Alterations in protein expression and lipid composition are associated with cellular aging and the development of diseases such as CVDs and Alzheimer. Advancements in high-throughput proteomics and lipidomics are enabling the identification of new biomarkers for aging and age-related conditions.

- **Functional Biomarkers**: Functional biomarkers, such as cognitive function tests, physical activity assessments, and cardiovascular health measures, are critical for evaluating the impact of aging and therapeutic interventions. These biomarkers are used in clinical trials to assess the effectiveness of potential anti-aging treatments and disease prevention strategies (López-Otín, 2013).

Biomolecular chemistry is instrumental in elucidating the mechanisms of aging, identifying biomarkers, and developing interventions for age-related diseases. As we gain a deeper understanding of these complex processes, it opens the door to new therapeutic strategies aimed at promoting healthy aging and extending lifespan.

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Polymer Chemistry Development

Zobia ARIF

Polymer chemistry development has undergone significant transformations in recent years, driven by advances in synthesis techniques, characterization methods, and nanotechnology. This chapter highlights recent developments in polymer chemistry, focusing on novel synthesis method, structure- property relationships, and emerging applications. New polymerization techniques, such as controlled radical polymerization and ring opening metathesis polymerization have enabled the design of complex polymer architectures with tailored properties. The integration of polymers with nanoparticles and biomolecules has opened up new avenues for application in energy, medicine and sustainability. This chapter provides an overview of the current state of polymer chemistry, highlighting key challenges and opportunities for future research and developments. The development of polymer chemistry has revolutionized various industries, including material science, medicine and energy. Polymer are versatile materials that can be tailored to exhibit specific properties, making them suitable for a wide range of applications. Recent advances in polymer chemistry have focused on developing sustainable and functional materials. Sustainable polymers are developed biodegradable and recyclable polymers to reduce environmental impact. Functional polymers are designed polymers with specific properties such as conductivity, self- healing or responsiveness to stimuli. Polymer nanocomposites are integrating polymers with nanoparticles to enhance mechanical, thermal or electrical properties. Polymers have wide range of applications including energy storage and conversion as used in batteries, fuel cells and solar cells. Biomedical applications of polymers are as these are used in drug delivery, tissue engineering and bio- sensors. Sustainable materials are being made by using polymers like packaging, textiles and construction materials. Future research in polymer chemistry will focus on developing sustainable, functional and responsive materials. Some key areas of research include circular economy, advanced materials and nanotechnology.

The rapid evolution of polymer chemistry has revolutionized the field of material science, enabling the development of innovative materials with tailored properties. Recent advances in synthesis techniques, characterization methods, and nanotechnology have transformed traditional polymers into sophisticated materials with unprecedented functionality. This chapter explores the latest breakthroughs in polymer chemistry, highlighting novel synthesis methods, structure- property relationships and emerging applications in fields such as energy, medicine and sustainability. By examining the current state of polymer chemistry, this chapter aims to provide insights into the future directions of this dynamic field and its potential to address pressing global challenges. The polymer chemistry has come a long way since its inception, with significant advancements in understanding the relationships between polymer structure, properties and applications. The development of new polymerization techniques, such as controlled radical polymerization and ring opening matethesis polymerization, has enabled the synthesis of complex polymer architecture with tailored properties

1. Introduction to polymer

1.1 Definition

The compound having greater size, high molecular mass and is made up of many smaller molecules named as ‘monomers’ is called polymer. Polymer is derived from two words as ‘poly’ means many and ‘mer’ means part, it is also called ‘macromolecule’ because of its bigger size. Polymers show different physical and chemical properties that can be changed by changing the type of monomers, number of monomers, arrangement of monomers, method of synthesis and its source like flexibility, strength, resistance to heat and chemicals and elasticity (Koltzenburg et al., 2017).

1.2 Historical overview

In early human societies, utilization and synthesis of polymer started from application of cotton, wool, linen and other natural materials in paper making and clothing. The nature, type, method and properties of these substances was not known in initial years of nineteenth century but the different combinations and mixing of different monomers to form macromolecule was started. In 1920, Hermann Staudinger had proposed the concept of polymers that consist of monomers which are combined by covalent bond instead of polymers as colloidal aggregates. In 1930, by extending Hermann’s concept, many polymers like nylon, bakelite, neoprene and many other artificial polymers were prepared. In 1950-1960, many other synthetic polymers like polyethylene and polypropylene were prepared. In 1970 and after it, very vast range of synthetic polymers were prepared by using modern materials (Feldman et al., 2008).

1.3 Importance in daily life and industry

Polymers are used in daily life as synthetic polymers like nylon, polyesters and others are used in clothing because of flexibility, durability and many other properties. Many other artificial polymers like polyvinylchloride etc. are used in building material, electrical wiring, pipes and many other materials due to flexible strength, hardness and durability. In pharmaceuticals, surgical implants, contact lenses, catheters and other medical devices are made up of different kind of polymers. Plastic bags, containers, preservative films and other materials are synthesized by using polymers like polypropylene, polyethylene etc. Automobile parts, tires and other transport material is also prepared by using synthetic polymers because of vehicle safety and fuel efficiency. Polymers are also used in making of daily used home utensils, toys, plastic appliances and other devices etc. In surface coating, elastomers, adhesives, man- made fibers and many other materials are being made up of polymers either natural polymers or synthetic polymers (Lu et al., 2023).

2. Classification of polymers

Polymers are classified into different classes on following basis:

- On the basis of origin or source
- On the basis of arrangement of monomers
- On the basis of type of polymerization

- On the basis of thermal properties
- On the basis of nature of monomers

Following are further types of polymers on the basis of above-mentioned factors.

2.1 Types on the basis of origin

Macromolecules or polymers are classified on the basis of origin or source or occurrence of these big molecules.

- ***Biopolymers:*** All the polymers which are present in living organisms or their source is natural are called biopolymers. These are also called 'natural polymers. For example, lipids, proteins, carbohydrates etc.

- ***Synthetic polymers:*** All the polymers which are present in non-living things or artificially prepared by man are called synthetic polymers. These are also called 'man-made or artificial polymers. For example, polyvinyl chloride, polyethylene, polyamide etc.

2.2 On the basis of arrangement of monomers:

Polymers are formed by smaller units called monomers which can be arranged in multiple ways and there symmetry decides the type of polymers which are as following:

- ***Linear polymer:*** A type of polymer which is formed by monomers that is arranged in straight line or linear form and these straight chains just move in parallel to other straight chain having monomers. For example, polyvinylchloride etc.

- ***Branched-chain polymer:*** A type of polymer which is formed by monomers that is arranged in such a way that a linear chain is further divided into branches that can be isolated or complex. For example, low density polyethylene (LDPE) etc.

- ***Cross- linked polymer:*** A polymer that is formed by the arrangement of monomers in such a pattern that linear chains of monomers are intertwined or inter-linked to form cross-linked polymer. For example, epoxy resins etc.

- ***Network polymer:*** A type of polymer which is formed by the arrangement of chains of monomers in such a way that chains are interlinked, branched, multiple linear and other forms in order to give a net complicated structure that is called network polymer. For example, bakelite etc.

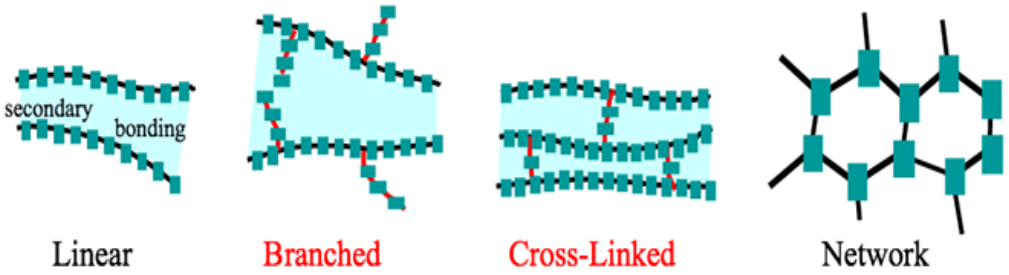


Figure 1. Types of polymers on the basis of arrangement of monomers

2.3 On the basis of type of polymerization

Polymerization is a process of polymer formation. A process in which smaller units called monomers combined together to form a larger molecule called polymer. These are the following types of polymers on the basis of type of polymerization:

➢ ***Addition polymer:*** A type of polymer which is formed when any unsaturated kind of monomers are bonded with each other to form a larger macromolecule is such a way that no group is substituted or replaced rather monomers are just added by 'addition reaction' that could take place in the presence of sunlight, peroxide or any other initiator which is called 'addition polymerization'. For example, polyvinyl chloride etc.

This process takes place in three steps named as:

- ✓ Initiation
- ✓ Propagation
- ✓ Termination

➢ ***Condensation polymer:*** A type of polymer which is formed when smaller molecules called monomers combined or bonded in such a way that during this reaction a smaller molecule like water, methane and others either be released or not which is called 'condensation reaction'. For example, polyamide, nylon-6,6 etc.

2.4 On the basis of thermal properties

Polymers can be classified on the basis of physical properties like response to heat or high temperature and stability or reactivity in the presence of high temperature. Following are the types of polymers on the basis of thermal properties:

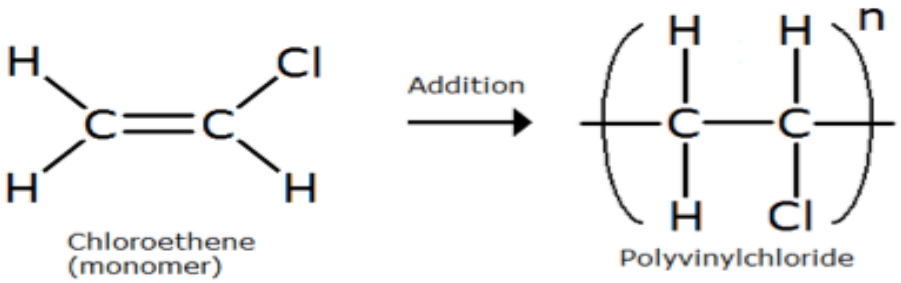
➢ ***Thermoplastic polymers:*** All the polymers which can be melted and softened on heating and can be remolded or reshaped again are called thermoplastic polymers. For example, toys, pipes etc.

- ***Thermosetting polymers:*** All the polymers which are hardened on heating and cannot be further reshaped or remolded again are called thermosetting polymers. For example, resins etc.

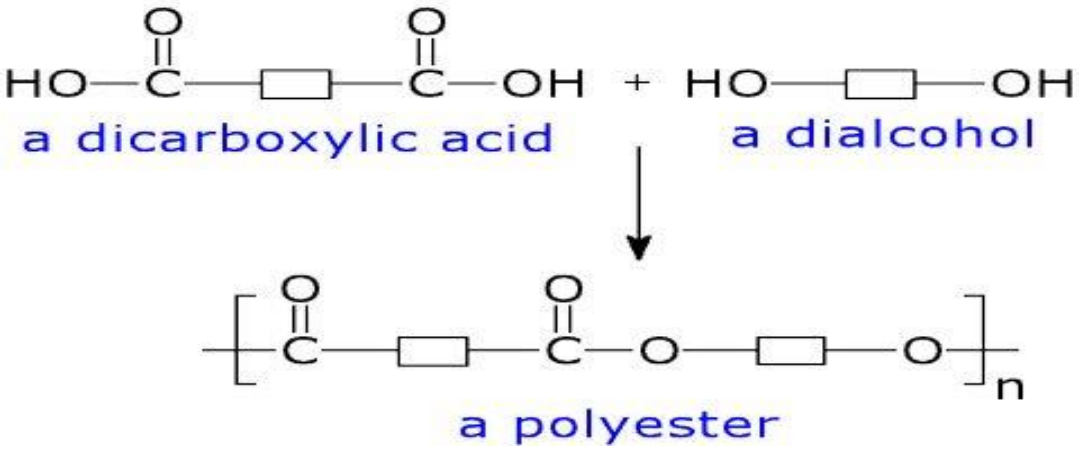
2.5 On the basis of nature of monomers

Polymers can be classified on the basis of type of reactant or monomers used during the process of polymerization for the formation of polymers and following are the classes on this base:

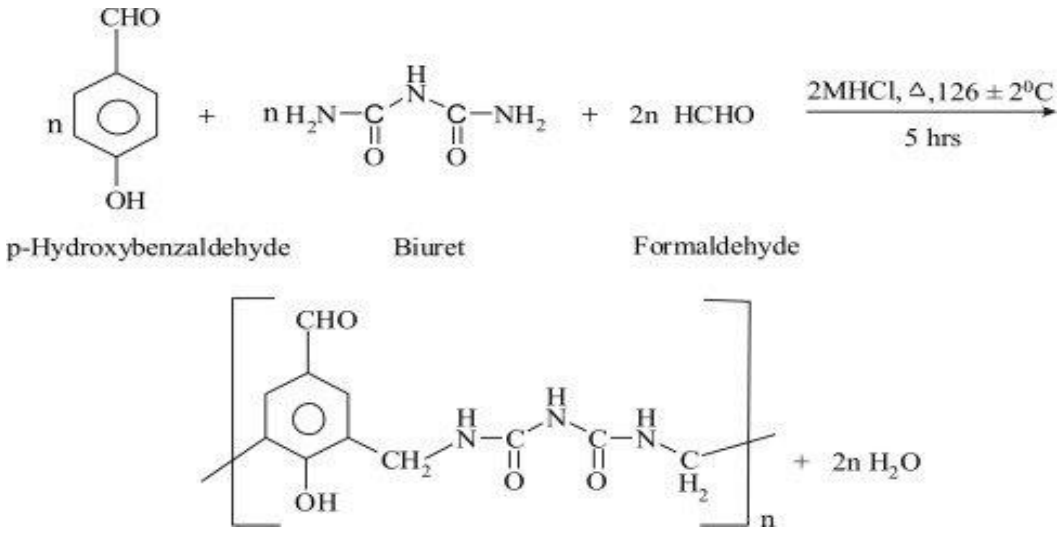
- ***Homo-polymer:*** 'Homo' means same, a type of polymer which is formed by the polymerization of similar type of monomers. For example, polyvinyl chloride is formed by the combination of number of vinyl chloride.



- ***Co-polymer:*** A type of polymer which is formed by the combination of two different type of monomers is called co-polymer. For example, a polyester is formed by combining carboxylic acid and other kind of monomer which is di alcohol or diol.



- ***Ter- polymer:*** A type of polymer which is formed by combining three different types of monomers together is called terpolymer. For example, a terpolymer named p-HBBF is formed by combining three types of monomers named as p-hydroxybenzaldehyde, biuret and formaldehyde (Tezuka et al., 2001).



3. Polymerization techniques

Polymerization is a process in which monomers are combined to form polymer. There are following methods for the formation of polymer that is:

- Addition polymerization
- Condensation polymerization
- Co-polymerization

3.1 Addition polymerization

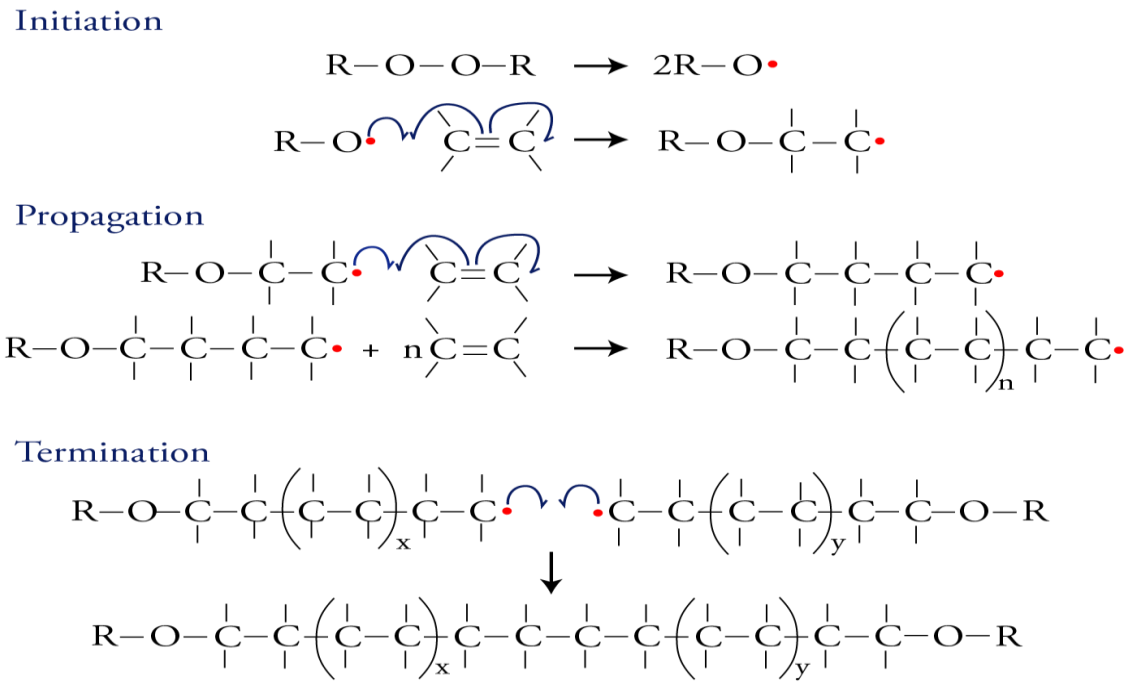
A type of polymerization in which monomers mostly unsaturated are combined to form polymer in such a way that unsaturated monomer is converted into saturated polymer by the 'addition reaction' and the polymer that is formed by this reaction is called 'addition polymer'. This reaction can be aided by any initiator that could be in the form of free radical, cation or anion. This reaction takes place in the following **three steps** named as:

- ❖ Initiation
- ❖ Propagation
- ❖ Termination

Addition polymerization technique is classified into further **two types**, which are on the basis of type of initiator which is used during this process is free radical (in the presence of sunlight), any positive ion called cation or any negative ion called anion, named as:

- ❖ Free radical addition polymerization
- ❖ Cationic or anionic addition polymerization

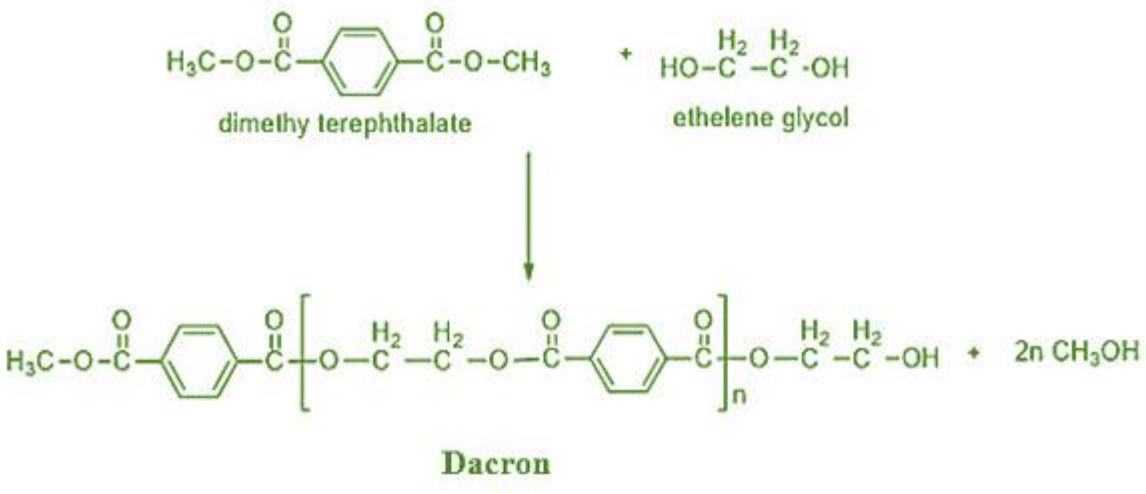
Following is an example of free radical addition polymerization:



3.2 Condensation polymerization:

A type of polymerization in which monomers are combined together in order to form a larger molecule that is macromolecule and during its formation either a small molecule like water, methane, carbon dioxide etc. could be released or not by a reaction named as 'condensation reaction' and the polymer that is formed is known as 'condensation polymer.

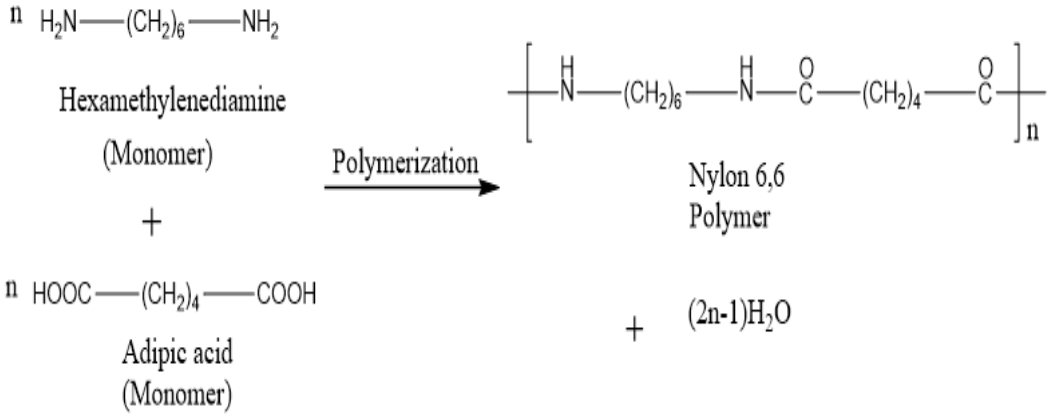
For example, dacryon which is a condensation polymer formed by condensation reaction of monomers named as dimethyl terephthalate and ethylene glycol by the removal of methanol.



3.3 Co-polymerization:

Copolymerization is a process in which two different species of monomers are combined to form a copolymer that is different than homomer and is mostly biopolymer. It is a simultaneous combination of two or more than two monomers and polymer that is formed by this reaction is known as ‘copolymer’.

For example, formation of a copolymer, nylon-6,6 formed by two monomers hexamethylene diamine and adipic acid is an example of copolymerization (Liu et al., 2020).



4. Structure- property relationship

The processing, structure, molecular weight, the way it is synthesized and many other factors determine the mechanical, thermal and physical properties of polymers. The structure of polymer involves the position of branching, type of branching, number of branching, cross-linking, linear chain arrangement, web networking of chains in polymers and the type of monomers used to form polymers, saturation or unsaturation, techniques used for synthesis of polymers, its source, conditions on which polymer is being made and many other factors like these influence the properties of polymers. Some of the factors are given below:

❖ Monomer type:

The building block of polymers called monomers, its structure and nature predict many properties of polymer like solubility, thermal properties, melting point and boiling point, stability, reactivity and polarity etc. For example, any polymer is dissolved into polar solvent like water, alcohol etc if its monomers are having polar nature and if its monomers are non-polar then this polymer is going to get dissolved into some non-polar solvent like benzene etc.

❖ Crystallinity:

Crystallinity involves the arrangement of monomers during the formation of polymer. As, the monomers are arranged in such a way that a three dimensional well arranged

'crystalline structure' is possible and also a random three dimensional, not very well arranged 'amorphous structure' is also possible. Most of the polymers are amorphous solids that consist of a smaller well-arranged region in this amorphous structure called '**crystallite'**. This crystallinity affects the stability, flexibility, rigidity and other mechanical properties of polymers. Studies shows that the randomly arranged amorphous part is less stiff and weak and weak or less strong than the crystalline region of polymer.

❖ **Chain length:**

The length of the chain in polymer is the measure of **molecular weight** of any polymer. The longer chain represents having larger number of monomers, greater molecular weight and this kind of polymer has greater strength and more stiffness than the polymer having less molecular weight due to small chain length.

❖ **Cross-linking:**

As the chains in polymers are arranged in different ways and if there is cross linking in the chains of polymer then it represents that structure of polymer is more compact, complex and more symmetrical which is the indicator of high-quality polymer with greater strength and heat resistance.

❖ **Chain arrangement:**

The chains of polymers are arranged in multiple arrangements to give different kind of polymers like linear chain polymer, branched chain polymer, cross linked polymer and networked polymer and many properties like flexibility, elasticity, toughness and thermal stability depend on the arrangement of monomers in the chain to form polymer.

❖ **Intermolecular forces:**

Chains of polymers have some kind of attractive forces due to the presence of partial positive and partial negative ends or polar end in the chains of polymer and these forces are also called 'inter-chain forces. These forces could be hydrogen bond, Vander Waal's forces, dipole- dipole forces, ion- dipole forces, dipole- induced dipole forces and many other temporary forces. Strength, melting point, glass transition temperature and other thermal or mechanical properties are dependent on inter-chain forces.

❖ **Glass transition temperature:**

The behavior of polymer is dependent on glass transition temperature which is 'temperature at which a change or transition occurs from a rigid, glasslike structure of an amorphous polymer or semi-crystalline polymer to more flexible, rubbery structure of polymer'. This is abbreviated as 'Tg'. Thermal expansion, flexibility, electrical conductivity, optical transparency and many other properties are depending on glass transition temperature as processing of polymer is supported by tg as below tg, the polymer shows lesser flexibility but above tg, polymer shows flexibility to this range that it can be molded into any other shape without getting fractured.

❖ **Melting temperature:**

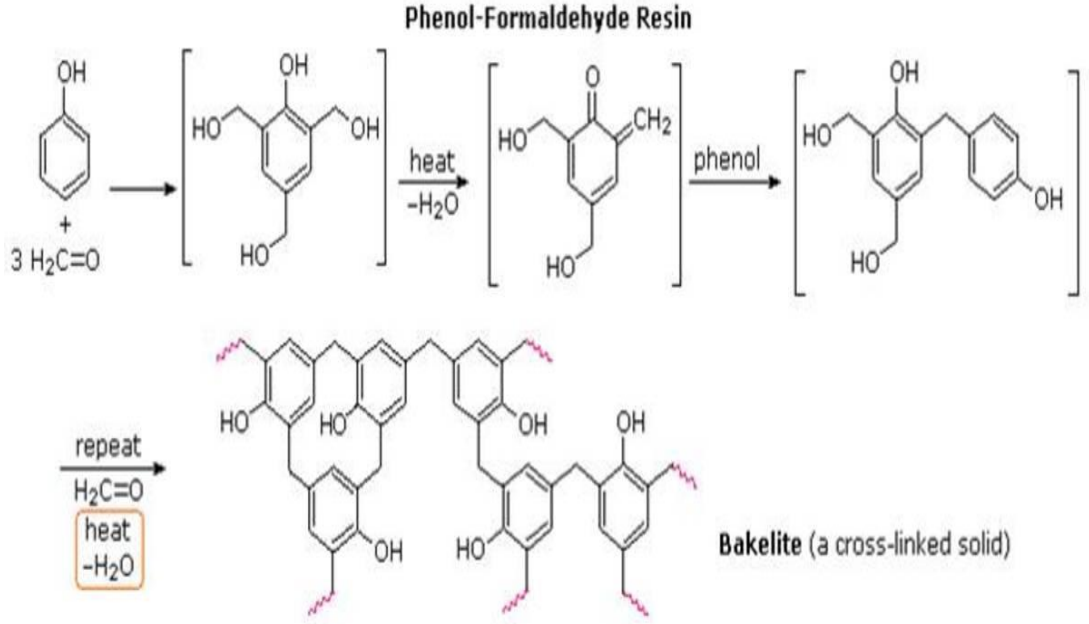
Melting temperature is the ‘temperature of any polymer at which regular and well-arranged crystalline regions in semi-crystalline polymer is converted into viscous-liquid state. This is represented as Tm. This temperature is also measure of thermal and chemical properties of polymers (Carraher et al., 2012).

5. Development milestones in polymer Chemistry

Polymer chemistry has advanced in last few years as it shows tremendous development when it comes to synthesize synthetic polymer having desirable properties. Some are given below:

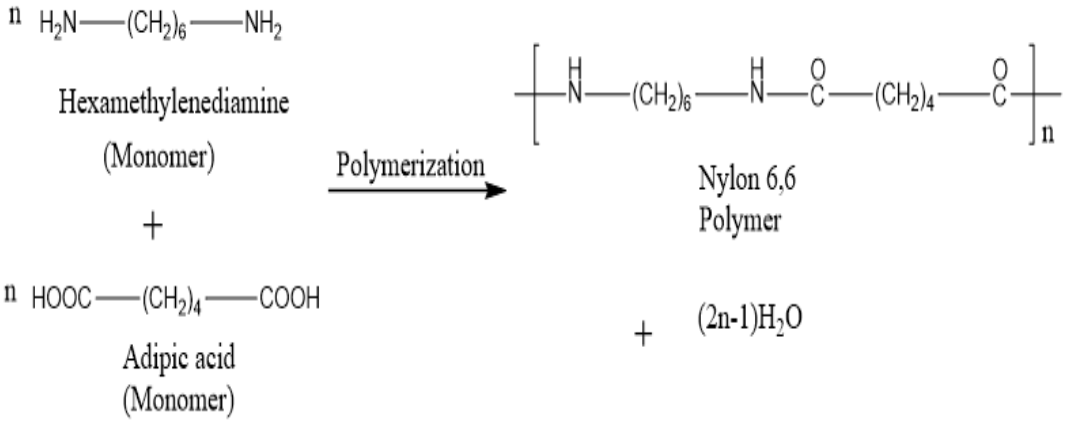
5.1 Synthesis of Bakelite:

Bakelite, first synthetic polymer, was synthesized in 1907 by Leo Baekeland. This synthesis led to many other inventions of synthetic plastics and polymers; this was synthesized by using phenol and methanal that is formaldehyde in controlled basic conditions with appropriate temperature and pressure. Bakelite is characterized by great durability, hardness and chemically resistance (Baekeland, 1909).



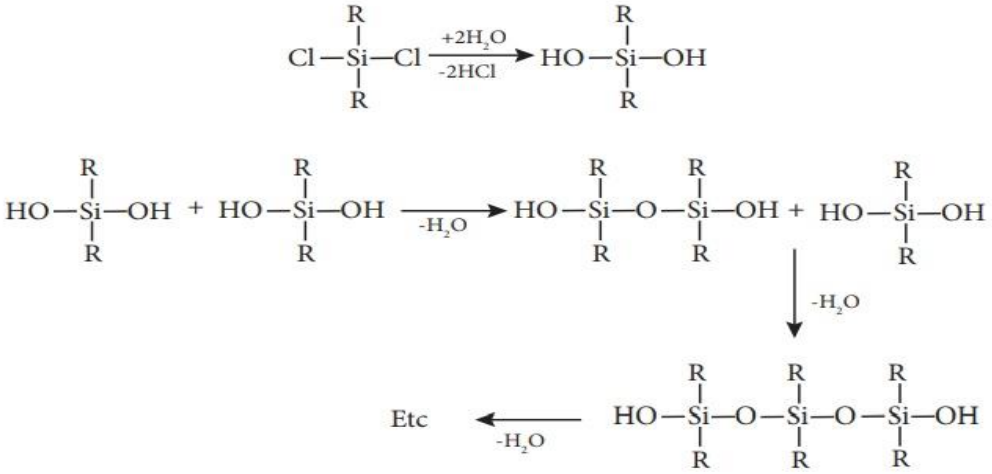
5.2 Synthesis of nylon

Nylon is a synthetic polymer which is actually a copolymer that is made up of two different species of monomers called adipic acid (a dioic acid, 1,6-Hexandioic acid) and hexamethylene diamine and the nylon that is formed as a result of this reaction is called nylon,6,6 because both monomers consist of six carbons each. Other forms of nylon are also being made in which carbon number of monomers is different. Nylon-6,6 is a condensation polymer as it is formed by condensation reaction in which removal of water occurs (Usuki et al., 1993).

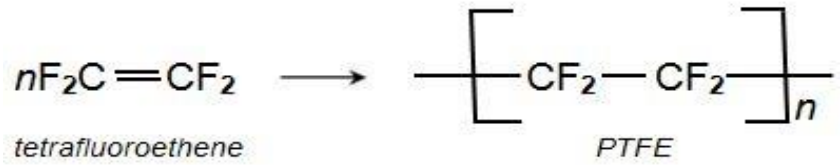


5.3 Development of silicones and Teflon

In 1823, Jackob Berzillius was the first scientist who has used excess of metallic potassium and metallic silicofluorure (K2SiF6) to undergo processing to extract **silicone** from it. It had been done by doing the reaction in silica container and heating small chunks of potassium and then washing away the residual by-products (Yilgör et al., 2014). The formation of silicone is given below:



Dr. Roy J. Plunkett has accidently prepared **Teflon** for the very first time when he was working on refrigerants. Full form of Teflon is 'polytertrafloroethylene' (PTFE) as it was discovered when he was working on a gas that is used as refrigerant named as tetrafloroethylene and he noticed the formation of white, waxy solid which was compressed and frozen then named as polytetrafloroethylene commonly known as Teflon (Kaur et al., 2001).



5.4 Emergence of bio-degradable and bio-polymers:

- In 1926, Maurice Lemoigne has prepared first bio-degradable polymer named as **polyhydroxybutyrate (PHB)** which is a polyester that is produced by multiple microorganisms and it was the first bioplastic that was discovered, identified and studied.
- Then **polyglycolic acid (PGA)** was first synthetic biodegradable polymer that was used in biomedical benefits and used as one of the key components in bio absorbable suture.
- One of the very first synthetic biodegradable polyester was **poly (lactic-co-glycolic acid) (PLGA)** that is also used in biomedical synthesis and also used as component in bio absorbable suture.
- Other than these above mentioned early bio degradable polymers, some of the other polymers like polylactic acid (PLA), polyanhydrides, plycaprolactone(PCL) and many other polymers were identified and then studied because of their vast applications in medical field due to biodegradability and other desirable characteristics (Shi et al., 2011).

6. Modern advances in polymer chemistry

Polymer chemistry has evolved extremely in the last few years and shows advances in synthesis, identification and profound studies related to many polymers because of their vast applications in industrial level, house-hold level, medicine field and many others. Some of the advances in the branch of polymer chemistry are given below:

❖ Smart polymers:

'Smart polymers are those polymers that shows visible large change or response to very small or fractional stimuli in environment like light, temperature, pressure, ionic strength and many other factors like these.' These polymers show reversible adsorption on the surface, change or alternation between hydrophobic state and hydrophilic state, gelation, destruction of surface graft, precipitation or collapse of hydrogel as **responses**. These polymers are temperature responsive, ionic strength responsive, light responsive and most responses of these polymers are reversible. This term was started when studies were started About the production of polymers or biomaterials that were prepared by the combination of biological activities of proteins with benefits of smart synthetic polymers. These smart polymers found their **applications** in development of diverse areas like drug delivery, molecular switches, regulated protein folding, gene therapy, microfluidics, bioseparation, reusable enzymatic catalysts and tissue engineering. Smart polymers are prepared by the conjugation of proteins with polymers and this linking of protein is either through engineering in a site- specific manner or random. The reactive amino acid could be bind in a particular position to trigger a particular kind of response to specific environmental stimuli (Roy et al., 2003).

❖ Conducting polymers:

Conducting polymers which are precisely called ‘conductive polymers. ‘These are the polymers which have the ability to conduct electricity and pass current that’s why show metallic conductivity and also can behave as semiconductors. These polymers have different mechanical properties than other polymers but show conductivity and also not thermoplastic in nature. These polymers and their properties can be altered or somehow changed by using dispersion method. These polymers are more similar to organic polymers which are organic and covalent in nature. These polymers find their vast applications in the different fields due to their property to conduct electricity. Some **applications** are like printing electronic circuits, radar absorptive coating, supercapacitors, solar panels, amplifiers, organic LEDs, bio-sensors, chemical sensors, transparent conductive layers, microwave-absorptive coatings and many other applications like these. The organic structure of these polymers consists of organic rings, long chains, aromatic rings, double bonds, and aromatic cycles along with other functional groups. These polymers are mainly **synthesized** by dehydrogenation, electro-co-polymerization and many other techniques and methods (Awuzie, 2017).

❖ Biodegradable polymer:

‘These are the polymers which can easily be decomposed by bacterial activities and then produce inorganic salts and gases, biomass, water and other organic materials in the form of product’. These polymers consist of ester, amide, ether and other functional groups and these polymers can be natural polymers obtained from natural sources and artificial or synthetic polymers which are man- made. Metal catalysts, ring opening polymerization and condensation polymerization reactions are used for the **manufacturing** of these polymers. These polymers are specialized due to non- toxic nature, high crystallinity, high surface area, good mechanical strength, hydrophobicity and many other such characteristics. These polymers find their **applications** in the making of nano- medicine, in the field of tissue engineering, drug- delivery, designation of metabolic pathways and other repairing of bone damage area and creation of damaged arteries and capillaries (Chandra et al., 1998).

❖ Recyclable and green polymers:

‘These polymers are sustainable, having least impact on the environment and also renewable, biodegradable polymers. These are the polymers which can easily be used, restored after collection and recycled again and again after giving them particular desirable properties. These polymers are the cause of least air pollution, water pollution, soil pollution and land pollution. Even on recycling and bacterial decomposition the biomass and other organic, inorganic biomaterial which is produced is least harmful for the environment. These polymers are **used** in pharmaceutical industries, in biomedical field, in constructions, packaging, electronics, traditional plastic’s replacement and many other applications (Hong et al., 2017).

❖ **High performance polymers:**

'All the polymers that have the capacity to bear extreme environmental conditions like high pressure, high temperature, effect of multiple reactive agents, effect of oxidizing and reducing agents, impact of inert agents and many other factors like these, but still these polymers have the capacity to retain their desirable properties to maximum are called high performance polymers.' These are also called heat resistant polymers and advanced engineering material and high temperature polymers because of their ability to withstand high temperature and vast applications in engineering field. These polymers need to follow some **criteria** like high decomposition temperature, high durability, and ability to withstand corrosive agents and radiations, ability to retain its characteristics even on attack of aggressive chemicals, electrical shock and mechanical stress. These polymers should have high glass transition temperature, minimal weight loss on even extreme high conditions of temperature and exceptional mechanical properties. These polymers have found their **applications** in the field of manufacturing of heavy machinery, gas industries, oil industries, production operations, drilling operations, automotive and aerospace industries, electronics and many other fields (Al Christopher et al., 2021).

7. Characterization of polymer techniques

- **GPC:**

GPC stands for 'gel permeation chromatography'. This technique is used to separate polymers on the basis of differences in molecular masses and sizes. In this technique, polymers are separated by using perforated gel made up of cross- linked polymer like dextran, polyamide or polystyrene that is filled in a column and then dissolved polymers (desired polymers dissolved into any suitable solvent) are passed or injected through this column. The polymers having greater molecular mass and larger size are not able to penetrate deeper into perforations that's why separated early than the polymers having lesser size and lesser molecular mass because of their greater ability to penetrate deep into perforations of gel that is filled in the column. This technique is also named as 'size exclusion chromatography that is abbreviated as SEC'. The amount or concentration of polymer that is eluted from this column is determined with the help of different detectors like light scattering detectors or refractive index (RI) detectors (Kissin, 1995).

- **FTIR and NMR:**

FTIR stands for 'Fourier transform infrared spectroscopy'. This technique use specific and particular absorption of infrared rays and particular patterns of absorption of infrared rays by any polymer is used to analyze the structure of polymer and identification of polymers. The presence of any functional group and specific feature related to the structure of polymer are also identified with the help of this technique. This technique also helped in the determination of type of polymer, effect of environmental factors on polymer and decomposition of polymers with the passage of time due to the presence of environmental factors, the quality of polymers is also assessed by using this technique, helps in the identification of components of polymers and their interaction with each

other that gives particular properties to polymer and polymers showing different kind of reaction and how these reactions are progressed are studied with the help of FTIR. NMR stands for 'nuclear magnetic resonance'. This technique is utilized to study the sequence or arrangement of monomers, substituents in any parent chain of polymer, movement and flexibility of polymers is also determined by this technique so other properties can also be predicted on this basis (Bhargava et al., 2003).

- **DSC and TGA:**

DSC stands for 'differential scanning calorimetry.' This technique is used for the determination of effect of heat on type of polymers, analysis and identification of different types of polymers on the basis of thermal properties, the effect of blending of different type of polymers and their nature, determination of optimal temperature for manufacturing of polymers, how polymers can be decomposed or degraded on multiple temperatures and also determination of glass transition temperature for different polymers. This technique is also used for the study of different physical properties which are related to their change in temperature and also helps in the determination of melting temperature, glass transition temperature and other such factors by measuring the difference in heat changes that occurs when heat is transferred between a sample that is any sample studied and a reference material. TGA stands for 'thermogravimetric analysis'. This technique helps to determine the stability of any polymer at different temperature, for determination of different additives, fillers and volatile components in any polymer, if moisture is absorbed or retained by any polymer then that's also determined by this technique, determination of temperature at which any polymer starts melting or undergo evaporation. This technique also helps in the study of mass change and composition change in any polymer when temperature is varied as the polymer is heated or cooled but this process is studied under specifically controlled conditions (Wong et al., 2002).

8. Applications of polymers

Polymers found vast applications but some of the applications are given below:

- Polymers are majorly used for the packaging of food material that could be beverages, dairy products or other food products. For example, polystyrene, polypropylene and other such polymers are used in packaging.
- Polymers are used in textiles and clothing as linen etc.
- Polymers are used for the making of thermal insulation which are also electrically insulators too for household or for buildings and also used in transportation.
- Polymers are also used in biomedical field as they are used in the synthesis of wound healers, making of surgical instruments, implantation of biomedical materials and also used in drug delivery system.
- Polymers are used in aerospace as because of higher thermal stability of some polymers.
- Polymers are also used for making some parts of automobile engines and vehicles as because of their stability, sensitivity and resistibility.

- Polymers are also used for making of semiconductors, batteries and some electronic devices.
- Polymers are used for the making of elastomers and also for the making of insulation used for storage containers.
- Polymers are used for the making of parts or components of space crafts like body panel, window, adhesive parts, instruments etc.
- Polymers are used in the making of helicopter, silicon nanocomposite coating for airbags that could be used in Mars exploration rover by NASA.
- Polymers are used in the making of components of military aircrafts.
- Polymers are used for the making of sea water pipes.
- Polymers are used for the making of optical glasses which are used under sea level.
- Polymers are used for the making of life saving jackets and cargo lines.
- Polymers are used for the prevention of soil erosion, for increasing water using plants.

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Pharmaceutical Chemistry Innovations

Tatheer FATIMA
Shamsa SHABBIR

1.1 Introduction

Pharmaceutical chemistry is an interdisciplinary branch of chemistry that collaborates with the principles of organic and inorganic chemistry, biochemistry, analytical chemistry, molecular biology, and pharmacology. It deals with the design, development, synthesis, and analysis of biologically active molecules that can be used for the production of different medicines. These pharmacologically active compounds can prevent or treat different diseases. Pharmaceutical chemistry has revolutionized modern pharmacological techniques and the Discovery of drugs (Silverman & Holladay, 2014).
Pharmacological chemistry carries a vast scope from the discovery of biological reactive compounds to the final results of the compound in the human body to cure that specific disease. This includes initial design of the active compound, then its integration into the delivery system of the human body in a controlled and effective manner (Katzung, Vanderah, & Trevor, 2021).

There are various steps:
1.1.1 Drug Design and Discovery: In the first step, using structure-activity relationships (SAR), the lead compound is identified, and it is screened through high-throughput screening techniques. After identification using molecular modeling, this compound is actively used in the desired medicine (Silverman & Holladay, 2014).

1.1.2 Synthesis of drug molecules: The efficient synthesis of drug molecules focuses on their wheel purity and scalability (Barrett, 2018).

1.1.3 Pharmaceutical analysis: In terms of pharmaceutical analysis, drug molecules are actively passed through HPLC analysis, gas chromatography analysis, mass spectrometry, or other qualitative and quantitative analyses of medicine and their metabolites (Watson, 2020).

1.1.4 Drug formulation and delivery: The most crucial step of drug is the drug delivery into the system. To ensure this tab is mandatory to formulate the drug according to the availability and the targeted delivery system. So the drug is formulated according to the different drug delivery systems, like nanoparticles, transdermal patches, or liposomes (Allen & Ansel, 2013).

1.1.5 Toxicology and pharmacokinetics: when the drug delivery system is successfully targeted, the drug evaluation in terms of its safety, metabolism, distribution, absorption, and its final excretion from the body is studied through in vitro and in vivo activities (Gibaldi & Perrier, 1982).

1.2 Importance of pharmaceutical chemistry:

Pharmaceutical chemistry is fundamental to respond to emerging medical challenges because it directly contributes to public health. Important contributions of pharmaceutical chemistry are as follows:

1.2.1 Drug innovation and therapeutics:

There are various life-saving medicines, such as those for HIV, cardiovascular disease, diabetes, and cancer, that are developed by using pharmaceutical chemistry. Day by day, these medicines are also innovative according to the challenges like antibiotic resistance and different viral mutations. So the IM pharmaceutical chemistry ensures continuous innovation in the therapeutic field.

1.2.2 Safety and efficacy:

Pharmaceutical chemistry involves the medicine's safety and its practical use. To ensure these qualities, strict analytical validations and testing are necessary for the approval of drugs.

1.2.3 Quality control and assurance:

ensuring equality and consistency of the pharmaceutical drugs is vital for public safety and regulation. Chemistry plays a critical role in establishing assurance and quality standards and detecting contaminants and impurities.

1.2.4 Interdisciplinary integration: this field not only contributes to the production of medicine but also contributes to other distinct fields like biotechnology, biomedical research, and material sciences for driving the process of pharmaceutical products.

1.2.5 Global health impact: today, the production of life-saving medicines like HIV vaccines, antibiotics, antiviral vaccines, and other critical medicinal products has a crucial impact in combating pandemics and improving life (Patrick, 2017).

1.3 Historical background

In ancient civilizations, the traditional medicinal system, such as Ayurveda, was a rich source for creating and curing infections. This system was primarily utilized in India, Chinese herbal medicines, and Greek remedies. These ancient civilizations mostly used medicinal plants for healing purposes as a folk medicine.

During the 19th century, these traditional medicines were transformed into modern pharmaceutical medicine when the active agents from these medicinal plants were isolated using various innovative techniques. This was a milestone in the history of pharmaceutical chemistry from the 18th to the 21st century.

In the early ages, a German pharmacist, Friedrich Serturner, isolated morphine from opium and initiated the isolation of active compounds. Then, in the late 19th century, by organic chemistry, Aspirin was designed in 1897 by Felix Hoffmann to relieve pain. In 1928, penicillin was discovered by Alexander Fleming, and it laid the foundation for antibiotics and pharmaceutical microbiology. In the 20th century, various synthetic drugs were developed, such as barbiturates, sulphonamides, and psychotropic drugs. From the 1970s to the present era, using computational chemistry with the help of computers, different drugs have been designed according to the target, setting a standard practice in the innovation of drug history (Sneader, 2005).

1.4 Emerging Trends in Drug Discovery and Design

(Computer-Aided Drug Design (CADD) and Structure–Activity Relationships (SAR))

As the world is changing, complexity in diseases is emerging. This complexity demands a safer and targeted therapeutic medication system. So that traditional trial and error methods are being replaced by sophisticated innovative approaches for drug Discovery and design.
Nowadays, the most demanding advanced techniques for the production of medicines are computer-aided drug design (CADD) and structure-activity relationships (SAR). These innovative techniques significantly reduce the cost, risk, and time associated with the pharmacokinetics.

1.4.1 Computer-aided drug design (CADD)

When a biologically active molecule is discovered, various competition and modeling tools and techniques are used for its design and optimization, which is referred to as computer-aided drug design. These techniques help to analyze the structure of the molecule and predict how this molecule will interact with its target using algorithms and molecular simulations. Active compounds can be targeted at different proteins, enzymes, or other receptors.
Computer-aided drug designing tools mostly approach two techniques

- **Structure-based drug design (SBDD)**
- **Ligand-based drug design (LBDD)**

- **Structure-based drug design (SBDD)**

This technique depends upon the attachment of the target molecule to the active side of the receptor. It is mainly based on the 3D structure of the target receptor or protein by which the active compound will attach. Using computer editing tools, the target molecule is actively docking with the site of the target protein or receptor, and it is identified by their binding affinity and molecular interactions.

- **Ligand-based drug design (LBDD)**

This technique is used to build a predictive model for molecule attachment when the 3D structure of the target is unknown.

There are various benefits and applications of the computer-aided drug designing technique, which include the prediction of potential toxicity before clinical testing, and it is a very cost-effective and time-effective technique. It gives high-throughput screening of millions of compounds virtually. Various practices have been used recently by using computer editing tools to design the pandemic drugs. The most important are COVID-19 vaccines and HIV protein inhibitors (Sliwoski et al., 2014).

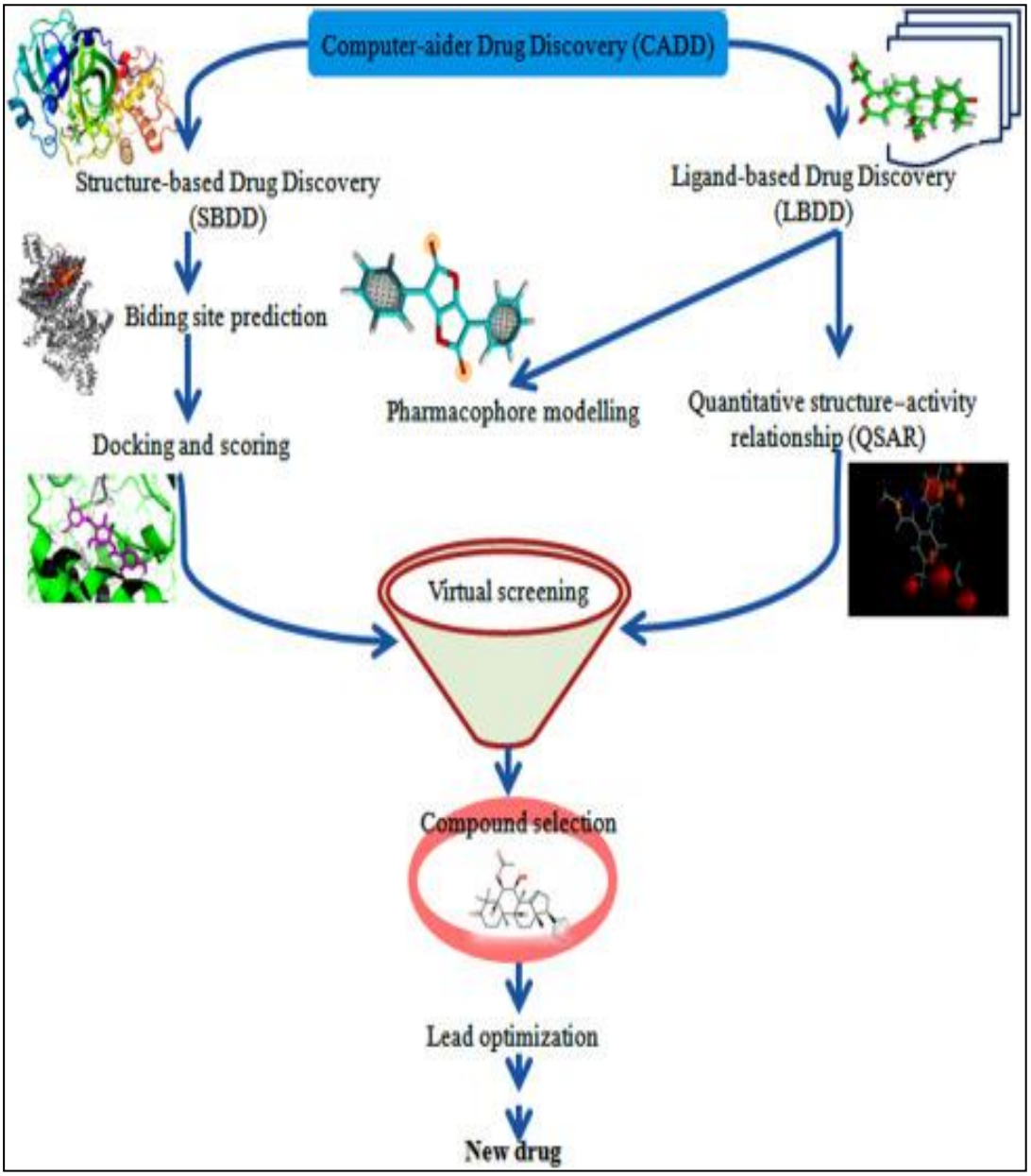

Figure 1. Computational Aided Drugs; SBDD and LBDD

1.4.2 Structure–Activity Relationships (SAR)

In the structure-activity relationship technique, chemists understand the structure of bioactive compounds in terms of their behaviour in the system. Moreover, in this technique, a few modifications in the target molecule are also made to observe how these changes will impact the pharmacological effect. If the structural modification causes greater potential in the biological system then it can assume a best compound with few modifications to target. Then this compound is targeted by the medicinal chemist for greater potential, selection, and safety. The various types of structure modifications that can be done in this technique make more effective active compounds in medicine.

Inorganic compounds' alkyl chain variation can be an effective way to make them more lipophilic and metabolically stable. Functional group alteration is also a good way to improve the binding and solubility of the target compound. Functional groups in the organic compounds like hydroxyl carboxyl and amines can be altered. In case of aromatic by active compounds, the ring size or the type of aromatic and heterocyclic ring can make the receptor binding more impactful. By changing the special orientation of the atoms or the stereochemistry address mint can be an effective way to enhance the selectivity and to reduce the toxicological effects of the medicine (Silverman & Holladay, 2014).

1.4.2.1 Quantitative SAR (QSAR)

In the quantitative structural activity relationship technique, mathematical models are developed that can relate structural descriptors like the target's molecular weight and electronic configuration to the biological activity. QSAR models can protect the activity of new active compounds even before their synthesis. SAR technique is very effective in the identification and optimisation of the selective compounds, and it helps in the selection of the most promising compound for biological activity. Moreover, this technique helps to understand which part of the compound can cause toxicity so that it can be redesigned for safer use. Is this also an effective technique, like computer-aided drug designing, to modify the molecule to enhance the quality of absorption, metabolism, bioavailability, and distribution of medicines? By using this technique, beta blockers like propranolol and non-steroidal anti-inflammatory drugs are developed, which leads to safer and more effective agents. CADD and SAR offer more productive, effective, and precise strategies to innovate pharmaceutical research. Together these two techniques form the backbone of pharmacokinetics and it enables the development of more effective and safer medicines. As well as machine learning and artificial intelligence is continuously evolving to be more powerful and help out the shape of the future of modern drug designing (Cherkasov et al., 2014).

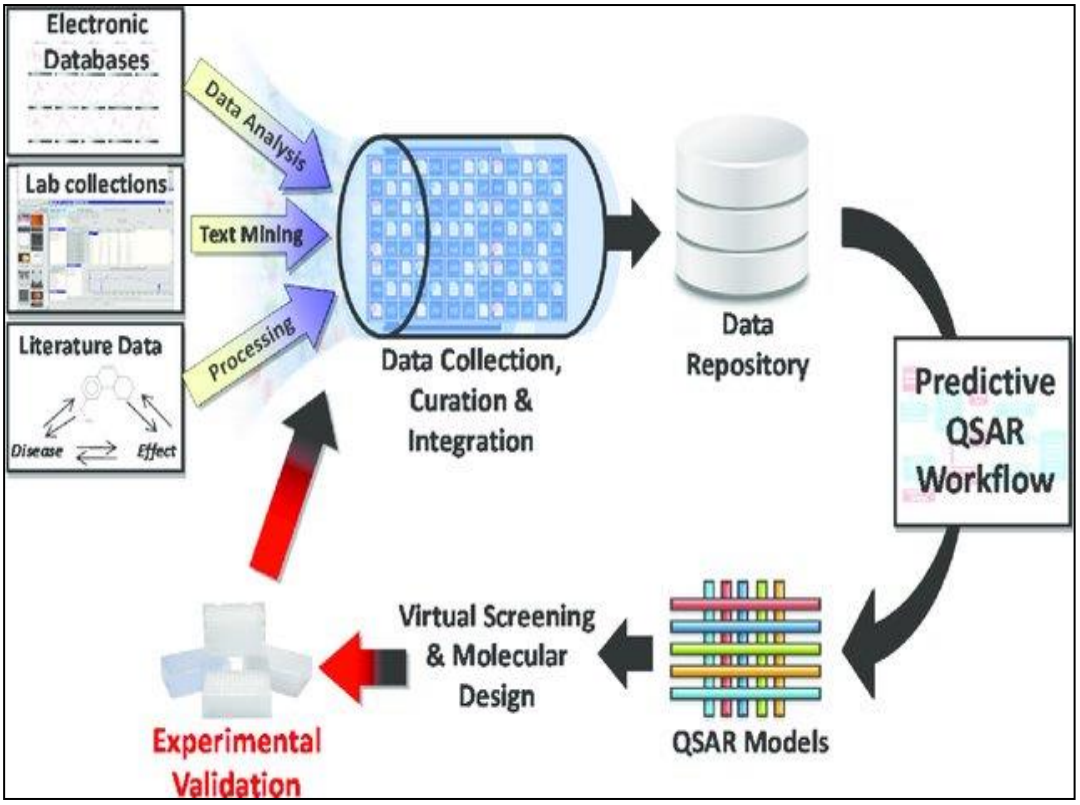

Figure 2. QSAR Analysis: Creative Biostructure Drug Discovery

1.5 Innovative Synthetic Approaches in Drug Development

The development of drugs lies at the heart of the synthesis of pharmacological compounds. The development of a drug depends upon the synthesis of pharmaceutical compounds. Ordinary leave for the multi-step drug synthesis processes was used, which included energy-intensive processes, toxic solvents, and hazardous agents. All those conventional methods effectively produced desirable yield and components, but also raised some environmental safety concerns as well as concerns about sustainability and cost efficiency. To minimize these challenges, pharmaceutical industries have evolved to innovative synthetic approaches that are considered not only cost-effective but also environmentally friendly. Microwave-assisted synthesis, flow chemistry, and Green chemistry are among the most emerging revolutionary techniques that are transforming how drugs are developed.

1.5.1 Green chemistry methods

This is the most effective and environmentally friendly method considered nowadays for the processing and production of the lord shield of medicine. This method has the least harmful substances for the generation of desirable compounds in drug development. In the production of medicine, Green chemistry is used to reduce waste material, energy use, and the environmental impact of compounds, while also maintaining the effectiveness of synthetic reactions. The development of drugs using Green chemistry involves minimizing waste and maximizing the incorporation of the material into the final product. Moreover, it enhances the safety of the solvent and reaction conditions, and ensures efficient use of renewable materials

and design for degradation. Green chemistry methodology is used for the replacement of solvents like chloroform and benzene with alternative materials such as water, ethanol, and supercritical carbon dioxide. Moreover, this methodology is integrated with many reactions that happen in one vessel without the need for solvent distribution, isolation, or purification. The very famous anti-HIV drug efavirenz was developed using Green chemistry methodology, which leads to the production of vaccines by reducing the amount of solvent used by 75% and also improving its overall yield (Anastas & Warner, 1998).

1.5.2 Flow chemistry

Flow chemistry is an advanced technology in which chemical reactions occur in a continuously flowing system as compared to traditional reactors. In this advanced method, reactants are placed into a reactor, and the reaction takes place as the material passes through the system. This process offers several benefits, particularly in terms of reaction parameters like pressure, temperature, time, and productivity, which can be precisely controlled. Moreover, in this methodology, reactions are safely conducted, especially those that are exothermic and involve explosive intermediates. Integration with the purification system of flowchartometry also gives the best control and streamlines production.

For drug production, slow chemistry has proven to be an innovative approach involving multiple steps, enabling this process in a single system without intermediates and waste. This process is beneficial for those reactions in which light or current is involved, as it simplifies the handling of such reactions. Another important feature of this groundbreaking innovation is a drug synthesis on demand, where pharmaceutical drugs can be produced on-site and as needed in emergencies in remote locations. Artemether is an important antimalarial drug produced using this innovative flow chemistry technique (Ley et al., 2015).

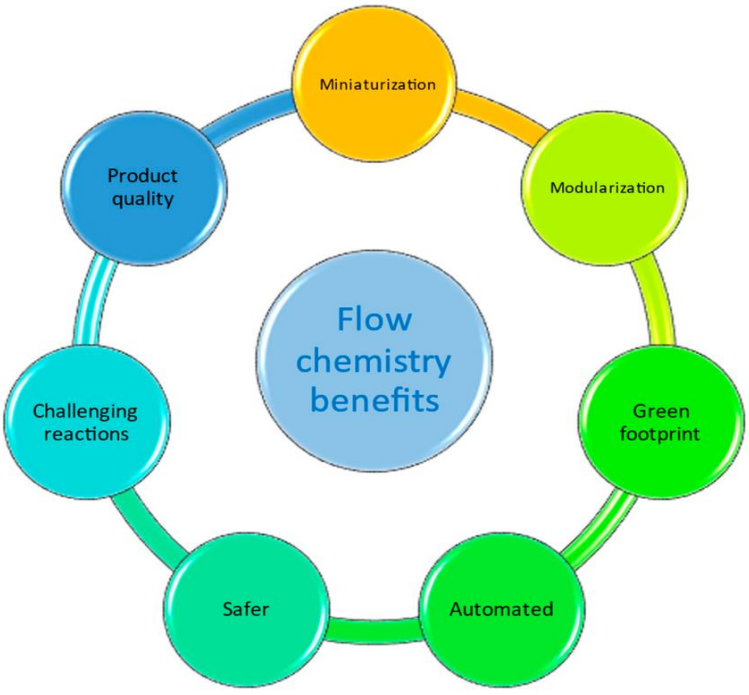

Figure 3. Benefits of Flow Chemistry In Pharmaceutical Industries

1.5.3 Microwave-assisted synthesis

In this advanced technique for the production of pharmaceuticals at an industrial level, microwave radiation is used to heat chemical reactions uniformly and rapidly. This method relies on conventional heating methods, which are conduction and convection, in which the reaction mixture is exposed to microwave radiation, which directly contacts polar molecules. As a result of this interaction, energy is transferred more efficiently, allowing reactions to occur at a significantly higher rate. This approach aims at reaction time, which typically takes more than several hours. This groundbreaking technology enhances production and reduces the formation of unwanted products, thereby improving the efficiency of the synthetic product. This method is environmentally friendly and cost-effective because less energy is used compared to the conventional heating reactions. Reactors are designed sufficiently to scale up the reaction as well as maintain production and efficiency at both the research and industrial levels. This microwave-assisted process is more efficient for the production of hydrocyclic compounds, which are the main structure of many therapeutics. It is also used for the production of peptides and polymers, where exact conditions are required. It is also used for screening of medicinal chemistry in library generation, which makes it possible to produce different molecular structures for biological testing. Quinoline is an example of this application, a compound used in antimalarial and anti-cancer drugs. Microwave cystic process utilized for the production of pure and high yield quality products over conventional methods to highlight the innovative potential in modern drug development and discovery (Kappe, 2004).

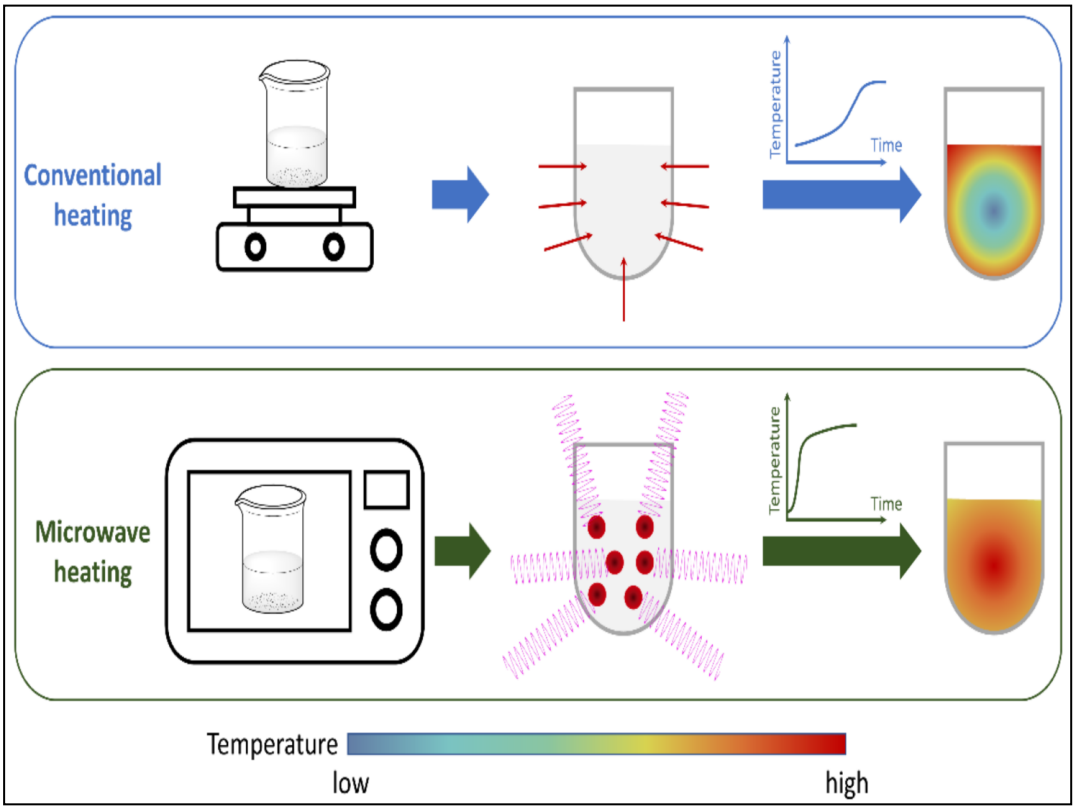

Figure 4. Microwave Assisted Drug production Vs Conventional Heating Method

1.5.4 3D printing in pharmaceutical chemistry

For the production and delivery of medicine, the integration of a 3D printing approach in pharmaceutical chemistry is a new frontier. September or additional manufacturing, this technique allows for custom drug preparation, ensuring the needs of every individual, as compared to the large batch production of uniform capsules or tablets. Freddy printers make it possible to create dosages with specific shapes and drug combinations and profiles that are challenging to achieve otherwise.

Personalized dosage and polypeals are the most advanced applications. Personalized dosage enables every individual patient to receive the exact quantity of medicine according to their needs. Other factors, such as genetic profile, weight, age, and metabolic rate, also affect this technique. It has maximum benefits with minimum side effects. While Poli pills are also one of the most promising approaches, in which multiple ingredients for the drugs are combined into an interesting tablet that improves complications in patients who are suffering from severe cardiovascular diseases or diabetes. These patients have to follow a complex medication prescription. Spritam is one of the landmark examples of this technology, which is designed using 3D printing techniques. Moreover, it is the first FDA-approved 3D printed tablet fish design for epilepsy patients. It dissolves quickly and provides convenience and precise dosage (Norman et al., 2017).

1.5.5 Machine learning and artificial intelligence

Machine learning and artificial intelligence are used to reshape the drug development and discovery. This technology has developed a dataset of chemical libraries to genomic sequences, a pattern that is difficult for humans. Artificial intelligence can design a powerful drug, and it can forecast the pharmacological activity and toxicity, as well as pharmacokinetics, to synthesize the drug. It can dramatically reduce the time for the production of new drug synthesis from its identification to the clinical testing. Moreover, automation in pharmaceuticals can increase the efficiency of drug formation. During the COVID-19 pandemic, pharmaceutical companies used artificial intelligence to identify potential antiviral drugs quickly (Vamathevan et al., 2019).

1.6 Future Prospects and global perspectives

Global health challenges, such as outbreaks of emerging viral diseases and other communicable diseases, require an emergence in technology innovation for drug production in pharmaceutical chemistry. These challenges require not only faster delivery of the drugs but also their adaptability to diverse populations and healthcare settings. The combination of brochures, including 3D printing, artificial intelligence, and advanced synthetic methods, can provide an approach for developing advanced medicines in limited settings. The interdisciplinary approach in pharmaceutical chemistry can be a bridge to solve the gap between designing a molecule and patient care. For example, collaboration between computational scientists and clinicians can produce predictive models that work efficiently.

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Nano-chemistry in Chemical Applications

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Yusra MAJEED

Muqadas ALEEM

With its innovative approaches to enhancing sustainability, efficiency, and selectivity in a variety of chemical processes, nanotechnology has emerged as a revolutionary tool in chemical applications. This chapter looks at the production, characteristics, and applications of nanomaterials in chemical sensing, energy storage, environmental remediation, and catalysis. Special focus is paid to the role of nanoparticles as advanced catalysts that speed up reactions while using less energy and producing less waste. This chapter also discusses the application of nanostructures in chemical sensors for extremely sensitive pollution detection and industrial process monitoring. Furthermore, the potential of nanotechnology in green chemistry techniques is explored, focusing on its function in environmentally friendly chemical production. This in-depth examination demonstrates how crucial nanotechnology has been in revolutionizing the chemical industry and paving the way for future advancements in chemical research and industrial applications.

The fast evolving science of nanotechnology has revolutionized a number of industries, including electronics, medicine, environmental research, and chemical engineering(Malik et al., 2023).Manipulating matter at the atomic or molecular level to create materials and technologies with unique properties not found in their larger-scale counterparts is the main focus of nanotechnology(Rafeeq et al., 2025).Nanotechnology and chemistry may now be used to build new materials, catalysts, and processes that are more functional, efficient, and sustainable. Chemistry studies the behavior and interactions of various compounds. By enabling researchers to precisely control the characteristics and actions of individual particles, nanotechnology has contributed to the transformation of chemistry(Mitchell et al., 2021). Numerous branches of chemistry have greatly profited from developments in nanotechnology, including the creation of novel nanomaterials, catalysts, drug delivery systems, and sustainable technologies. The usual size of nanomaterials ranges from 1 to 100 nanometers, which defines them(Khan et al., 2022). They frequently have characteristics that are entirely distinct from those of their mass counterparts. Better conductivity, magnetism, strength, and reactivity are the results of enhanced surface energy, a greater surface area-to-volume ratio, and quantum effects. As a result, nanomaterials enable the development of low-impact energy sources, enhance chemical processes, and progress a variety of industries(Rahman et al., 2025).

Chemistry has been greatly revolutionized by nanotechnology, which has enabled the development of catalysts that speed up and accurately regulate chemical reactions(Chadha et al., 2022). Enhancing a range of industrial processes utilized in the manufacturing of fine chemicals, petrochemicals, and medications requires the employment of nano-catalysts.

Furthermore, nanotechnology is making it easier to develop innovative drug delivery methods that enable medical professionals to deliver drugs directly to specific body areas for targeted therapy, enhancing therapeutic results. Additionally, nanotechnology is making a substantial contribution to the resolution of environmental problems such as pollution, water treatment, and waste management(Manzari et al., 2021).Nanotechnology improves absorption, breakdown, and removal methods, enabling efficient pollution treatments. Innovations in nanotechnology are driven by the desire for industry to operate in a more ecologically responsible way. Using nanotechnology in the realm of chemistry presents a number of difficulties. Concerns regarding safety, the impact on the environment, and moral dilemmas may arise with the introduction of new materials and technology. Because nanoparticles can be hazardous to humans and the environment, proper use of these technologies necessitates a thorough assessment of potential dangers and ongoing regulatory oversight(Isibor et al., 2024).

Nanotechnology in Chemistry

The field of nanotechnology has developed to encompass many scientific fields and successfully combines fields like chemistry, physics, biology, and materials science(Haleem et al., 2023). The integration of chemistry with other disciplines has had a significant impact and has the potential to change a wide range of fields. Chemists can create new materials with distinctive properties for use in catalysts, polymers, and composites by manipulating atoms and molecules at the nanoscale(Mitchell et al., 2021). Atom-by-atom engineering of nanomaterials is now possible because to synthetic techniques and computer technologies. They have special qualities that have a wide range of uses in chemistry. Nanotechnology is essential to the development of catalytic reactions in chemistry. Usually used in chemical reactions, traditional catalysts frequently have drawbacks such poor selectivity, sluggish reaction speeds, and restricted recyclability(Tahir et al., 2021). However, the increased surface area and active sites provided by nanocatalysts—which are frequently made of nanoparticles or nanostructured materials—lead to faster, more effective reactions with improved selectivity. These catalysts are especially useful in the synthesis of biofuels, petrochemicals, and fine chemicals, where accuracy and productivity are critical. At the core of this chemical revolution is the creation of nanomaterials(Mukhtar et al., 2022). By manipulating their size, shape, and composition at the molecular level, nanomaterials can be designed to have particular qualities. For instance, because of their small size and high surface-to-volume ratio, metal nanoparticles like gold, silver, and platinum have shown exceptional catalytic activity. Similar to this, materials created by mixing nanoparticles with polymers or other materials, known as nanocomposites, have improved mechanical, thermal, and electrical properties that make them perfect for a variety of uses, such as energy storage devices, coatings, and sensors(Sharma et al., 2021).

In pharmaceutical chemistry, nanotechnology has advanced the creation of drug delivery methods in addition to catalysis and material design(Sultana et al., 2022). Due to their small size, nanoparticles can be designed to more accurately deliver medications to certain body parts, minimizing adverse effects and enhancing therapeutic effectiveness. In the treatment of

cancer and other chronic diseases, when conventional techniques frequently fall short of providing sufficient therapeutic dosages to the intended site, this focused approach to medication administration is especially helpful. Beyond industrial uses, nanotechnology plays a significant role in chemistry.(Baryakova et al., 2023) By facilitating the creation of more environmentally friendly and sustainable chemical processes, it also tackles important environmental issues. Because nano-based materials can improve reactions that break down contaminants or make it easier for pollutants to be absorbed, they are being employed more and more in environmental applications like energy production, pollution control, and water purification(Saravanan et al., 2021). The future of science and technology will be redefined by the novel materials, processes, and applications made possible by the convergence of nanotechnology and chemistry as the area develops further. However, the widespread usage of nanomaterials raises safety, ethical, and environmental problems that must be carefully considered in light of this rapid advancement(Inbathamizh et al., 2023).

The Fundamentals of Nanotechnology: Principles and Methods

Scientific research and industry innovation now rely heavily on nanotechnology, which is commonly defined as the manipulation of matter at the atomic, molecular, and supramolecular scales. Fundamentally, the design, synthesis, and use of materials and technologies whose shapes, characteristics, and uses arise from their nanoscale dimensions (1–100 nanometers) constitute nanotechnology. Understanding the fundamental ideas and techniques that underpin nanotechnology is crucial to comprehending how it affects chemistry(Khan et al., 2022).

Nanoscience and Nanotechnology: Defining the Scope

Despite their frequent interchangeability, "nanoscience" and "nanotechnology" are not synonymous. Understanding the behavior of matter at this minuscule size is the main goal of nanoscience, which is the study of phenomena and material manipulation at the nanoscale(Manzoor et al., 2025). The use of this knowledge to design and build buildings, systems, and gadgets with special qualities is known as **nanotechnology**. Physics, chemistry, biology, and engineering concepts are combined in nanotechnology to produce novel instruments, materials, and systems(Panda et al., 2021).

Key Principles of Nanotechnology

There are many principles that enable the manipulation and creation of nanomaterials. Some followings are the key principles that acknowledged the field:

a. **Quantum Effects:** Materials behave very differently at the nanoscale than they do at the macroscale. This is due to the fact that when particle size drops, quantum mechanical effects become more noticeable. Materials' electrical, optical, and chemical characteristics may alter as a result of these quantum phenomena. For instance, because

of a quantum mechanical phenomenon called surface plasmon resonance, gold nanoparticles have distinct optical characteristics from bulk gold(Zhang et al., 2023).

b. **Ratio of Surface to Volume:** The surface-to-volume ratio sharply rises as materials are reduced to the nanoscale. Compared to their bulk counterparts, nanomaterials are far more reactive due to their increased surface area, which also increases the number of active sites for chemical reactions. In catalysis, where a larger surface area results in higher catalytic activity, this characteristic is particularly crucial(Pozzi et al., 2024).
c. **Self-Assembly:** The process by which molecules spontaneously arrange themselves into structured nanomaterials is known as self-assembly, and it is one of the most fascinating concepts in nanotechnology. Without the aid of outside forces, self-assembly uses a molecule's inherent characteristics, such as hydrophobicity or electrostatic interactions, to propel the creation of nanostructures. In chemical science, this idea has enormous promise for creating nanostructured materials(Gupta et al., 2022).
d. **Comparing Top-Down and Bottom-Up Methods:** Nanotechnology includes both top-down and bottom-up methods for creating materials at the nanoscale. Using mechanical, chemical, or photolithographic techniques, the top-down process breaks down bigger materials into nanoscale components. In contrast, the bottom-up strategy builds materials atom by atom or molecule by molecule, frequently through the use of self-assembly processes or chemical reactions(Tripathy et al., 2023).

Nanomaterials in Chemical Chemistry: Synthesis and Characterization

Advanced techniques and methods are needed for the synthesis of these materials, and characterization is essential to guaranteeing that the materials fulfill the requirements needed for different applications. The synthesis and characterization of nanomaterials within the framework of chemical chemistry will be examined in this chapter.

Nanomaterials' Significance in Chemistry:

Compared to their bulk equivalents, nanomaterials have exceptional features because of size-dependent processes that take place at the nanoscale. These consist of new mechanical behaviors, improved electrical and optical characteristics, greater surface area, and improved reactivity. Because of these characteristics, nanomaterials can be used in a variety of fields, such as environmental cleanup, medicine delivery, energy storage, sensors, and catalysis(Atif et al., 2022).Nanomaterials are essential to chemistry because they can improve the characteristics of materials, increase the efficiency of chemical reactions, and create new technologies that were previously impractical with conventional materials. Many fields of industrial chemistry and chemical engineering have undergone radical change as a result of the creation of nanomaterials, which has made it possible to create novel energy sources, improved medication delivery systems, and more effective chemical processes(Baig et al., 2021).

Types of Nanomaterials in Chemistry

Nanomaterials can be classified into various categories based on their shape, size, and composition are shown in image 1. Some of the common types of nanomaterials used in chemistry include:

a. Nanoparticles: Solid particles with at least one dimension in the nanometer (1–100 nm) range are called nanoparticles. They may consist of carbon, polymers, metals, metal oxides, and other substances. Because of their tiny size and large surface area, which offer a large number of active sites for chemical reactions, nanoparticles are commonly utilized in catalysis. Heterogeneous catalysis frequently uses metal nanoparticles, such as gold and silver nanoparticles, which can improve reaction speeds and selectivity(Wu et al., 2022).

b. Nanotubes: Tubular formations that have dimensions in the nanometer range are called nanotubes. Carbon nanotubes (CNTs), which have remarkable mechanical, electrical, and thermal characteristics, are the most often researched nanotubes. CNTs can be used as catalysts or catalyst supports, sensors, batteries, and supercapacitors. In chemical chemistry, they are especially useful for improving the functionality of materials in chemical reaction processes and energy storage devices(Rashko et al., 2022).

c. Nanowires and Nanorods: Despite having nanoscale dimensions, these one-dimensional nanostructures may reach lengths of many micrometers. Although they are commonly employed in electrical and optoelectronic applications, nanowires and nanorods may also be found in chemistry, namely in the creation of fuel cells, high-performance sensors, and catalytic materials(Kirubakaran et al., 2025).

d. Quantum dots: Due to quantum confinement phenomena, semiconductor nanoparticles known as quantum dots have special electrical and optical characteristics. These materials find use in chemical sensors, bioimaging, and optoelectronics, such as light-emitting diodes (LEDs) and photovoltaic systems. Fluorescence-based detection techniques for chemical and biological studies also employ quantum dots in chemistry(García de Arquer et al., 2021).

e. Nanocomposites: Nanomaterials (such nanoparticles, nanotubes, or nanowires) combined with a matrix material (like polymers, metals, or ceramics) are called nanocomposites. Properties like strength, conductivity, and thermal stability are frequently increased when nanoparticles are included into the matrix. Drug delivery, catalysis, and coatings are just a few of the chemical processes that employ nanocomposites(Hassan et al., 2021).

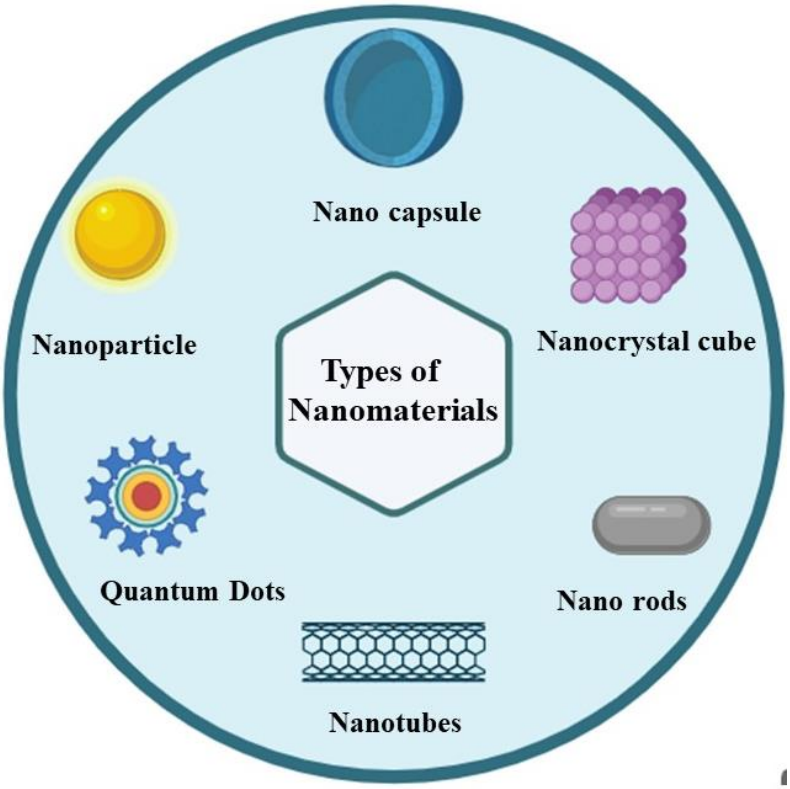

Figure 1: Varius types of Nanomaterial

Techniques for Nanomaterial Synthesis

The controlled construction of atoms or molecules into tiny structures is known as nanomaterial synthesis. Top-down and bottom-up techniques are the two primary strategies for creating nanomaterials.

Top-Down Approaches: Top-down approaches are based on transforming large materials into nanoscale shapes. This is used to make lots of nanomaterials, especially when exact measurements are not vital(Abid et al., 2022). Top-down methods generally rely on these types of approaches.

a. Milling: Ball milling and other mechanical operations are used to reduce pieces of bulk material into tiny nanoparticles. While this technique is often applied for making metal and ceramic nanoparticles, it may sometimes lead to contamination from materials used for milling(Ogbezode et al., 2024).

b. Lithography: Electron-beam lithography and Photolithography uses electrons or beams of light to form tiny patterns on surfaces. Lithography is preferred in the semiconductor field and is also useful for developing sensors and photonic gadgets(Butt et al., 2024).

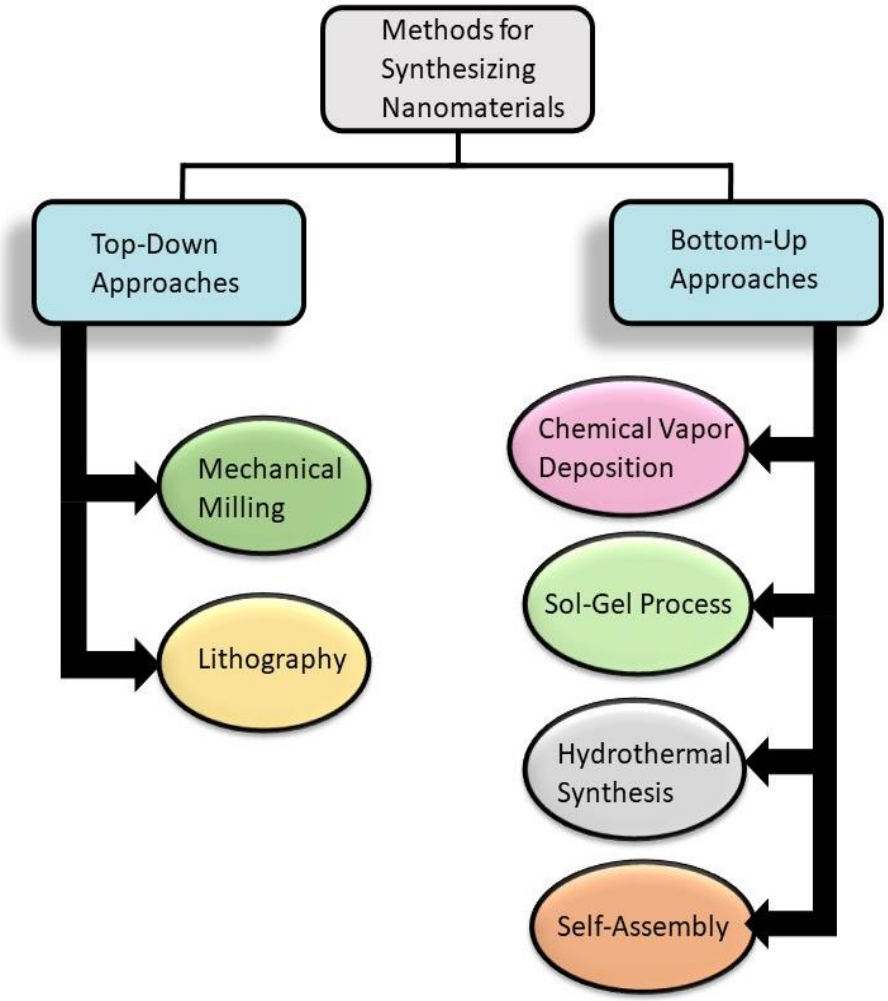

Figure 2: Flow diagram of method of synthesis of nanomaterial

Bottom-Up Approaches:

This method involves building up nanomaterials from atoms or molecules, typically using chemical reactions or self-assembly techniques. These methods are capable of producing very high-quality and precisely controlled nanomaterials (Jiang et al., 2022). Common bottom-up techniques include:

a. Chemical Vapor Deposition (CVD): CVD refers to introducing a gas into a chamber, reacting it on a surface and forming solid nanomaterials. Carbon nanotubes, graphene and metal oxide nanoparticles are produced using CVD. The shape and size of the nanomaterials can be regulated almost exactly using this procedure(Sabzi et al., 2023).

b. **Sol-Gel Process:** In sol-gel, a sol is turned into a gel and further steps are used to create nanomaterials. This coding is often used for preparing silica and titania oxide nanoparticles, as well as preparing thin films and coatings(Bokov et al., 2021).

c. **Hydrothermal Synthesis:** Hydrothermal synthesis means that reactions take place between substances in water when heated to a high temperature and placed under high pressure. This technique finds great use when generating metal oxide nanoparticles such as titanium dioxide and zinc oxide which are important in catalysis, photovoltaics and protection of the environment(Thonge et al., 2024).

d. **Self-Assembly:** Self-assembly allows molecules to arrange themselves at the nanoscale level without any help from outside forces. The process is commonly applied when making nanostructures such as nanoparticles, nanowires and thin films. Manufacturing nanomaterials by self-assembly can be efficient as well as cost-effective(Sinha et al., 2021).

Characterization of Nanomaterials

Exploring the qualities of nanomaterials is crucial to understand their features and make certain they meet the targeted specifications in various fields. Many methods are applied to understand the size, form, structure and chemical properties of nanomaterials.

Microscopic Techniques:

a. **Scanning Electron Microscopy (SEM):** Imaging the surface of nanomaterials is often done with the SEM technique. SEM creates detailed images of the dimension and shape of nanoparticles and nanostructures by examining them with an electronic beam(Chu et al., 2021).
b. **Transmission Electron Microscopy (TEM):** TEM is capable of imaging nanomaterials at an even finer scale than SEM, by allowing scientists to look inside them at the atomic level. One advantage of TEM is its ability to see nanoparticles' crystals, composition and size(Zheng et al., 2023).
c. **Atomic Force Microscopy (AFM):** AFM uses a pointed tip to move across a sample and assess its topography as well as how strong the nanomaterials are. AFM is widely used to determine how large, shaped and rough nanoparticles and nanostructures are (Joshi et al., 2022).

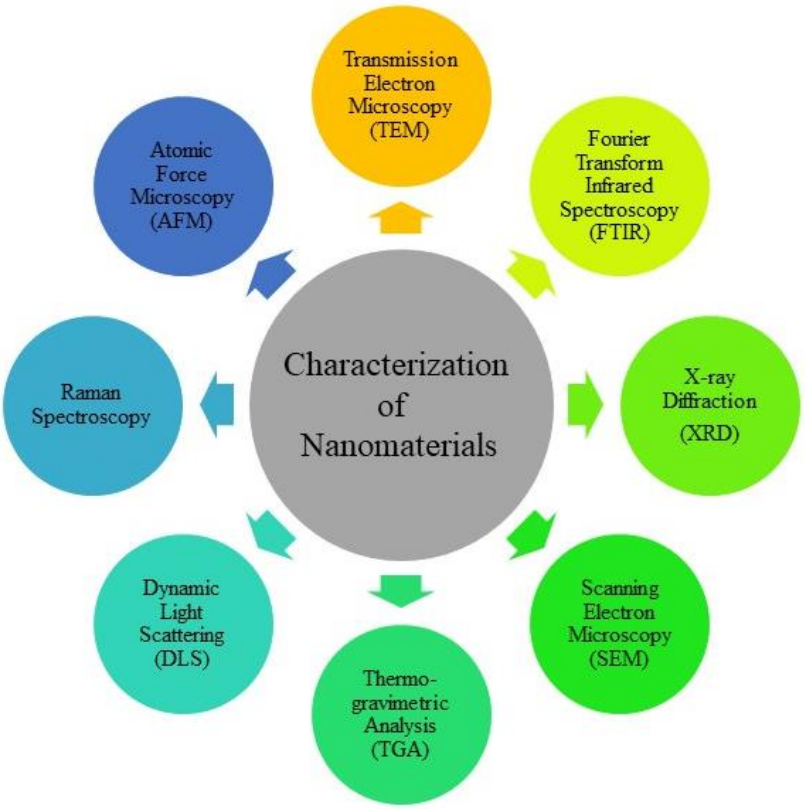

Figure 3: Techniques used for characterization of nanomaterial

Spectroscopic Techniques:

a. **X-ray Diffraction (XRD):** XRD is a technique used to examine the structure of nanomaterials. It allows the researcher to identify the different phases present and determine the size of the quartered material (Pandey et al., 2021).
b. **Fourier Transform Infrared Spectroscopy (FTIR):** FTIR is employed to discover the types of functional groups and bonds in nanomaterials. It helps investigate the surface chemistry of nanoparticles and detect any organic or inorganic atoms attached to them (Fadlelmoula et al., 2022).
c. **Raman Spectroscopy:** Raman spectroscopy can detect the vibrations happening within molecules. This outlines the organization of small atoms in the carbon-based nanomaterials graphene and carbon nanotubes(Orlando et al., 2021).
d. **Dynamic Light Scattering (DLS):** It is common to use DLS to measure the size of nanoparticles present in a liquid mixture. It counts on light scattering by the elements in the fluid and is particularly effective in figuring out the hydrodynamic size of nanoparticles(Jia et al., 2023)
e. **Thermogravimetric Analysis (TGA):** During TGA, the harmful components of a material are removed as it undergoes heating, allowing for the identification of its main components. It is used to detect the level of organic content in nanocomposites and observe how nanomaterials burn off at high temperatures(Escalante et al., 2022).

Applications of Nanomaterials in Chemical Chemistry

Special properties found in nanomaterials are making new possibilities available in chemistry. Some of the best uses for these materials include:

a. **Catalysis:** Chemists often use nanomaterials as catalysts or supports because they are highly reactive and have a large surface area. They can increase how fast and selective a chemical reaction is(Chadha et al., 2022).
b. **Sensors:** Manufacturing sensitive chemical and biological equipment involves the use of nanomaterials. Since sensors are small and have a wide surface area, they can spot small changes or specific molecules(Flynn et al., 2023).
c. **Energy Storage:** Using nanomaterials in batteries, supercapacitors and fuel cells increases the capacity for both storing and using energy. Adding nanomaterials to them can improve each device's efficiency and how much data it stores or uses (Yogeswari et al., 2022).
d. **Environmental Remediation:** Air, water and soil are purified using nanomaterials. They are good at absorbing or facilitating the breakdown of dangerous materials due to their high reactivity (Chen et al., 2023).

Applications of Nanotechnology in Chemical Engineering and Industry

By using nanotechnology, chemical engineering processes and industries are being enhanced, while new materials and methods for better efficiency are being developed. Due to being very small, having lots of surface and showing unique electronic and light properties, nanomaterials are suitable for many applications in chemical engineering and large-scale industries(Mohammad et al., 2022).This chapter focuses on the use of nanotechnology in fields such as chemical engineering, industry and areas related to catalysts, materials, manufacturing and sustainability.

Nanotechnology in Catalysis

Applying nanotechnology to chemical engineering mostly focuses on the area of catalysis. Catalysts help temple reactions go faster, without getting used up and they are necessary in industrial procedures for petrochemical refining, making drugs and developing chemicals.

Because nanomaterials offer a greater number of reactive sites, they are preferred for catalytic activities. It has been demonstrated that nanoparticles made from platinum, gold and silver are better catalysts than the bulk forms of these metals(Sabater et al., 2024).

Heterogeneous Catalysis: Because nanoparticles are small, they are commonly used in heterogeneous catalysis. Because nanoparticles have a large surface area, they can assist in more efficient catalytic processes by interacting with a high number of reactants. The process is used in hydrogenation, oxidation and reactions where carbon couples with other carbons(Vogt et al., 2022)

Enzyme Mimicry: Thanks to nanotechnology, scientists have developed synthetic catalysts similar to enzymes. They are designed particles that can replace biological enzymes by carrying out catalytic activities. Unlike natural enzymes, nanozymes can withstand harsh environments, can be used again and again and are very stable(Zhang et al., 2021)

Nanomaterials in Material Science

Nanotechnology is contributing to the growth of new materials with better properties. Engineers are able to produce substances with distinctive features by manipulating materials at an extremely small scale..

a. **Nanocomposites:** In nanocomposites, tiny particles or features called nanoparticles are mixed with a base material. Nanomaterials can boost the mechanical, electrical and thermal performance of the base material. Carbon nanotubes are used in these fields to help improve the strength, conductivity and durability of important materials (Silva et al., 2021).
b. **Smart Materials:** Because of nanotechnology, there are smart materials that react to things such as temperature, pH levels and light. They may alter their shape, color or other characteristics when exposed to changes around them. Smart materials can be used in sensors, actuators and systems that deliver drugs (Su et al., 2022).
c. **Nanocoatings:** When nanocoatings are applied to a material's surface, they change and improve its properties. They may increase the coatings' ability to resist corrosion, abrasion and wear and also help the surface repel water and clean itself. From cars to electronics, nanocoatings are applied in various industries to increase the useful life of different products(Li et al., 2023).

Nanotechnology in Manufacturing

Nanotechnology is helping the manufacturing industry build materials and products that have better capabilities than before. Nanomaterials have helped to increase the efficiency of several manufacturing methods.

Nanoelectronics and Semiconductors: Advances in electronics and semiconductors have largely been made possible by a focus on nanotechnology. Because electronics have become smaller, it is possible to manufacture chips, transistors and memory devices that are both faster and use less energy. Some scientists are investigating carbon nanotubes and graphene to replace silicon in transistors, as they are both faster and more flexible (Song et al., 2024).

Nanomanufacturing: Nanomanufacturing is the process of creating large supplies of nanomaterials and nanodevices. Chemical vapor deposition (CVD), molecular beam epitaxy (MBE) and electrospinning are among the methods they can use. Nanomanufacturing is predicted to improve the way electronics, medicine and energy industries produce nanomaterials at reasonable costs (Cui et al., 2024).

Additive Manufacturing (3D Printing): Nanotechnology is now finding use in 3D printing methods. Adding nanomaterials to 3D printing allows manufacturers to design items that are both strong and light. It matters a lot in these industries because the materials must be easy to use and long lasting (Agrawal et al., 2021).

Energy Applications of Nanotechnology

Nanotechnology is making a significant contribution to energy production, storage and efficiency. Using nanomaterials in various types of energy systems improves performance, uses less energy and allows for developing new methods of energy generation (Shah et al., 2022).

Solar Cells: Nanotechnology is making a significant contribution to energy production, storage and efficiency. Using nanomaterials in various types of energy systems improves performance, uses less energy and allows for developing new methods of energy generation(Wang et al., 2022).

Energy Storage: By using nanotechnology, it is possible to boost the capabilities of batteries and supercapacitors. In practice, materials on the nano-scale are blended with lithium-ion batteries to strengthen their efficiency, fast charging, energy storage and performance. Graphene-based options and carbon nanotubes are being evaluated as alternatives to chemical batteries in supercapacitors (De Andrade et al., 2021).

Fuel Cells: Nanotechnology is being applied to make fuel cells function better and turn fuel into electricity. Researchers apply platinum nanoparticles to the electrodes of fuel cells to help the reactions occur more quickly and efficiently. Applying nanomaterials in fuel cells may result in more sustainable and cleaner sources of energy (Arshad et al., 2023).

Nanotechnology in Drug Delivery and Pharmaceutical Chemistry

Nanotechnology has emerged as a groundbreaking force in the field of pharmaceutical chemistry, transforming how drugs are designed, delivered, and monitored within the human body. One of the most significant contributions of nanotechnology is its application in drug delivery systems, which has the potential to enhance therapeutic efficacy, reduce side effects, and improve patient compliance. This chapter explores the principles, methods, and key advancements in nanotechnology-based drug delivery, along with its implications in pharmaceutical research and development (Mazayen et al., 2022).

Nanodrug Delivery Systems

To use a nanodrug delivery system, experts employ carriers as small as 1 nanometer and as large as 100 nanometers to target specific cells or tissues (Lv et al., 2024). They provide more benefits than traditional drugs given orally which are given bellow:

Enhanced bioavailability

Improved solubility of poorly water-soluble drugs

Prolonged drug circulation time

Controlled and sustained release of drugs

Targeted delivery to specific tissues or cells

By improving drug pharmacokinetics and biodistribution, nanotechnology helps overcome some of the major limitations in conventional therapies.

Types of Nanocarriers

Nanocarriers are engineered platforms designed to encapsulate drugs and deliver them effectively. Common types include:

a. Liposomes

Liposomes are spherical vesicles composed of lipid bilayers. They can encapsulate both hydrophilic and hydrophobic drugs and are biocompatible and biodegradable. Liposomal formulations are already used in treating cancers and fungal infections. An example includes Doxil®, a liposomal formulation of doxorubicin (Jiang et l., 2023).

b. Polymeric Nanoparticles

These are composed of biodegradable polymers like PLGA (poly lactic-co-glycolic acid) and are ideal for sustained and controlled drug release. They can be engineered to respond to environmental stimuli (pH, temperature) for site-specific delivery (Spirescu et al., 2021).

c. Solid Lipid Nanoparticles (SLNs)

SLNs are made from solid lipids and provide a matrix system for drug entrapment. They are stable and suitable for oral, topical, and injectable formulations (Arabestani et al., 2024).

d. Dendrimers

Dendrimers are branched, tree-like macromolecules that offer multivalency and precise structural control. They have internal cavities and external functional groups for drug attachment and targeting (Mittal et al., 2021).

e. Nanocrystals

Nanocrystals enhance the solubility and dissolution rate of poorly soluble drugs. Their small size increases surface area, thus improving bioavailability (Lin et al., 2023).

f. Carbon-Based Nanomaterials

Fullerenes, carbon nanotubes, and graphene are explored for drug delivery, particularly in cancer therapy, owing to their high surface area and unique physical properties (Ayanda et al., 2024).

Targeted Drug Delivery

A key advantage of nanotechnology in drug delivery is **targeted delivery**, which ensures that the drug reaches only the diseased tissue, minimizing toxicity to healthy cells (Manzari et al., 2021).

a. Passive Targeting

Exploits the enhanced permeability and retention (EPR) effect seen in tumors, where leaky blood vessels allow nanocarriers to accumulate more readily(Li et al., 2023)

b. Active Targeting

Involves modifying the surface of nanocarriers with ligands such as antibodies, peptides, or aptamers that bind specifically to receptors overexpressed on diseased cells (e.g., cancer cells) (Tianet al., 2022).

c. Stimuli-Responsive Delivery

Nanocarriers can be engineered to release their payload in response to specific stimuli, such as acidic pH in tumors or the presence of certain enzymes, ensuring site-specific drug release (Zhang et al., 2022).

Nanotechnology in Cancer Therapy

Cancer therapy has seen the most remarkable advances with nanotechnology. Nanocarriers can enhance the therapeutic index of anticancer drugs and reduce multidrug resistance. **Example:** Liposomal doxorubicin (Doxil®) reduces cardiac toxicity while maintaining anticancer efficacy (Alrushaid et al., 2023).

Polymeric micelles are used for delivering paclitaxel and other hydrophobic chemotherapeutics (Kotta et al., 2022).

Magnetic nanoparticles can be used for both drug delivery and hyperthermia (heating tumors to kill cells selectively) (Stueber et al., 2021).

Nanotechnology in Gene Therapy

Gene therapy aims to introduce, silence, or repair genetic material in cells. Nanoparticles can safely carry nucleic acids (DNA, siRNA, mRNA) across cell membranes, protecting them from degradation.

Lipid nanoparticles (LNPs) were pivotal in the success of mRNA vaccines for COVID-19.

Chitosan and PEI-based nanoparticles are widely researched for gene delivery due to their positive charge and ability to compact DNA (Liet al., 2024).

Nanotechnology in Infectious Disease Treatment

In infectious disease treatment, nanotechnology improves drug delivery to infection sites, enhances antimicrobial efficacy, and reduces resistance.

Silver nanoparticles show potent antibacterial and antiviral properties(Al-Awsi et al., 2023)

Nano carriers are being developed to deliver antibiotics in a controlled manner to minimize resistance development (Kumaret al., 2023).

Targeted nanocarriers help in crossing barriers like the blood-brain barrier to treat infections like tuberculosis and meningitis (Kesharwani et al., 2021).

Transdermal and Ocular Drug Delivery

Nanocarriers have been integrated into transdermal patches, creams, and ocular inserts for more effective delivery.

Nanoemulsions and **nanogels** facilitate deeper skin penetration of drugs.

Ocular inserts with nanoparticles prolong drug residence time and improve absorption across corneal membranes (Ranjbar et al., 2023).

Regulatory and Safety Considerations

While nanotechnology presents promising opportunities, there are several regulatory and safety concerns:

Toxicity and biocompatibility must be rigorously evaluated.

Long-term stability and **clearance mechanisms** of nanocarriers remain under investigation.

Regulatory approval processes for nanoformulations are still evolving, with agencies like the FDA requiring extensive safety profiling (Wang et al., 2021).

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Chemistry of Renewable Energy

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Tatheer FATIMA

1. Introduction to Renewable Energy Chemistry

Global energy demand, driven by industrialization and population growth, reached ~604 EJ in 2023, with fossil fuels still supplying ~80% . This dependence fuels both resource depletion and climate change, making decarbonization urgent. Renewable energy is often framed in engineering or policy terms, yet its core is inherently chemical: every energy conversion—solar to electricity, biomass to biofuel, water to hydrogen—is governed by reaction mechanisms, material properties, and interfacial processes.(Holechek, Geli, Sawalhah, & Valdez, 2022)

Chemistry enables optimization of energy technologies through advanced materials design, catalytic efficiency, and stability control. In photovoltaics, semiconductor doping, defect passivation, and compositional tuning (e.g., halide perovskites) directly influence efficiency and degradation (Ašmontas & Mujahid, 2023) Hydrogen systems depend on electrolysis kinetics, electrocatalyst performance, and chemical storage strategies. Bioenergy relies on catalytic and biochemical conversions—transesterification, fermentation, and anaerobic digestion—tailored to feedstock and process chemistry. Electrochemical storage technologies hinge on redox chemistry, with advances in lithium-ion batteries tied to novel electrode and electrolyte chemistries (Tarascon & Armand, 2001)

This chapter positions chemistry as the unifying discipline in renewable energy. Section 2 covers fundamental thermodynamic, electrochemical, photochemical, and catalytic principles. Sections 3–6 examine solar energy, hydrogen, bioenergy, and electrochemical storage, while Section 7 explores emerging areas like CO_2 reduction and artificial photosynthesis. Section 8 concludes with challenges and opportunities. By grounding the discussion in chemical principles, the chapter aims to provide mechanistic insights necessary for advancing renewable energy innovation.

2. Fundamental Chemical Principles

The chemistry of renewable energy is rooted in thermodynamics, electrochemistry, photochemistry, and catalysis, which define how energy is harvested, converted, and stored. These principles provide the molecular framework for advancing renewable systems.

2.1 Thermodynamics of Energy Conversion

Thermodynamics sets the limits of energy efficiency. The first law ensures energy conservation, while the second law imposes entropy-driven constraints. For instance, the

Shockley–Queisser limit (~33%) for single-junction photovoltaics arises from photon absorption and recombination losses.(K. Wang et al., 2022) Likewise, Gibbs free energy (ΔG) defines the minimum 1.23 V required for water splitting under standard conditions.

2.2 Electrochemistry and Charge Transfer

Electrochemistry governs batteries, fuel cells, and electrolyzers. The Nernst equation links cell potential to reactant activity, predicting performance. Key factors include electrode–electrolyte interfaces, double-layer effects, and redox kinetics. In lithium-ion batteries, intercalation chemistry is dictated by redox potentials and ion diffusion at the nanoscale.(Manfo & Şahin, 2023)

2.3 Photochemistry and Light–Matter Interactions

Solar technologies rely on photon absorption to create electron–hole pairs. Efficient separation and transport require optimized band gaps, exciton dynamics, and carrier mobility. In photo electrochemical cells, band alignment with redox potentials determines reaction feasibility.

2.4 Catalysis in Renewable Energy

Catalysts accelerate energy reactions without altering thermodynamics. Electro-catalysts like Pt, MoS_2, and Ni–Fe oxides reduce over potentials in hydrogen and oxygen evolution. In bioenergy, enzymatic and heterogeneous catalysts drive biomass conversion. Performance depends on turnover frequency, activation energy, and long-term stability. (Anekwe et al., 2025)

Scope Ahead

These foundations connect molecular processes to material innovations, providing a framework for evaluating present technologies and guiding future breakthroughs in sustainable energy chemistry.

3. Solar Energy Conversion

Solar energy conversion transforms sunlight into usable electricity or chemical fuels via light–matter interactions, charge separation, and redox reactions. From a chemistry perspective, these processes hinge on semiconductor band structures, catalytic surfaces, and stability engineering.

3.1 Photovoltaic Systems

Silicon-Based Solar Cells

Silicon dominates photovoltaics due to its abundance, non-toxicity, and well-understood crystal chemistry. In the photovoltaic effect, photons with energy above the 1.1 eV band gap excite electrons from the valence to the conduction band, producing electron–hole pairs. (Unold & Schock, 2011)

Key chemical steps include:

- **Purification:** Metallurgical-grade Si is upgraded to solar-grade (>99.9999%) via chloro-silane chemistry (Siemens process).
- **Doping:** Boron (p-type) or phosphorus (n-type) atoms adjust conductivity.
- **Surface passivation:** Dielectric layers (SiNx, Al_2O_3) saturate dangling bonds to reduce recombination.
- **Encapsulation:** EVA polymers shield cells from UV and moisture degradation. (Raman, Gurusamy Thangavelu, Venkataraj, & Krishnamoorthy, 2021)

Perovskite Solar Cells (PSCs)

Hybrid perovskites (e.g., $CH_3NH_3PbI_3$) offer strong absorption, long carrier lifetimes, and tunable band gaps.

- **Structure:** ABX_3 lattice with organic cation (A), metal cation (B), halide anion (X).
- **Synthesis:** Solution-processed films via solvent coordination control.
- **Stability:** Sensitive to heat, moisture, and oxygen; improved via grain boundary passivation and cation substitution (formamidinium, Cs). (Wu et al., 2018)

3.2 Photo catalysis for Solar Fuel Production

Water Splitting & Hydrogen Evolution

Photocatalytic water splitting comprises:

- **Oxygen Evolution Reaction (OER):**
$$2H_2O \rightarrow O_2 + 4H^+ + 4e^-$$
catalyzed by RuO_2, IrO_2, or Co_3O_4.
- **Hydrogen Evolution Reaction (HER):**
$$4H^+ + 4e^- \rightarrow 2H_2$$
catalyzed by Pt or MoS_2.

Semiconductors like TiO_2, g-C_3N_4, and doped Fe_2O_3 absorb light, creating electron–hole pairs that drive reactions. Proper band edge alignment with water redox potentials is essential for efficiency and stability.(Xiao et al., 2020)

CO_2 Reduction Chemistry

Solar-driven CO_2 conversion produces CO, CH_4, or CH_3OH via multi-electron transfers:

Catalysts include Re/Mn bipyridyl complexes and Cu/Ag nanostructures, which stabilize intermediates like *COOH. Functionalized surfaces and co-catalysts improve selectivity and yield.

3.3 Organic and Dye-Sensitized Solar Cells (DSSCs)

Organic Photovoltaics (OPVs)

These use π-conjugated polymers or small molecules for light absorption and charge transport. Molecular design tunes band gaps and absorption.

DSSCs

In DSSCs, a dye (often Ru-based or metal-free organic) bound to mesoporous TiO_2 absorbs light and injects electrons into the TiO_2 conduction band.

- **Electrolyte:** I^-/I_3^- mediates hole transfer; cobalt complexes give higher voltages but lower stability.
- **Anchoring:** Carboxylate or phosphonate groups bind dyes to TiO_2, improving electron injection. (Liu et al., 2017)

Case Study: Halogen Doping in PSCs

Replacing part of iodide with bromide or chloride in $CH_3NH_3PbI_3$ reduces defects and improves crystal quality. Doping passivates grain boundaries, boosts charge mobility, and enhances resistance to moisture and heat. Resulting devices show longer operational lifetimes with minimal efficiency loss. (X. Wang, Yang, Zhong, Yu, & Pan, 2024)

4. Hydrogen as a Renewable Energy Carrier

Hydrogen (H_2) has emerged as a versatile and sustainable energy vector, capable of decarbonizing multiple sectors including transportation, industry, and grid energy storage. Its high gravimetric energy density (120 MJ kg^{-1}) and the potential for production from renewable sources make it a key component of future energy systems. However, the deployment of hydrogen technology relies on advancements in production, storage, and utilization pathways, each governed by unique chemical principles.

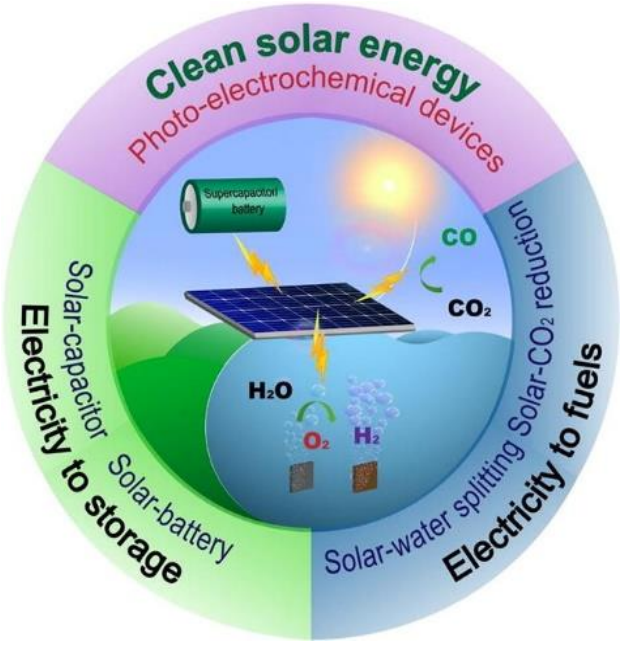

Figure 6: Solar Energy *(Zhang et al., 2020)*

4.1 Hydrogen Production Methods

a) Electrolysis of Water

Electrolysis is the electrochemical splitting of water into hydrogen and oxygen using an external power source:

$$2H2O(l) \rightarrow 2H2(g) + O2(g)\Delta G \circ = 237.13\ \text{kJ mol} - 1$$

The efficiency and scalability of electrolysis depend on the electrolyte type and electrode materials:

- **Alkaline Electrolysis (AEL)**: Utilizes aqueous KOH or NaOH (20–40 wt%) as the electrolyte. Nickel-based electrodes facilitate the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Advantages include low cost and durability, but AEL systems operate at lower current densities (~0.2–0.4 A cm^{-2}).
- **Proton Exchange Membrane Electrolysis (PEMEL)**: Employs a solid polymer electrolyte (e.g., Nafion®) allowing operation at higher pressures and current densities (~2 A cm^{-2}). Precious metal catalysts (Pt for HER, IrO_2 for OER) are required, which increases cost but improves performance and dynamic response—ideal for coupling with intermittent renewable power sources.
- **Solid Oxide Electrolysis Cells (SOEC)**: Operates at 700–1000 °C using ceramic electrolytes (yttria-stabilized zirconia, YSZ). The high temperature reduces the electrical energy requirement by supplying part of the energy as heat, often sourced from industrial waste heat. SOEC offers high theoretical efficiency (>90%) but faces challenges in long-term stability. (S. Wang, Lu, & Zhong, 2021)

b) Photocatalytic Water Splitting

This method uses semiconductor photo catalysts (e.g., TiO_2, g-C_3N_4) to directly convert solar energy into chemical energy via the photoexcitation of electrons and holes, which drive HER and OER. The main challenge is improving quantum efficiency through bandgap engineering, co-catalyst loading, and surface modification.

c) Thermochemical Water Splitting

High-temperature thermochemical cycles (e.g., sulfur–iodine cycle) utilize concentrated solar power or nuclear heat to drive endothermic reactions that produce H_2 without direct electricity input. The process involves multiple chemical steps and high system complexity, but it eliminates the need for large-scale electrolysis units. (Hye-Won & and Jin-Soo, 2018)

4.2 Hydrogen Storage Chemistry

Efficient storage is critical to match hydrogen supply with demand while ensuring safety and energy density targets.

a) Metal Hydrides

Hydrogen reacts with metals or alloys to form solid hydrides (e.g., MgH_2, $LaNi_5H_6$) through reversible absorption/desorption:

$$M + \frac{x}{2}H^2 \rightleftharpoons \text{MHx}$$

These materials offer high volumetric density but require thermal energy for desorption (30–350 °C depending on hydride type). Research focuses on nano-structuring, doping, and catalysis to lower desorption temperatures and improve kinetics.

b) Liquid Organic Hydrogen Carriers (LOHCs)

Compounds like methylcyclohexane or dibenzyltoluene store hydrogen via catalytic hydrogenation and release it by dehydrogenation. LOHCs benefit from existing liquid fuel infrastructure; however, their round-trip efficiency is limited by the heat requirements of dehydrogenation.

c) Chemical Storage Routes

Hydrogen can be stored in the form of ammonia (NH_3) or formic acid (HCOOH), which act as hydrogen-rich molecules. Ammonia offers high hydrogen density (17.8 wt%) and is easily liquefied, but requires catalytic cracking for release. Formic acid decomposition is an attractive low-temperature route for portable applications. (Tarasov, Lototskyy, & Yartys, 2007)

4.3 Hydrogen Utilization

Hydrogen can be directly combusted or converted into electricity through fuel cells, with the latter offering higher conversion efficiencies.

a) Proton Exchange Membrane Fuel Cells (PEMFCs)

PEMFCs operate at 60–80 °C using a solid polymer electrolyte. The hydrogen oxidation reaction (HOR) occurs at the anode:

$$\mathrm{H}^2 \rightarrow 2H^+ + 2e^-$$

Protons migrate through the membrane to the cathode, where they react with oxygen to produce water:

$$\frac{1}{2}O^2 + 2H^+ + 2e^- \rightarrow H_2O$$

Advantages include fast start-up and high power density, making PEMFCs suitable for transport and portable electronics. Challenges include catalyst cost and durability.

b) Solid Oxide Fuel Cells (SOFCs)

SOFCs operate at 600–1000 °C with ceramic electrolytes conducting O^{2-} ions. The cathodic reaction reduces oxygen:

$$\mathrm{O}^{2-} + 4e^- \rightarrow 2\mathrm{O}^{2-}$$

These oxide ions migrate to the anode, where they oxidize hydrogen:

$$\mathrm{H}^2 + O^{2-} \rightarrow H_2\mathrm{O} + 2\mathrm{e}^-$$

SOFCs achieve electrical efficiencies >60% and can internally reform hydrocarbon fuels, but high operating temperatures necessitate advanced materials to prevent degradation. (Yue et al., 2021)

Case Study – Large-scale PEM Electrolysis in Europe
Europe is at the forefront of scaling green hydrogen via PEM electrolysis, driven by the EU's 2030 hydrogen strategy. Projects such as the **REFHYNE plant** in Germany (10 MW capacity) use renewable electricity to produce 1,300 tons of hydrogen annually for industrial use, replacing fossil-derived H_2 in refineries. The high-pressure PEM system allows direct pipeline injection, reducing compression costs. Ongoing advancements focus on catalyst

durability, stack scaling, and integration with offshore wind farms to maximize renewable utilization. (Reksten, Thomassen, Møller-Holst, & Sundseth, 2022)

5. Bioenergy and Biochemical Pathways

Bioenergy harnesses chemical energy stored in biological materials—such as plant matter, algae, and waste biomass—through conversion processes that produce renewable fuels. The core advantage of bioenergy is its carbon cycle compatibility: carbon dioxide emitted during combustion is partially offset by the CO_2 absorbed during feedstock growth.

5.1 Biofuels

5.1.1 Transesterification Chemistry in Biodiesel Production

Biodiesel is produced by converting vegetable oils or animal fats—mainly composed of triglycerides—into fatty acid methyl esters (FAMEs) via **transesterification**. The general reaction involves reacting triglycerides with a short-chain alcohol (methanol or ethanol) in the presence of a catalyst (typically NaOH, KOH, or enzymatic lipases):

$$\text{Triglyceride} + 3\text{MeOH} \xrightarrow[\text{Catalyst}]{\text{T}} 3\text{FAME} + \text{Glycerol}$$

Key factors influencing yield include:

- **Catalyst type**: Homogeneous (alkali, acid) vs. heterogeneous catalysts.
- **Alcohol-to-oil ratio**: Excess alcohol shifts equilibrium toward FAME production.
- **Reaction temperature**: Typically 50–65°C for base-catalyzed processes.

Biodiesel offers high cetane numbers and lubricity, with reduced emissions of particulates, CO, and unburned hydrocarbons compared to petro-diesel. However, oxidative stability and cold flow properties remain challenges. (Salaheldeen et al., 2021)

5.1.2 Fermentation Pathways for Bioethanol

Bioethanol production involves fermenting carbohydrate-rich biomass—such as sugarcane, corn, or lignocellulosic residues—into ethanol via yeast or bacterial metabolism. In **Saccharomyces cerevisiae**, the biochemical pathway proceeds as:

1. **Glycolysis**: Glucose is converted to pyruvate, generating ATP and NADH.
2. **Alcoholic fermentation**:

$$Pyurvate \xrightarrow{Pyurvate\ Decarboxylase} Acetaldehyde + CO_2$$

$$Acetaldehyde \xrightarrow{Alcohol\ Dehydrogenase} Ethanol$$

For **lignocellulosic feedstocks**, pretreatment and enzymatic hydrolysis are required to release fermentable sugars from cellulose and hemicellulose. Advances in genetically engineered microbes aim to improve tolerance to ethanol toxicity and broaden substrate utilization. (Singh et al., 2022)

5.2 Biogas Chemistry

5.2.1 Anaerobic Digestion

Biogas is generated via **anaerobic digestion** of organic waste under oxygen-free conditions, producing a methane-rich mixture (CH_4 50–70%, CO_2 30–50%). The process occurs in four biochemical stages:

1. **Hydrolysis**: Complex polymers (carbohydrates, proteins, lipids) are broken down into monomers by extracellular enzymes.
2. **Acidogenesis**: Monomers are fermented into volatile fatty acids (VFAs), alcohols, H_2, and CO_2.
3. **Acetogenesis**: VFAs are converted into acetic acid, H_2, and CO_2.
4. **Methanogenesis**: Methanogenic archaea convert acetic acid and H_2/CO_2 into methane:

$$CH_3COOH \rightarrow CH_4 + CO_2$$
$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

5.2.2 Methanogenesis Reactions and Efficiency

Two primary pathways dominate:

- **Acetoclastic methanogenesis**: Responsible for ~70% of methane production.
- **Hydrogenotrophic methanogenesis**: Uses H_2 as the electron donor, particularly under low acetate conditions.

Biogas upgrading involves removing impurities such as H_2S and moisture, yielding biomethane suitable for grid injection or vehicle fuel. (Kianfar & Mahmoud, 2024) (Park et al., 2019)

Table 1: Energy applications of Different bioproducts

Product	Feedstock Type	Key Chemistry	Energy Application
Biodiesel	Oils, fats	Transesterification	Diesel engines
Bioethanol	Sugars, starch, lignocellulose	Fermentation	Gasoline blending
Biogas	Organic waste, manure	Anaerobic digestion	Heat, power, CHP

6. Electrochemical Energy Storage

Electrochemical energy storage technologies underpin portable electronics, electric vehicles (EVs), and renewable energy integration. Their performance depends on charge-storage mechanisms, electrode/electrolyte chemistry, and cycle life.

6.1 Lithium-Ion Batteries

Lithium-ion (Li-ion) batteries dominate the market due to high energy density and efficiency. Their operation relies on **intercalation chemistry**, where Li^+ ions shuttle between the cathode (commonly $LiCoO_2$, $LiFePO_4$, or layered nickel-manganese-cobalt oxides) and the graphite anode. During charging, Li^+ ions intercalate into graphite layers; during discharge, they return to the cathode.

The **electrolyte**, typically $LiPF_6$ dissolved in carbonate solvents, ensures ion transport but must remain stable over wide voltage windows. A crucial feature is the **solid electrolyte interphase (SEI)** that forms on the anode. This thin passivation layer prevents further electrolyte decomposition while allowing Li^+ diffusion, ensuring stability and safety. However, SEI instability causes capacity fade and limits cycle life. (Ngoy et al., 2025)

6.2 Next-Generation Batteries

To overcome limitations of Li-ion, several alternatives are emerging:

- **Sodium-ion batteries (SIBs):** Replace lithium with sodium, an earth-abundant element. SIBs use layered oxides or Prussian blue analogs as cathodes, offering lower cost but reduced energy density.
- **Zinc-air batteries:** Rely on Zn oxidation at the anode and oxygen reduction at the cathode. They feature very high theoretical energy density and safety but suffer from sluggish oxygen kinetics and electrode degradation.
- **Solid-state batteries:** Replace flammable liquid electrolytes with solid ionic conductors (ceramics, polymers, or sulfides). This enables pairing of high-capacity **Li-metal anodes**, boosting energy density and safety. Yet challenges include interfacial resistance and dendrite formation. (Xu et al., 2023)

6.3 Supercapacitors

Supercapacitors bridge the gap between batteries and conventional capacitors. They provide high power density and rapid charging but lower energy density.

- **Electrical double-layer capacitors (EDLCs):** Store charge via ion adsorption at electrode–electrolyte interfaces, typically using porous carbons.
- **Pseudocapacitors:** Use fast surface redox reactions in transition-metal oxides or conducting polymers, enhancing capacitance.

Supercapacitors excel in applications requiring burst power (e.g., regenerative braking, grid stabilization) but cannot replace batteries for long-term storage.(Pathak et al., 2023)

Case Study: Development of Solid-State Li-Metal Batteries for EV Applications Solid-state Li-metal batteries are a frontier in EV energy storage. By replacing flammable liquid electrolytes with solid ceramic or polymer electrolytes, these systems promise **2–3 times higher energy density** than conventional Li-ion, while improving safety. Research efforts in Japan and Europe have demonstrated pouch cells exceeding 400 Wh/kg. Key breakthroughs include **sulfide electrolytes** with high ionic conductivity and engineered interfaces to suppress Li dendrite growth. Automakers such as Toyota and BMW are investing heavily, aiming for commercialization by 2030. While scalability and cost remain barriers, this technology could revolutionize EVs by delivering longer driving ranges and faster charging with reduced fire risk.(Agarwal & Anand, 2025)

Table 2: Different Battery types and their properties

Battery Type	**Energy Density (Wh/kg)**	**Cycle Life (cycles)**	**Approx. Cost (USD/kWh)**	**Key Advantages**	**Limitations**
Lithium-Ion (Li-ion)	150–250	1,000–3,000	120–200	High efficiency, mature technology, portable	Safety risks, limited raw materials
Sodium-Ion (Na-ion)	100–160	1,000–2,000	50–100	Low-cost, abundant sodium, safer operation	Lower energy density, early stage
Zinc–Air	200–400 (theoretical)	300–800	30–80	Very high theoretical energy density, cheap materials	Limited rechargeability, slow kinetics
Solid-State Li-metal	300–500	1,000–10,000 (projected)	200–400 (currently high)	High energy density, improved safety	Expensive, scaling challenges

7. Emerging and Less-Covered Areas

7.1 Solar-Driven CO_2-to-Methanol Conversion

The conversion of carbon dioxide (CO_2) into methanol offers a sustainable route for carbon recycling and renewable fuel production. Methanol is a versatile platform chemical and liquid fuel, making it an attractive target in the context of climate change mitigation. The process involves CO_2 hydrogenation, typically requiring three molecules of hydrogen per CO_2 to yield methanol and water:

$$CO2+3H2 \rightarrow CH3OH+H2OCO_2 + 3H_2 \rightarrow CH_3OH + H_2OCO2+3H2 \rightarrow CH3OH+H2O$$

Catalysts play a pivotal role in improving the selectivity and efficiency of this reaction. Copper–zinc oxide–alumina ($Cu/ZnO/Al_2O_3$) catalysts remain the industrial benchmark, while emerging alternatives include molecular complexes, single-atom catalysts, and nanostructured semiconductors that can directly harness solar photons to activate CO_2. Solar-driven systems often couple water splitting with CO_2 reduction, thus eliminating reliance on fossil-derived hydrogen. Mechanistically, hydrogenation proceeds via intermediate species such as formate (HCOO*), formaldehyde (H_2CO*), and methoxy (CH_3O*), with catalyst surface structure strongly influencing product yield. (Sajnani et al., 2025)

7.2 Artificial Photosynthesis

Artificial photosynthesis aims to replicate nature's ability to convert sunlight, water, and CO_2 into chemical energy. Unlike photovoltaic devices, which generate electricity, these systems produce fuels such as hydrogen, methanol, or hydrocarbons. Molecular catalysts—often based on transition metals like ruthenium, cobalt, or manganese—enable water oxidation and CO_2 reduction steps. Bio-inspired designs also draw from photosystem II (PSII), employing semiconductor–molecule hybrid assemblies that mimic chlorophyll's light absorption and charge transfer. (Kathpalia & Verma, 2023)

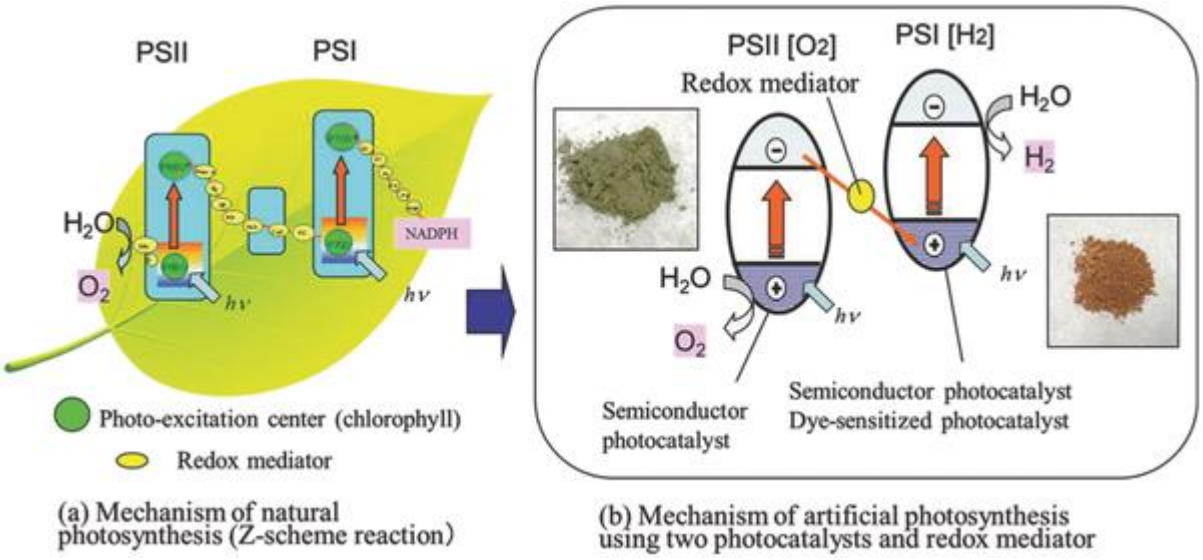

Figure 7: Artificial Photosynthesis

Recent efforts focus on integrating light-harvesting semiconductors (e.g., TiO_2, perovskites) with catalytic centers to achieve efficient charge separation and long-term stability.(Miseki & Sayama, 2018). Although artificial photosynthesis remains in its infancy, breakthroughs in tandem photoelectrochemical cells and molecular co-catalysts have shown promise for scalable fuel production. The broader vision is to create a "solar refinery" capable of sustainable fuel synthesis, thereby reducing dependency on fossil fuels.

Table 3: Key Roles of different energy systems

Energy Source	Principle	Key Role of Chemistry
Solar Energy	Sunlight → electricity & fuels	Semiconductor design (Si, perovskites); band-gap tuning; photocatalysts for water splitting & CO_2 reduction.
Hydrogen	Water electrolysis → H_2 fuel	Electrocatalysts for HER/OER; materials for storage (metal hydrides, LOHCs); membranes in fuel cells.
Bioenergy	Biomass → biofuels & biogas	Transesterification (biodiesel); fermentation (bioethanol); anaerobic digestion & methanogenesis chemistry.
Electrochemical Storage	Redox reactions in batteries & capacitors	Intercalation chemistry (Li-ion, Na-ion); solid electrolytes; double-layer & pseudocapacitance mechanisms.

8. Challenges, Opportunities, and Future Perspectives

8.1 Stability and Scalability Issues

A major challenge in renewable energy chemistry is the stability and scalability of catalytic and photoactive materials. Many high-performance catalysts, such as perovskites or molecular complexes, suffer from rapid degradation under operational conditions. (Michael, 2025) Similarly, noble-metal-based systems, though efficient, face prohibitive cost barriers that limit large-scale deployment. Achieving long-term durability and low-cost production is therefore essential for industrial adoption.

8.2 Integrating Chemistry with Engineering and Policy

The transition to renewable energy requires more than breakthroughs in chemistry; it demands integration with engineering, economics, and policy frameworks. For example, scaling solar-to-fuel systems requires not only efficient catalysts but also robust reactor designs, energy infrastructure, and favorable policy incentives. (Tuller, 2017) A multidisciplinary approach linking fundamental chemistry to applied technology and climate policy is key to bridging the gap between laboratory success and societal impact.

8.3 Future Outlook

Future advances will rely heavily on the discovery of new functional materials and accelerated innovation pathways. Emerging techniques such as artificial intelligence (AI) and machine learning are poised to revolutionize materials discovery by predicting structure–function relationships and optimizing catalysts. By 2050, a roadmap combining advanced chemistry, sustainable engineering, and global policy cooperation could enable renewable energy systems to become the backbone of a carbon-neutral economy. (Sammu & Gray, 2025)

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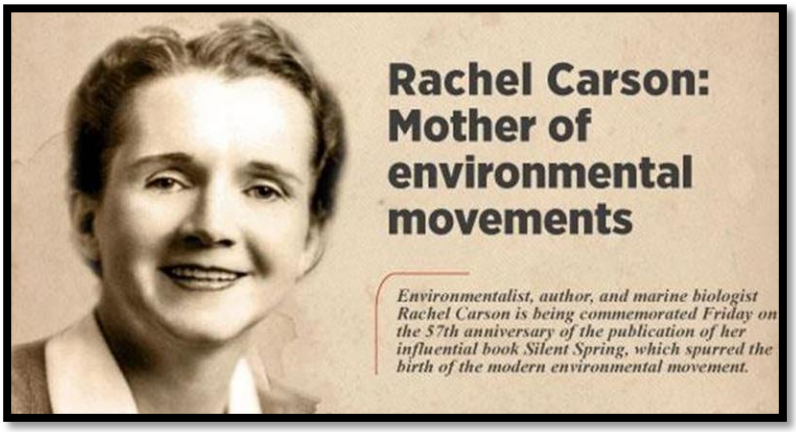
Environmental Chemistry Innovations

Momina ZUBAIR

1.1. Introduction

What exactly is "environmental chemistry"? The term 'environmental chemistry' may not have a specific definition, as its meaning varies among individuals. Nevertheless, ecological chemists play a very significant role in solving different global challenges such as ozone layer depletion and climate change, as well as also follow some local or regional issues such as acid rain, water pollution, and air pollution, etc *(Andrews et al., 2009).*

An old Chinese proverb states, "If we don't change our path, we'll end up exactly where we're going." This concept is significant today for humanity. The tiny part of the universe that supports all life is Earth, but human is on a dangerous pathway that could destroy their own homes. Almost 2 billion years ago, oxygen that was produced by sunlight altered the Earth as many photosynthetic organisms, such as cyanobacteria. Since no other life is such the most important on Earth, particularly its atmosphere. At present, humans can create significant changes by utilizing fossil fuels to produce energy.



Some concerned citizens have started to take action for the security of Earth’s future as risks to the planet mount and for humanity. Various efforts have been made for decades to

maintain the important ecosystem, such as in the early 1900s, when soil erosion was caused by farming in the United States. The Dust Bowl in the 1930s forced the government to take action for soil preservation according to climate change. In 1962, Rachel Carson's Silent Spring prompted global environmental change and mentioned the danger of pesticides in the environment (Manahan, 2011).

1.2. What is environmental chemistry

Environmental chemistry is the scientific study of biological and chemical processes found in natural settings such as water, soil, air, and living organisms. Its main purpose is to pay attention to pollution from industry, farming, and transportation. Since the revolution in the industrial field, human activities have significantly changed these natural systems, which has caused issues like water pollution and air pollution. Many fields have to work to find solutions that decreases the harm to living organisms and support eco-friendly practices (Enneboog, 2025). Environmental chemistry examines very carefully the risk characteristics of all the chemical compounds present in the environment. It plays a vital role in assessing the new significant products and their environmental impact. This field of science also safeguards the groundwater from the dust, soil, and various waste particles. It also prevents the water surface from sedimentation, pollutants, and radioactive microbiological parameters (Gooijer, 2022).

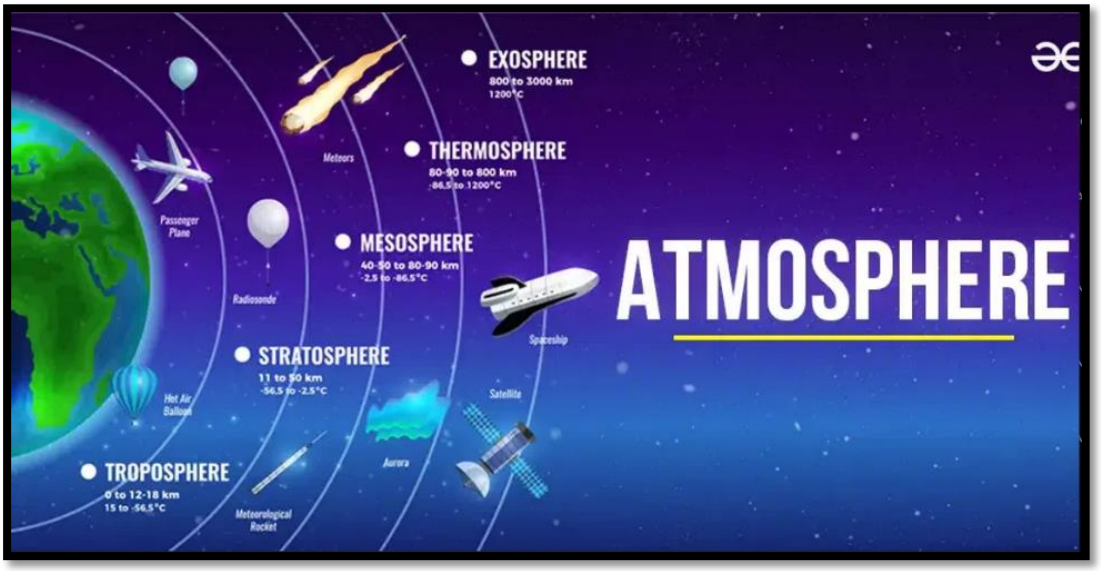
1.3. Essential role of Chemistry

Our lives are inescapably linked to Chemistry. Everything we eat, the environment where we live, and our bodies are all made up of chemicals. This is according to the concept that chemistry is the study of matter, and all matter is fundamentally chemical. Moreover, it controls the agricultural land that produces the food, the drinking water, and the atmosphere where we breathe. The human body has complex chemical reactions that carry out countless chemical mechanisms significant for life, and also a lot of chemical components present within us.

However, the different environmental chemical techniques, for example, the use of ecotoxicants and chemical indicators, are utilized to improve the soil quality. Out of this, some unwanted contaminants such as gasoline, motor oil. Sediments, carbon compounds, hydrocarbons, and metals can accumulate on roadways, roofs, impermeable surfaces of parking lots, and inside cities. Different fields were working on the management of waste, and cleaner production can be used in environmental chemistry.

1.4. Study of chemical processes in nature and how human activities affect them

There are various multidisciplinary scientific areas of chemical and biological processes that take place in the natural world, and studies that examine how human activity affects the natural ecosystem. It investigates the different long-term fates of natural and man-made chemicals that are present on the Earth, chemical and biological changes, origin, ecological impact, and their distribution. By fusing the concept with chemistry, the hydrosphere, lithosphere, biosphere, and atmosphere were all collected under a single umbrella (Team, 2024).



Different types of chemical reactions, such as organic and inorganic reactions that take part in changing the environmental condition; besides this, physical chemistry take an important part in contaminating the environmental chemistry. When the different chemicals enter the environment, they interact with the living organisms, water, soil, and the air, and can be categorized into ecosystems for plants and animals, also including humans. However, the final location of chemical impact is determined by the physical process, such as adsorption, sedimentation, and volatilization. Once the chemical dispread, it can decompose by biological or chemical mechanisms. The initial chemical degradation in water or oxidation in air, reduction, and hydrolysis (Speight, 2018).

Most of the reactive gases containing chlorine and bromine destroy the stratospheric ozone layer through a catalytic cycle, which includes two or more independent chemical reactions.

Therefore, a single chlorine and bromine atom can destroy hundreds of ozone molecules before they expel into the stratospheric layer. This means that the tiny amount of chlorine and bromine can have a huge effect on the ozone layer. A very unique fact arises in the early spring or late winter season, which is known as the polar region, when a significant increase of chlorine monoxide, which is the most reactive gas that leads to substantial ozone depletion. In the given figures, the ozone destruction cycle is discussed (https://csl.noaa.gov/assessments/ozone/2006/chapters/Q9.pdf).

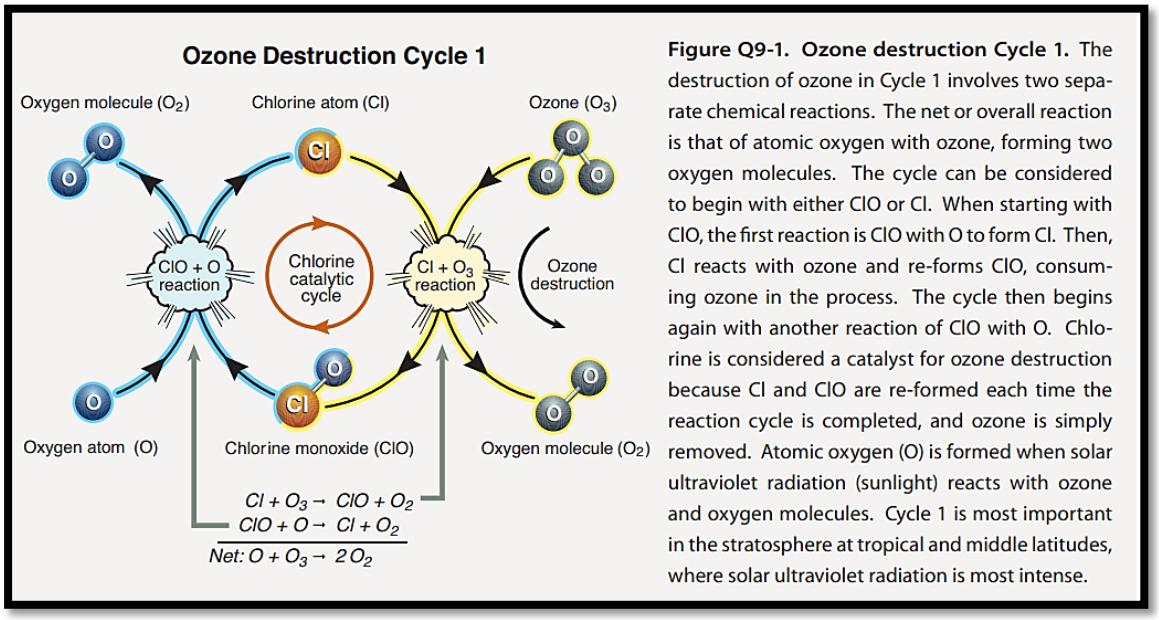


Figure Q9-1. Ozone destruction Cycle 1. The destruction of ozone in Cycle 1 involves two separate chemical reactions. The net or overall reaction is that of atomic oxygen with ozone, forming two oxygen molecules. The cycle can be considered to begin with either ClO or Cl. When starting with ClO, the first reaction is ClO with O to form Cl. Then, Cl reacts with ozone and re-forms ClO, consuming ozone in the process. The cycle then begins again with another reaction of ClO with O. Chlorine is considered a catalyst for ozone destruction because Cl and ClO are re-formed each time the reaction cycle is completed, and ozone is simply removed. Atomic oxygen (O) is formed when solar ultraviolet radiation (sunlight) reacts with ozone and oxygen molecules. Cycle 1 is most important in the stratosphere at tropical and middle latitudes, where solar ultraviolet radiation is most intense.

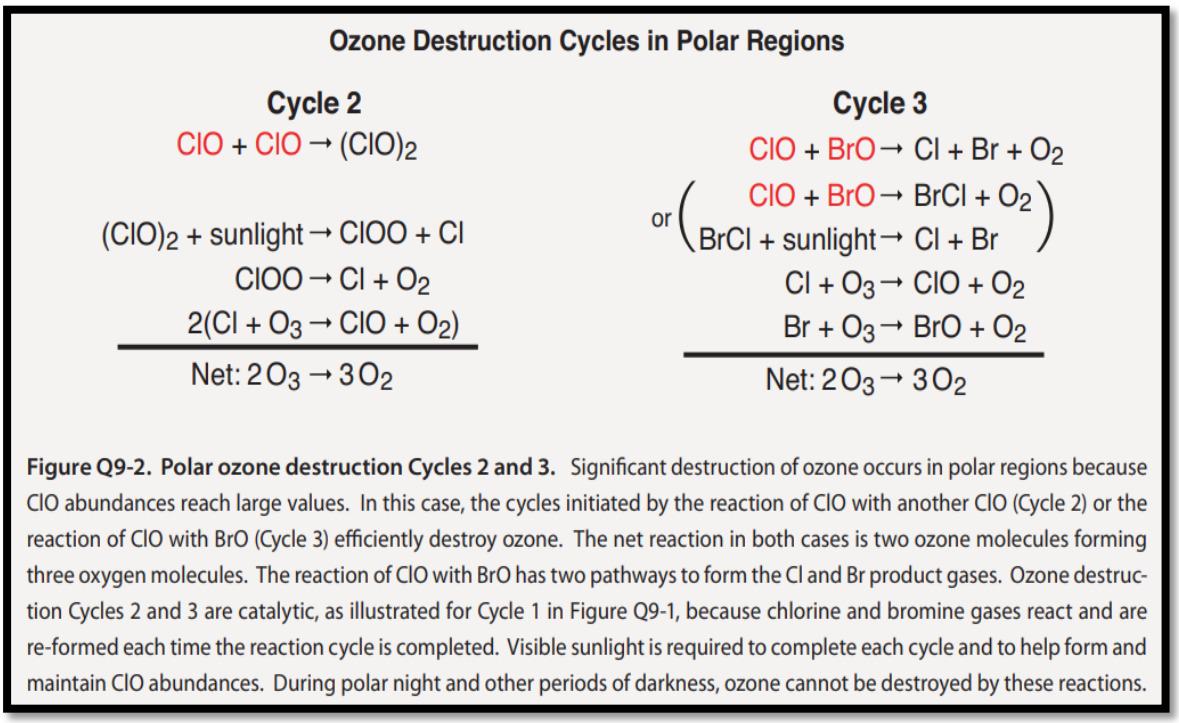
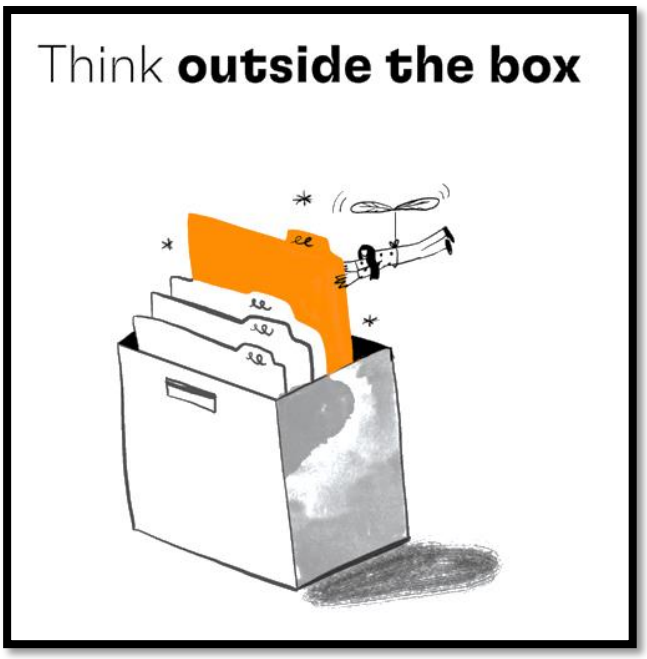


Figure Q9-2. Polar ozone destruction Cycles 2 and 3. Significant destruction of ozone occurs in polar regions because ClO abundances reach large values. In this case, the cycles initiated by the reaction of ClO with another ClO (Cycle 2) or the reaction of ClO with BrO (Cycle 3) efficiently destroy ozone. The net reaction in both cases is two ozone molecules forming three oxygen molecules. The reaction of ClO with BrO has two pathways to form the Cl and Br product gases. Ozone destruction Cycles 2 and 3 are catalytic, as illustrated for Cycle 1 in Figure Q9-1, because chlorine and bromine gases react and are re-formed each time the reaction cycle is completed. Visible sunlight is required to complete each cycle and to help form and maintain ClO abundances. During polar night and other periods of darkness, ozone cannot be destroyed by these reactions.

‘‘A nation destroy its soil destroy itself.’’ The primary reason for environmental destruction is Humans. Since the time when the ancient civilization began altering the land according to their survival. Various our activities such as spreading pollution, overconsumption, and deforestation have all led to major irreversible damage. In the current scenario, we are losing the most important natural resources, such as fertile soil, clean water, and biodiversity, very quickly. We have no more society if we destroy the environment. Leonardo DiCaprio said ‘‘Our planet’s alarm is going off, and it is time to wake up and take action’’

1.5. Why does innovation matter?

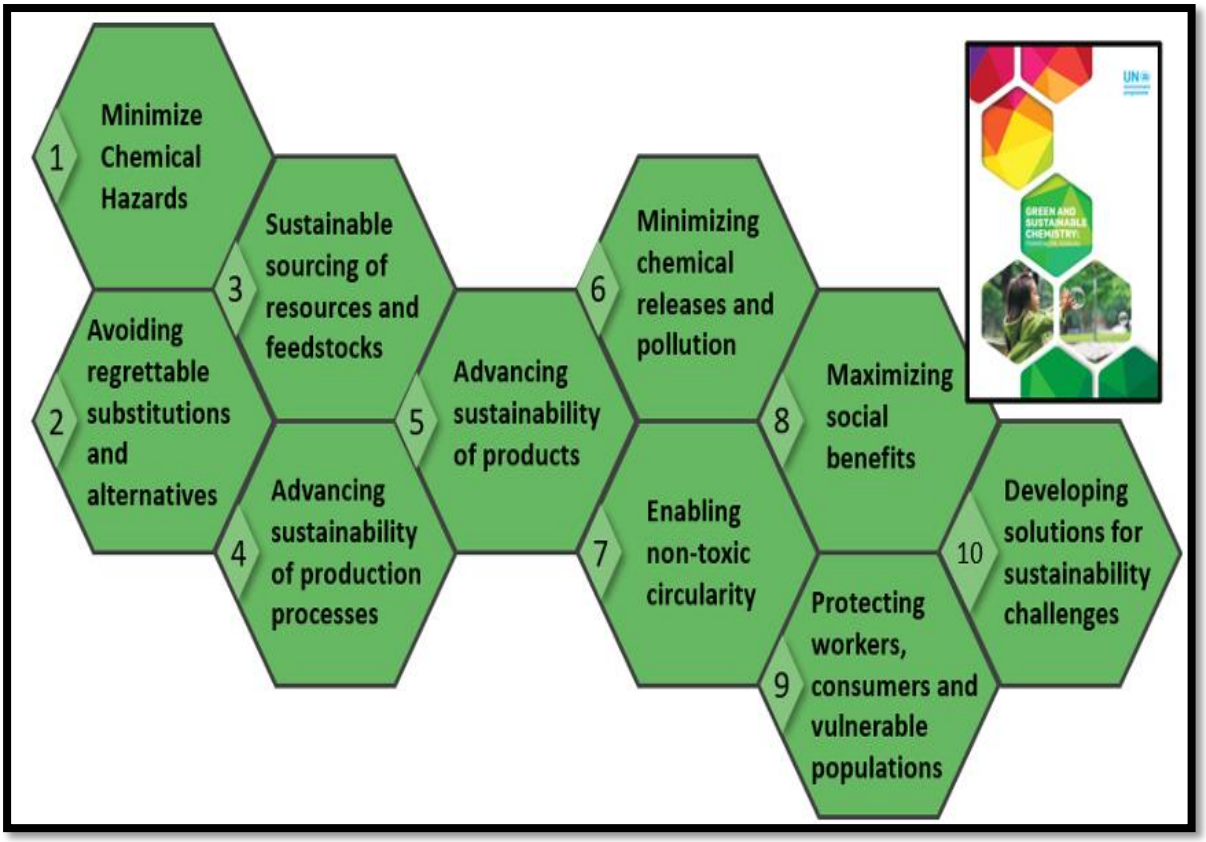


The innovation in environmental chemistry is very significant for the protection of living life, especially human health. And also to detect and eliminate the new toxic pollutants before they come across the environment and make pollution. Various interventions have been made possible, such as modern tools that can now able to detect tiny particles in drugs, pesticides, industrial chemical waste, and pharmaceuticals in water sources to help clean up all. Moreover, intelligent material and modern catalytic techniques are also more effective for the degradation of toxic pollutants faster, preventing long-term damage to the ecosystem. various example of innovation that provides real-time data to government and corporations to make quick or smart actions include lab-on-a-chip devices and AI-powered tools for monitoring environmental pollution. Today, after continuous hard work and efforts in research and technology, environmental chemists are not only able to solve the current issues but also predict the upcoming possible risks and ensure economic growth doesn’t come at any cost to damage our Earth.

1.6. Key Areas of Environmental Chemistry Innovations

Many of the scientists are creating more effective methods to detect and remove the pollutants and fight climate change. The all-new innovative solutions help to promote the cleanliness of our planet’s air, water, soil, and most importantly, they improve human health.

1.6.1. Green & Sustainable Chemistry



According to the Environmental Protection Agency (EPA), green chemistry involves the production of chemical products and processes that are environmentally safe, hence preventing pollution. It maximum chemical products were made in such a way that they break down into environmentally safe components that have no longer in the environment to create pollution and cause harm to the environment. Rather than considering a separate branch of science, green chemistry is responsible multidisciplinary approach to science founded on social, ecological, and chemical. Green chemistry inspires the innovation and development of novel research (Ivanković, 2017). In order to accomplish the global sustainable development targets, there have ten objectives shown in the given figure to seeks the progress in chemistry and foster the innovation. The UNEP work with more than 100 expert stakeholders to develop the main objectives and considerations for the green and sustainable chemistry. These objectives or goals add to traditional chemistry by focusing what we want to show and the sustainability. In the current situations after ensuring that chemistry is fully compatible with the global goals and to encourage the new ideas and they fully connect to potential of chemistry with the 2030 sustainable development agenda (https://www.unep.org/).

1.6.2. Principles of green chemistry

Paul Anastas and John warner in 1998 formulated 12 principles of "Green Chemistry''. They encourage the industrialists, government officials and scientist to adopt their activities that decrease or reduce the usage of hazardous material. These 12 principles have made significant contribution to the formation of new philosophy on the bases of their usefulness, specificity, and their relevance. These 12 principle are given below as

1. **Atom efficiency:** modified the synthesis methods to incorporate the raw material into its final product and decrease the waste of it.
2. **Prevention of waste:** Design the chemical methods as the minimum waste and the maximum usage into products.
3. **Safe chemical synthesis:** Developing the chemicals that are less dangerous or zero toxicity to human life as well to environment.
4. **Safe reaction condition and solvents:** Select that route of reaction which is safe for environment and the solvent used during the reaction also non hazardous
5. **Renewable stock material:** The raw material used is derived from sustainable sources such as crop and waste.
6. **Catalytic reaction:** Select the catalytic chemical reaction over the stoichiometric reagents to decrease the waste.
7. **Degradable substances:** At the end of chemical reaction the remaining chemical will convert into harmless components.
8. **Real time pollution monitoring:** The by-products during the synthesis regulating to avoid the waste production.
9. **Derivative reduction:** If possible to avoid the use of blocking or protective groups or any other temporary change.
10. **Prevention of accidents:** Select those type of chemicals and their routes to reduce the risk of explosion.

11. Energy efficient process: For ideal chemical reaction conducted at ambient temperature and pressure. If the chemical reaction takes place at low temperature and pressure.

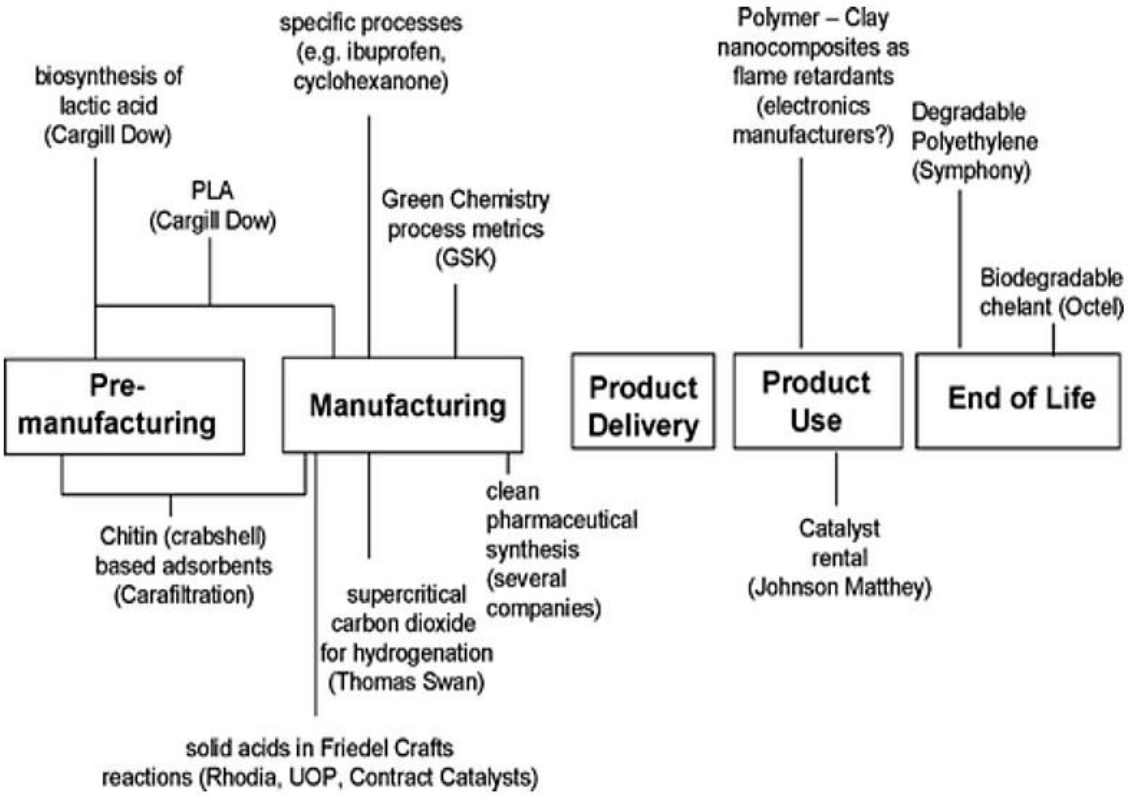
12. Safe route of route of reaction: Design the safe chemicals that are effective and non-toxic at all (Soltys et al., 2021).

Examples of green chemistry

1.6.3. Pollution Remediation Technologies

There are a number of various technologies discovered for pollution remediation, such as:

- Activated carbon-based technology
- Air sparging
- Bioremediation
- Groundwater circulating wells
- Nanoscale material for environmental site remediation
- Soil vapour extraction



1.6.4. Renewable Energy & Carbon Capture

The efficiency and cost of switching to 2050 clean energy of wind-water solar (WWS) could bring large significant values. The renewable systems are much more useful than fossil fuels, that why they cut global energy usage, which is more than half of the total usage. Around

60% of would save households by producing electricity cheaper, which affects the energy bills. Due to the burning of fossil fuels, which causes air pollution in the current time, the death rate is decreasing which has about 5 million usages of coal, oil, and gas is reduced (https://environmentamerica.org/center/). Since 2010 scalability of solar and wind has decreased from 89% to 69%, but enhancing the competitiveness of renewable energy sources without involving carbon capture (Bennett, et al., 2025).

1.7. Challenges & Future

- One of the main challenges is climate change, global warming, ozone layer depletion, deforestation, and solid waste management out Among all these issues, the most important challenge is the economic barriers.
- In the future, environmental chemistry depends on the interdisciplinary innovation that combines with artificial intelligence, biotechnology, chemistry, and the various rules that follow a low-carbon, minimum waste economy. For success in this field, we need Global collaborations, funding, as well as raising public awareness to increase the essentials.

1.8. Conclusion

Environmental chemistry has the main goal of detecting, preventing, and resolving the different types of pollution to make the environment clean and safe for living purposes. It gives an idea to understand the behaviour of chemicals in nature and analyse the new routes that are non-hazardous. Due to the cleaning project, it protects the groundwater, soil, and air from sediments and toxins also observes the harm, such as microbes and radiation.

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