GHEMZONE 2025

THE ANNUAL DEPARTMENTAL MAGAZINE

THEME : RECENT DEVELOPMENTS IN CATALYSIS FOR RENEWABLE ENERGY AND SUSTAINABLE FUTURE

DEPARTMENT OF CHEMISTRY MAITREYI COLLEGE University of Delhi

Cover Page Design: Muskan Kumari, B.Sc. (P) Physical Science, IIIrd year

CHJn

Copyright @ 2025, Maitreyi College

All rights reserved by the editor

No part of this publication be reproduced or stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, or otherwise without the prior permission of the editor and co-editors.

Book Title : CHEMZONE 2025 Editors : Dr Ritu Gaba, Dr Ankita Chaudhary, Dr Gazala Ruhi, Dr Hema Bhandari ISBN : 978-93-92603-16-7 Publisher : FA DIGITAL PRODUCTIONS 18A/20 Zakir Nagar, Jamia Nagar, New Delhi- 110025 Mob: +91 9810674877 Edition : 2025

For purchase or trade inquiries, contact: Department of Chemistry, Maitreyi College University of Delhi Bapu dham, Chanakyapuri, New Delhi, Delhi 110021 E-mail: chemistry@maitreyi.du.ac.in

TEACHER'S



Dr. Ritu Gaba Associate Professor Physical Chemistry



Dr. Ankita Chaudhary Associate Professor Organic Chemistry



Dr. Hema Bhandari Associate Professor Organic Chemistry



Dr. Gazala Ruhi Assistant Professor Physical Chemistry

EDITORIAL BOARD

STUDENT'S



Tanu Sarkar

II Year



Kalpana Yadav II Year



Stuti Sharma II Year



Sukreeti Singh II Year



Bharti Mahajan I Year



Pragya I Year



Ishita Bhadana III Year



Tanya Kumari II Year



Monika III Year



Contents

| 1. EDITORIAL ADDRESS | 01 |
|---------------------------------------------|----|
| 2. FROM THE PRINCIPAL'S SANCTUM | 02 |
| 3. VICE-PRINCIPAL'S MESSAGE | 03 |
| 4. CONVENOR'S MESSAGE | 04 |
| 5. INTRODUCTION TO THE CHEMISTRY DEPARTMENT | 05 |
| • FACULTY | |
| NON -TEACHING STAFF | |
| TEAM CHEMZONE | |
| CHEMISTRY COUNCIL | |
| 5. EVENTS AND ACTIVITIES | 10 |
| ORIENTATION 2024 | |
| • TEACHER'S DAY 2024 | |
| • SEMINARS | |
| CHEMSOPHY'25 | |
| • FAREWELL 2025 | |
| EDUCATIONAL EXCURSIONS 2025 | |
| 7. ARTICLES | 20 |
| • FACULTY | |
| • STUDENTS | |
| • ALUMNI | |
| 8. STUDENT'S CORNER | 86 |
| • FUNFACTS | |
| • MEMES | |
| ACHIEVEMENTS | |
| BLOG SECTION | |
| | |
| CHEM/ZONE 201 | |

EDITORIAL ADDRESS

Presenting Chemzone, Chemistry E-magazine 2025

t is a great privilege and pleasure to release the next issue of our annual magazine 'Chemzone'. Just as a rainbow is an embodiment of hopes, pleasure and aspirations represented as VIBGYOR across the horizon in a

manner soothing to eyes and mind, the annual magazine too intends to capture and represent diverse facts of the Radha Sairam Chemical magazine Society. The espouses the department's spirit which is built up within the department through collective actions, thoughts and aspirations. It captures momentous moments of the department and is a compilation of immense effort and creativity put forward by both teachers and students. Chemzone represents the ardour, honesty, deference and respect we have for chemistry. To put it briefly, the magazine presents an abstract collection of scientific interpretive methodologies including articles by both teachers and students.

blogs, students perspective on different topics, critical coverage of scientific research and memorable notes by alumini. recent advancements and news in the field of chemistry and some fun filled facts, memes and crossword. The enthusiastic write ups and achievements by the students are indubitably sufficient to hold the interest and admiration of readers. We are confident that the positive mindset, hardwork, persistent efforts and creative ideas of the students and the Teachers will surely captivate readers and take them to the enchanting realm of chemistry with unalloyed joy and pleasure. This platform gives our team the opportunity to express profound gratitude to the principal, convenor and faculty members of the department who were always there as our guiding light and source of inspiration .Thanks to the students for contributing to the magazine by whichever way they could. Thank you for encouraging the editorial board with valuable suggestions.

> Warm Regards, Editoral Board

CHEMZONE 2025

From The Principal's Sanctum



Prof. Haritma Chopra

Greetings from Maitreyi College,

Dear Readers,

It gives me immense pleasure to present the third edition of **CHEMZONE**, the Chemistry emagazine of Maitreyi College for the year 2025. This edition is a testament to the unwavering commitment of our students and faculty to scientific inquiry, innovation, and sustainability. The theme of this volume, Recent Developments in Catalysis for Renewable Energy and a Sustainable Future, resonates deeply with the global call for greener and cleaner technologies. Our students have enthusiastically explored the crucial role of catalysis in transforming the energy landscape, showcasing how chemistry can drive solutionsto some of the most pressing challenges of our times. At Maitreyi, we believe in nurturing not only academic excellence but also the curiosity and creativity that fuel scientific breakthroughs. Through initiatives like **CHEMZONE**, we provide our students a platform to express their ideas, collaborate on emerging scientific issues, and sharpen their critical thinking and communication skills.

I extend my heartfelt congratulations to the student editorial team and the faculty members for their collective efforts in bringing out this insightful edition. May this e-magazine continue to inspire young minds to innovate for a sustainable and inclusive future.

Best Regards, Prof. Haritma Chopra Principal Maitreyi College

Vice-Principal's Message



Prof. Pinkey B Gandhi

Dear Readers,

It gives me great pleasure to share my observations in the third edition of CHEMZONE, the chemistry e-magazine of Maitreyi College for the year 2025. This edition explores the theme 'Recent Developments in Catalysis for Renewable Energy and Sustainable Future' for greener and more sustainable technologies.

The global energy plight and environmental challenges have made it obligatory to shift towards cleaner, greener and more sustainable processes from the existing conventional processes. Catalysis plays a significant role in developing efficient and eco – friendly energy solutions.

Having Organic Chemistry specialisation, my core research interest has always been use of different types of catalysts for synthetic processes . Recently during a study for the synthesis of nanoparticles, l explored the use of Enzymes present in plant extracts and microbes as biocatalysts. These bio catalysts offer exceptional selectivity and function under mild environment friendly conditions. For example hydrogenase enzymes are being explored for their ability to produce hydrogen gas as a clean fuel with high efficiency. Similarly enzymes derived from fungai are being used as catalysts for green oxidation reactions as well as applications in biofuel Cells.

Through genetic engineering scientists have designed tailor made microbes that can convert biomass into useful fuels and chemicals, hence reducing dependency on fossil resources. The above mentioned studies highlight that how natural solutions can lead the way towards a sustainable future.

Dear students, as future scientists you may explore these innovative and impactful areas of research and contribute towards a sustainable future. Wishing the Department continued success and many more such insightful editions of CHEMZONE in the years ahead.

Best Regards Prof.Pinkey Bajaj Gandhi Vice-Principal Maitreyi College

Convenor's Message



Dr. Ritu Gaba

Science knows no country, because knowledge belongs to humanity, and is the torch which illuminates the world." — Louis Pasteur

Dear Readers,

It is with immense pride and joy that I present the latest edition of **CHEMZONE**, the e-magazine of the Department of Chemistry, Maitreyi College. As the Teacher-in-Charge, I have had the privilege of witnessing the vibrant synergy of ideas and creativity that has shaped this edition.

This year's theme, "Recent Developments in Catalysis for Renewable Energy and a Sustainable Future," could not be more timely. As the world grapples with the dual crises of energy scarcity and environmental degradation, catalysis emerges as a powerful tool—offering cleaner, greener, and more efficient alternatives for energy conversion and storage. Through this theme, our students have explored how innovative catalytic processes can pave the way toward a sustainable future. Their contributions reflect not only scientific understanding but also a deep sense of responsibility towards the planet.

This magazine is a tribute to the curiosity, critical thinking, and collaborative spirit that define

our department. Each article reflects a unique perspective, adding to the richness of this collective endeavor.

I extend my heartfelt thanks to our Principal Prof. Haritma Chopra and Vice Principal, Prof. Pinkey Bajaj Gandhi for their constant encouragement and for providing us the platform to showcase this emagazine. Their support has been instrumental in nurturing a culture of academic excellence and creative expression.

My deepest gratitude also goes to the student editorial team, the faculty members, and all the contributors who made this edition possible. May Chemzone continue to share meaningful dialogue among us all.

Dr. Ritu Gaba Teacher-in-Charge Department of Chemistry Maitreyi College

CRAFTING MOLECULES, CREATING MINDS: THE CHEMISTRY DEPARTMENT

Established in 1967, the Department of Chemistry at Maitreyi College has evolved into a vibrant center of academic excellence, driven by a commitment to nurturing comprehensive knowledge seekers who not only excel in the field of chemistry but also grow into responsible citizens contributing meaningfully to nation-building.

With a focus on fostering both intellectual and ethical growth, the department offers a dynamic and inclusive learning environment supported by a highly qualified and diligent faculty. Our teaching methodologies are rooted in conceptual clarity and experiential learning, aiming to strengthen the fundamentals of chemistry through an engaging undergraduate curriculum.

The department currently offers B.Sc. (Hons) Chemistry, and actively contributes to interdisciplinary programs such as B.Sc. (Prog) Physical Sciences and B.Sc. (Prog) Life Sciences. Additionally, we support the academic needs of students from other departments including Physics, Botany, Zoology, and Mathematics, reflecting our collaborative academic culture.

Our infrastructure includes four spacious and well-equipped laboratories for demonstrations, experimentation, and researchoriented project work, along with an instrumentation laboratory housing sophisticated instruments to facilitate undergraduate research. The department also boasts a dedicated library with over 500 books, smart classrooms, and access to computers and laptops for both staff and students.

Behind the seamless functioning of our practical sessions is a team of 13 skilled laboratory staff members, who play a pivotal role in managing our laboratories efficiently.

Through a fine blend of rigorous academics, hands-on training, and research exposure, the department provides a firm base to inculcate scientific temperament, critical thinking, and entrepreneurial skills among students. We strive to empower our students to face the challenges of the competitive world with confidence, curiosity, and integrity.





Prof. Pinkey B Gandhi Professor Organic Chemistry



Prof. Manju Mehta Professor Organic Chemistry



Dr. Sandhya Gupta Associate Professor Inorganic Chemistry



Dr. Gita B Narula Associate Professor Inorganic Chemistry



Dr. Padma Saxena Associate Professor Physical Chemistry



Prof. Ramesh Kumari Professor Physical Chemistry

Meet the Mentors



Behind every successful experiment and inspired student stands a dedicated mentor. Our esteemed faculty members bring a wealth of knowledge, research experience, and passion for teaching. Their guidance not only shapes academic journeys but also sparks curiosity and innovation in the ever-evolving world of chemical sciences.



Dr. Rajni Johar Associate Professor Inorganic Chemistry



Dr. Pratibha Chaudhary Associate Professor Organic Chemistry



Dr. Hema Bhandari Associate Professor Organic Chemistry CHEMZONE 2025



Dr. Ritu Gaba Associate Proîessor Physical Chemistry



Mr. Kamal Sharma Assistant Professor Organic Chemistry



Dr. Durgesh Kumar Assistant Professor Applied Chemistry



Dr. Lata Vodwal Associate Professor Organic Chemistry



Dr. Gazala Ruhi Assistant Professor Physical Chemistry



Dr. Preeti Yadav Assistant Professor Inorganic Chemistry



Mr. Roop Singh Meena Assistant Professor Inorganic Chemistry



Dr. Ankita Chaudhary Associate Professor Organic Chemistry



Dr. Navneet Kishore Assistant Professor Organic Chemistry



Dr. Nishu Assistant Professor Organic Chemistry

The Non-Teaching Staff

The non-teaching staff of the Chemistry Department at Maitreyi College, DU, play a vital role in ensuring smooth operations. From managing inventories to maintaining and assisting with equipment, their dedication supports both students and faculty, contributing significantly to the department's efficiency, safety and professional environment.



Mr. Satish Kumar, Mr. Aman Mudgal, Mr. Hansraj Saklani, Mr. Vinod Kumar Rai, Mr. Harish Chandra, Mr. Mohanlal, Mr. Madan Kishor, Mr. Ravindra Singh (Store Incharge), Mr. Raju Shah, Mr. Lalit Kumar, Mr. Devraj Singh, Mr. Omprakash Roul and Mr. Tribhuwan Singh

CHEM COUNCIL 2025

Our Beloved Team

President



Ishita Bhadana

Vice President



Tanu Sarkar

General Secretary



Kamakshi Sehgal





Prachi Bidhuri

Joint Secretary



Bharti Mahajan

Social Media

Head

Volunteer Head



Tanuu



Stuti Sharma



Creative

Head

Monika



Kalpana Yadav



Deepti



Pragya CHEMZONE 2025

EVENTS &



ACTIVITIES



ORIENTATION 2024



The Orientation Day for new students of the Chemistry Department was held on August 29, 2024. The session was aimed to introduce students to the faculty members and provide them with essential information about the department, college and academic guidelines. The session began with Dr. Ritu Gaba, TIC (Teacher-in-Charge) of the department, warmly welcoming the students. She introduced herself and other faculty members of the department, giving students an opportunity to get familiar with the teachers they will be learning from.

Following the introduction, Mr. Kamal Sharma delivered an insightful presentation about the college and the department. He spoke about the rich teaching experience of the staff, their qualification and the department's commitment to providing a supportive academic environment. Mr. Kamal also gave a thorough explanation of the internship opportunities available to students, the process of applying for internship and how these internships play a crucial role in practical learning and career development.

Dr. Preeti Yadav addressed the students regarding lab safety protocols. She emphasized the importance of following safety guidelines when working in the lab and exaplained the various in place to ensure a safe learning environment. She also advised to always seek guidance from lab supervisors when in doubt. The orientation ended with the brief Q&A session where students had the opportunity to ask questions and clarify any doubts they had. Overall, the day helped the students get an understanding of their academic journey and what to expect during their time in the department.





Special Lecture on "Foundation For Success"

On September 10, 2024, our college had the honor of hosting Mrs. Monica Dhawan, a seasoned professional with over 20 years of experience in leadership roles. The event, titled "*Foundation for Success*," was an enlightening session that covered key principles for achieving success in both personal and professional life.

Key takeaways-

- Self-Awareness
- Goal setting
- Resilience & Adaptability
- Effective Communication
- Network & Mentorship
- Continuous Learning
- Time Management & Productivity

Teacher's Day' 24

The Department of Chemistry celebrated Teacher's Day on September 5, 2024, at the college level. The event was organized by students to express gratitude towards their teachers.

The room was beautifully decorated, and the celebration began with a welcoming gesture and introductory speeches by students Shristi and Bharti. A Hindi poetry recital added a heartfelt touch to the event. The program included a cake-cutting ceremony, refreshments, and fun games such as Bingo, Dumb Charades, and Riddle solving.

The celebration successfully honored the teachers and strengthened the bond between students and faculty.











Lecture on "Exploring the Fundamentals of Protein Folding"

The Radha Sairam Chemical Society hosted an enlightening lecture on "The Basics of Protein Folding: In-Cell Insights" on February 19, 2025. Delivered by protein science expert Prof. Parmit K. Chowdhury, the session delved into the question: Can we predict the structure of a protein from its amino acid sequence? The event opened with a warm welcome by hosts Kashish and Taniya, followed by Saraswati Vandana and lamp lighting. Prof. Chowdhury's lecture highlighted the critical role of protein folding in cellular processes and its implications in disease. An engaging Q&A session followed, where students posed thoughtful showcasing their queries, curiosity and understanding. The event concluded with a vote of thanks by Dr. Ritu Gaba. Participants praised the session for its clarity, interactivity, and insightful exploration of protein folding mechanisms.







Career Counselling Workshop

On March 6, 2025, a workshop at Maitreyi College guided students on global and Indian career opportunities. Mr. Jitin Chawla shared insights on job markets, higher education and profile building. He emphasized both international options and India's growing sectors. The session was interactive and informative, helping students reflect on their career paths. Students were encouraged to ask questions and engage in discussions, making the session lively and enriching. Mr. Chawla highlighted the importance of staying adaptable in a rapidly changing job market and stressed the value of networking and continuous learning. Participants left with a clearer understanding of how to align their passions with career goals and the steps needed to achieve them. The workshop concluded with a Q&A session, where attendees received personalized advice and encouragement, leaving them inspired and motivated to pursue their aspirations with confidence.

CHEMSOPHY'25

Radha Sairam Chemical Society, Department of Chemistry, Maitreyi College organized its Annual Academic Fest, "CHEMSOPHY '25" on March 28, 2025. The event commenced with an inaugural guest lecture by Prof. Rajeev Gupta, Senior Professor at the University of Delhi, as part of the *'Luminaries of Indian Sciences'* lecture series. Five different events were organized under the aegis of the fest:

1. IMPATICA (POWERPOINT PRESENTATION)

Theme for the competition was "Artificial Intelligence in Science :Transforming the Future." The judges for the event were Prof. Ramesh Kumari and Dr. Preeti Yadav. It was conducted in Room no. 62, Maitreyi College. There were a total of 15 participants and the event showcased students' creative and technical presentation skills. The winners of the event were Vaibhav Kumar Mishra and Shreya Saha from ARSD college.

2. LAB RELAY

It was a solo participation event where contestants answered ten Chemistry-related questions within a strict one-minute time limit per question .The judges for the event were Dr. Padma Saxena, Dr. Durgesh Rawat, Dr. Nishu Nain and Dr. Raghavi Khattar. There were a total of 21 participants and the event tested participants' knowledge, quick reasoning, and adaptability under time constraints. The winners of the event were Vaishali (First position from Maitreyi College) and Aashika Jain (Second position from Gargi College)

3. CHEM QUIZ

This event was a chemistry quiz conducted in two phases: a written test followed by a team -based quiz with multiple rounds ,including a rapid fire segment. The judges of the event were Dr. Gazala Ruhi, Prof. Manju Mehta, Dr. Sandhya Gupta, Dr. Pooja Saluja and Dr. Navneet Kishore. There were a total of 20 participants and the event enhanced students' subject knowledge, problem-solving and teamwork skills. The winners of the event were Shweta Yadav and Saloni Bharati from Maitreyi college.



CHEMZONE 202

CHEMSOPHY'25

4. SCRIBBLE SCRABBLE

This was a team-based visual communication game where one member drew a word or concept and the other guessed it. The judges of the event were Dr. Hema Bhandari and Mr. Roop Singh Meena. There were a total of 30 participants and this event fostered creativity, team work and quick thinking. The winners of the event were Manak and Radhika from Gargi College and Kajal from Maitreyi College.

5. TREASURE HUNT

It was a team-based competition testing participants' wits and agility through a series of clues and challenges across the Science Block. The judges of the event were Mr. Kamal Sharma and Dr. Rajni Johar Chhatwal. There were a total of 41 participants and it challenged participants to think on their feet and act quickly, promoting teamwork and problem solving skills. The winners of the event were a team from Physics department of Maitreyi College.









Punjabi And Hindi Department, Maitreyi College University Of Delhi, Chanakyapuri, New Delhi, Delh 110021, India Lat 28.592185° Long 77.177645° 28/03/2025 12:30 PM GMT +05:30

FAREWELL 2025



April 22, 2025, a memorable farewell for the On graduating class was held in NSB Seminar Hall. The event was filled with creative and engaging activities, including energetic dance routines, melodious songs, heartfelt video and Miss farewell contest. The teachers extended their warm blessings, leaving attendees with a mix of happy and emotional farewells. A shared sentiment expressed during the event highlighted the importance of embracing new beginnings and cherishing the memories made. Students from both first and second years participated whole heartedly bidding a tearful goodbye to their seniors and III years also expressed their mixed emotions. Though parting is always bittersweet, this farewell signified the start of promising futures and lasting achievements for the graduates. The event came to an end by declaration of results for Miss farewell contest and DJ session.



EXPERIENTIAL LEARNING: VISITS

Visit to National Physical Laboratory (NPL)

The Foundation Day of NPL is celebrated as an 'Open Day', where students from all institutes were welcomed. On October 1,2024, from Maitreyi College, University of Delhi, a total of 19 students along with 2 teachers visited the National Physical Laboratory. NPL is famously known as the time keeper of India as it maintains the Indian Standard Time (IST) along with the other 6 units of measure.

We had Dr. Anupriya as our guide for visiting the labs. Under her guidance, we visited the Liquid Nitrogen and Helium Plant. At the next laboratory, we were given insight on the process of Thin Film Deposition and its importance in combating air pollution through a video lecture. Thereafter we visited the Solar Panels. There we came to know about the working of solar panels. He talked about the viscosity of these fluids and how Nonfluids Newtonian have vast applications in space programs and automobile braking systems.

We received positive feedback from all the participants and the beneficiaries. Students showed a keen interest in participating in workshops and internships organized by the CSIR-NPL.







CHEN CAREER

Chem Career India: National-Level Seminar Opens New Avenues for Aspiring Chemists

The Royal Society of Chemistry (RSC), in collaboration with the Department of Chemistry, School of Natural Sciences, Shiv Nadar University, organized a National-level seminar titled "*Chem Career India*" on 12 September, 2024. The event aimed to guide students in exploring diverse career opportunities in the field of chemistry.

The session commenced with a welcome address emphasizing the need for such initiatives to support students in making informed career choices. The seminar featured distinguished speakers and experts from academia and industry:

Prof. Akhilesh K. Verma (University of Delhi) delivered the opening lecture on career paths available to chemistry graduates, including higher education, academic research, and roles in the chemical industry.

Prof. Sebastian Chirambatte Peter spoke on emerging careers in chemical sciences, shedding light on fields like green chemistry, nanotechnology, and environmental science.

Dr. Samik Kumar Hait and Dr. Gurmeet Singh provided insights into industry-related opportunities, focusing on skills required for roles in pharmaceuticals, biotechnology, and materials science.



PM Hilary White, Head of Membership Development, RSC UK, highlighted the benefits of RSC membership, including access to global networks, research resources, and professional development tools. An interactive panel discussion followed, where students posed career-related questions to the experts, gaining valuable guidance. The event concluded with an intercollegiate quiz competition, where students from Maitreyi College proudly secured 3rd position.

A total of 18 students from Maitreyi College participated in the event. The feedback was overwhelmingly positive, with students expressing a clearer understanding of career options and industry requirements.

This enriching seminar was a milestone for chemistry students, offering clarity, confidence, and connections to navigate their future paths in the chemical sciences.

Visit to Rail Neer Plant, Hapur

A group of 23 enthusiastic students of B.Sc. (Hons) Chemistry, accompanied by faculty members Dr. Preeti Yadav, Dr. Durgesh Kumar, and Dr. Navneet Kishore, visited the Rail Neer Plant in Hapur, Uttar Pradesh on May 8, 20205. The visit was organized under the guidance of Dr. Ritu Gaba, with an aim to provide students with industrial exposure to water purification and packaging processes.

We were warmly welcomed and guided through various sections of the plant. The visit began with a detailed explanation by Dev Sir on the multi-stage purification process which included carbon filtration, ultrafiltration, reverse osmosis, and ozone treatment. Students also witnessed the manufacturing of PET bottles using high-pressure air molding with advanced Himens machinery.

Later, experts briefed us on the quality control laboratory, where chemical parameters like pH, TDS, hardness, chloride, and microbiological parameters such as yeast, mould, coliform, and TPC were tested.

The visit concluded with an interactive Q&A session, followed by a buffet lunch and a warm vote of thanks. The experience was highly informative and offered valuable practical insight into industrial chemistry applications.

Students expressed keen interest in similar industrial visits that connect classroom learning with real-world applications.







Articles

EDUCATORS & STUDENTS

HEXPANDING THE HORIZON OF OUR KNOWLEDGE

ARTICLES BY EDUCATORS

- Engineered Biomolecular Catalysts: Shaping the Future of Catalyts Dr. Ritu Gaba, Department of Chemistry, Maitreyi College
- Revolutionizing Green Catalysis with Deep Eutectic Solvents: A Sustainable Leap Forward Dr. Ankita Chaudhary, Department of Chemistry, Maitreyi College
- From Sunlight to Sustainability: Understanding Photocatalysis Dr Rajni Johar Chhatwal, Department of Chemistry, Maitreyi College
- Unravelling the Mystery: Beyond the Genetics Dr. Nishu Nain, Department of Chemistry, Maitreyi College
- A New Paradigm in Wastewater Treatment: The Carbon Quantum Dot Approach Dr. Gazala Ruhi, Department of Chemistry, Maitreyi College
- The Photocatalyst Revolution: Light Activated Remediation of Organochlorine Pesticides Dr. Hema Bhandari, Department of Chemistry, Maitreyi College
- Critical Role of Eco-friendly H₂O₂ Catalyst in Wastewater Treatment Dr. Navneet Kishore, Department of Chemistry, Maitreyi College

In the quest to revolutionize sustainable chemistry and improve industrial processes, scientists have turned to the very foundation of life itself: enzymes. Enzymes are naturally occurring proteins, responsible for accelerating biochemical reactions in living organisms, have inspired the development of engineered biomolecular combine catalysts that the efficiency of biological systems with the precision synthetic chemistry.¹ These of engineered catalysts are not just changing how we think about catalysis, they are opening doors to innovations that could reshape entire industries, from pharmaceuticals to energy Enzymes accelerate production. chemical reactions with remarkable speed and specificity. The efficiency and specificity of these molecular machines have inspired scientists to create artificial systems that mimic or even enhance their functions.

ENGINEERED BIOMOLECULAR CATALYSTS: SHAPING THE FUTURE OF CHEMISTRY

Dr. Ritu Gaba Department of Chemistry Maitreyi College

The idea of engineered biomolecular catalysts arose from the realization that the principles governing biological catalysis could be applied in industrial settings. By harnessing and modifying the molecular structures of enzymes, researchers can create tailored catalysts that exhibit high activity and selectivity for specific reactions,² while also being more sustainable and environmentally friendly compared to traditional chemical catalysts. In recent years, the focus has shifted from simply mimicking enzymes to creating catalysts with customized properties that meet specific industrial demands. This engineering of biomolecular catalysts often involves sophisticated techniques in molecular biology, directed evolution. immobilisation and computational modeling to design enzymes that not only catalyze reactions more efficiently but can also withstand extreme conditions or be tuned to interact with nonbiological substrates.

Mechanisms of Biomolecular Catalysis

To understand the appeal of engineered biomolecular catalysts, it is essential to understand how enzymes function at the molecular level. Enzymes lower the activation energy of a chemical reaction, making it easier for the reactants to reach the transition state and eventually convert into products. Unlike traditional catalysts, which often require high temperatures or harsh chemicals, enzymes typically work under mild conditions, in aqueous solutions, at physiological temperatures and neutral pH. This remarkable efficiency is due to the enzyme's three-dimensional structure, which provides a specific and complementary binding site for the substrate. The enzyme's active site is often a finely tuned microenvironment where substrates are precisely oriented, and unfavorable interactions are minimized. The enzyme catalyzes the transformation by stabilizing the transition state or facilitating the breakdown of bonds, typically using

a combination of acid-base catalysis, covalent catalysis, and metal ion coordination.

When enzymes are engineered, scientists can tweak their structures to optimize these catalytic mechanisms. By modifying the active site, changing amino acid residues or by introducing new cofactors researchers can enhance the enzyme's ability to catalyze a reaction, broaden its substrate scope, or improve its stability and resistance to harsh conditions.³ Various approaches to enzyme engineering have been developed⁴ to enhance the functionality, stability, and efficiency of enzymes for industrial, medical, and research applications these include directed evolution, substrate engineering, computational design, immobilization, and structure-guided engineering (Figure 1).

One of the most groundbreaking techniques in the development of engineered biomolecular catalysts is directed evolution. This approach mimics the process of natural selection, subjecting a library of genetic variants to selective pressure in the laboratory. By introducing mutations in the gene encoding the enzyme, researchers can create a diverse range of enzyme variants, each with slightly different properties. These variants are then tested for their catalytic performance, and the best candidates are selected for further rounds of mutation and screening. Over several generations, the enzyme evolves to exhibit improved properties, whether its faster reaction rates, broader substrate specificity, or greater resistance to inhibitors or extreme conditions. Directed evolution has enabled the creation of highly efficient and robust enzymes for a wide range of industrial applications, from biofuel production to waste management.

Substrate engineering complements this by modifying the structure of the enzyme's substrate to achieve better compatibility and catalytic performance. Computational design plays a critical role by using bioinformatics tools and molecular modeling to predict beneficial mutations, allowing for rational and targeted improvements. Immobilization of enzymes on solid supports enhances their stability, reusability, and ease of separation from reaction mixtures, making processes more cost-effective and scalable. Lastly, structure-guided engineering utilizes detailed structural information of the enzyme to inform site-specific modifications, enabling precise enhancements in activity, selectivity, or resistance to harsh conditions. Together, these methods form a powerful toolkit for tailoring enzymes to meet specific functional demands in diverse applications.

Notable Examples of Engineered Biomolecular Catalysts⁴

1. Cytochrome P450 Enzymes in Drug Development and Toxicology

Cytochrome P450 enzymes (CYPs) are a family of enzymes that play a critical role in the metabolism of drugs and other xenobiotics in the liver. Their ability to oxidize organic compounds has made them invaluable in the pharmaceutical industry. However, natural P450s often have limited substrate specificity and poor stability outside their native environment. Researchers have successfully engineered P450 enzymes to overcome these limitations. For example, by using directed evolution, scientists have developed versions of these enzymes that can catalyze reactions with new substrates, improving the efficiency of drug metabolism and enhancing the production of high-value pharmaceutical intermediates. Additionally, these engineered P450s are now being used in the synthesis of complex compounds, including those with challenging stereochemistry, that would be difficult or impossible to create using traditional synthetic methods.



Figure 1: Enzyme Engineering Approaches

2. Polymerase Enzymes for DNA Synthesis

DNA polymerases are enzymes that play a central role in the replication of genetic material. The engineering of DNA polymerases has revolutionized biotechnology, especially in the realm of synthetic biology, where the demand for efficient and precise DNA synthesis is high. By optimizing DNA polymerases for better accuracy, processivity, and resistance to inhibitors, researchers have developed enzymes capable of synthesizing long strands of DNA with high fidelity, an essential step in gene synthesis, cloning, and genome editing. Notably, the development of thermostable polymerases, such as Taq polymerase, has enabled polymerase a chain reaction

(PCR), a widely used technique that has had a profound impact on fields ranging from medical diagnostics to environmental monitoring. Today, engineered polymerases are being further optimized to perform new functions, such as the synthesis of non-natural nucleotides or the incorporation of unnatural bases into DNA, which could open the door to creating novel genetic systems.

3. Laccase and Peroxidase Enzymes in Green Chemistry

Laccases and peroxidases are enzymes that catalyze the oxidation of a wide range of organic compounds. These enzymes have found use in green chemistry, particularly in the development of more environmentally friendly chemical processes. One notable example is the use of engineered laccases to degrade environmental pollutants, such as dyes and plastics, without the need for harsh chemicals or extreme conditions. In one of the cases, researchers engineered a laccase enzyme to break down lignin, a major component of plant biomass that is typically difficult to process. This modification could potentially improve the efficiency of biomass conversion in biofuels production, making it a cleaner and more cost-effective alternative to fossil fuels. Similarly, peroxidases have been engineered to catalyze the polymerization of phenolic compounds in the production of bioplastics, offering an eco-friendly alternative to petroleum-based plastics.

4. Metalloenzymes for Carbon Dioxide Reduction

One of the most exciting frontiers in engineered biomolecular catalysis is the reduction of carbon dioxide (CO₂) into valuable chemicals, a process that could play a critical role in combating climate change. Nature has evolved metalloenzymes, such as carbon monoxide dehydrogenases and hydrogenases, that catalyze CO₂ reduction, but these enzymes are often slow, inefficient, and difficult to engineer. Researchers are now engineering metalloenzymes⁵ to improve their catalytic efficiency and

selectivity for CO₂ reduction. One innovative approach involves the incorporation of artificial metal centers into the enzyme's structure, creating hybrid metalloenzymes with enhanced activity. These engineered catalysts could eventually be used in processes that convert CO₂ into fuels, plastics, or other useful chemicals, potentially transforming the way we deal with greenhouse gases.

5. Artificial Enzyme Catalysts: A Step Beyond Nature

While engineered enzymes are already making a significant impact, researchers are also pushing the boundaries by creating entirely artificial catalysts that combine the efficiency of enzymes with the versatility of synthetic chemistry. For example, designer enzymes made from small organic molecules or synthetic peptides are being developed to mimic enzyme-like activity, offering advantages such as tunability, stability, and resistance to harsh chemicals. One notable example is the development of artificial metalloenzymes, where synthetic ligands are incorporated into a protein scaffold to create a catalyst with the properties of both a biological enzyme and a metal catalyst. These hybrid catalysts are being designed to perform reactions that are difficult to achieve with either traditional enzymes or synthetic catalysts alone, opening up new possibilities in industrial chemistry.

The Future of Engineered Biomolecular Catalysts

As research in engineered biomolecular catalysts continues to advance, the potential applications are vast. In addition to the examples mentioned above, engineered enzymes hold promise for a wide range of industries, including food processing, environmental remediation, and energy production. The ability to fine-tune enzyme activity will allow for the development of highly efficient, sustainable, and cost-effective processes that could replace traditional chemical methods in many industries.

However, challenges remain. Firstly, the scalability of engineered enzyme reactions can sometimes be a hurdle, particularly when it comes to producing large quantities of a specific enzyme. Additionally, while engineered enzymes can exhibit remarkable properties, they often need to be optimized for industrial conditions, which can involve high temperatures, extreme pH levels, or the presence of toxic chemicals. Researchers are addressing these challenges by exploring new methods of enzyme stabilization, such as encapsulation or immobilization on solid supports.

Despite these challenges, the future of engineered biomolecular catalysts is undoubtedly bright. With advances in genetic engineering, computational modeling, and synthetic biology, the next generation of biomolecular catalysts promises to be even more efficient, adaptable, and versatile. Whether its reducing carbon emissions, creating sustainable biofuels, or designing new medicines, engineered enzymes will undoubtedly continue to be a driving force in shaping the future of chemistry.

REFERENCES

- 1.Renata, H.; Wang, Z. J.; Arnold, F. H. Expanding the Enzyme Universe: Accessing Non-Natural Reactions by Mechanism-Guided Directed Evolution Angew. Chem., Int. Ed. 2015, 54, 3351
- 2. Nastri, F., Chino, M., Maglio, O., Bhagi-Damodaran, A., Lu, Y. Lombardi, Design and engineering of artificial oxygen-activating metalloenzymes A. Chem. Soc. Rev. 2016, 45, 5020
- 3. Hilvert, D. Design of Protein Catalysts Annu. Rev. Biochem. 2013, 82, 447
- 4. Bren, K. L. Engineered Biomolecular Catalysts J. Am. Chem. Soc. 2017, 139, 14331–14334
- 5.Kosko R. M., Kuphal K. L., Salamatian A. A., Bren K. L. Engineered metallobiocatalysts for energyrelevant reactions *Curr. Opin. Chem. Bio.* 2024, 84, 10254

REVOLUTIONIZING GREEN CATALYSIS WITH DEEP EUTECTIC SOLVENTS: A SUSTAINABLE LEAP FORWARD

Dr. Ankita Chaudhary, Department of Chemistry, Maitreyi College

Introduction: Chemistry at a Crossroads

In view of the escalating demand for advanced sustainable technologies, chemistry is undergoing a profound transformation. A clear paradigm shift is underway—from traditional dependence on hazardous solvents and expensive metal-based catalysts toward greener, safer, and more environmentally responsible alternatives. One of the most groundbreaking innovations in green chemistry is the development of Deep Eutectic Solvents (DESs)—a

| Property | Deep Eutectic Solvents (DESs) | Ionic Liquids (ILs) |
|-----------------------|-------------------------------------------------------------------|--------------------------------------------------------|
| Definition | Mixtures of HBD and HBA forming a eutectic liquid at room temp | Salts composed entirely of ions, liquid below 100°C |
| Cost | Low-cost, generally made from readily available constituents | Expensive and often require multi-step synthesis |
| Preparation | Simple mixing and heating; no purification requires | Often need complex synthesis and purification |
| Tosicity | Generally low; many are biodegradable and non-toxic | Some ILs can be toxic and less biodegradable |
| Tunability | Easily tunable by selecting different HBD/HBA combinations | Highly tunable due to wide variety of cations/anions |
| Thermal Stability | Good thermal stability | Excellent thermal stability |
| Vapor Pressui †††† | e Negligible | Negligible |

new class of environmentally friendly liquids that has rapidly transformed the landscape of catalysis. These simple yet powerful mixtures are reshaping how we think about catalysis offering a cleaner and more sustainable approach to chemical processes.¹⁻³

What Are Deep Eutectic Solvents?

The term "Deep Eutectic Solvent" was coined by Abott and co-workers in 2003,⁴ and are formed by mixing two or more components, typically a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA).

Deep Eutectic Solvents are also known as deep eutectic ionic liquids (DEILs), low transition temperature mixtures (LTTMs), low melting mixtures (LMMs), all emphasising their unique physical properties. The interaction between HBD and HBA, produces a eutectic mixture with a melting point significantly lower than that of the individual constituents. Choline chloride, urea, glycerol and organic acids are amongst the commonly used components in DES, many of which are non-toxic, derived

from renewable resources and biodegradable. Although Ionic Liquids (ILs) and Deep Eutectic Solvents (DESs) share similar physical properties and applications, they are chemically distinct and belong to two separate classes of substances (Table 1).⁵

What sets DESs apart is not just their green origin, but their remarkable stability, low flammability, and ease of preparation. Majority of them can be made by simply heating and mixing the components, without the need for any purification steps. These characteristics make DESs ideal candidates for replacing conventional solvents in both academia and industrial set up.



Figure 1: Properties of Deep Eutectic Solvents.

DESs as Catalysts: A Chemical Game-Changer

Beyond their role just as green solvents, DESs are proving to be multifunctional agents that can also serve as catalysts. Their ionic nature and ability to undergo extensive hydrogen-bonding permit them to stabilize the reaction intermediates, enhance the solubility of polar compounds as well as act as Brønsted or Lewis acids or bases, based on their composition. This role of simultaneously as solvent and catalyst significantly reduces the usage of chemicals in a reaction thereby minimizing waste and simplifying process design. Due to burgeoning environmental consciousness, Deep Eutectic Solvents (DESs) have emerged as viable candidates for sustainable and eco-friendly alternatives in catalysis owing to their various advantages like easy reproducible preparation, inexpensive, environmentally benign nature, wide liquid range, excellent thermal stability, negligible vapour pressure, recyclability, and adjustable properties.⁶ One of the most exciting aspects of DESs is their tunability; by adjusting the HBD and HBA; researchers can design task-specific DESs tailored for specific chemical transformations, thereby opening the door to a wide array of industrial applications such as biosensor development, extraction process, electrochemistry, biocatalysis, food analysis, gas capture, pharmaceutical industry etc.⁷⁴⁰

Conclusion: A New Era in Catalysis

DESs are ushering in a new era of green catalysis by fusing sustainability, safety, and efficiency. DESs have the potential to become a fundamental component of sustainable chemistry as research and industry applications expand, transforming not just what we synthesize but also the process.

REFERENCES

1. Chaudhary, A. Odyssey of Deep Eutectic Solvents as Sustainable Media for Multicomponent Reactions: An Update. Mini Rev. Org. Chem., 2022, 19, 156-189.

2. Liu, P.; Hao, J-W.; Mo, L-P.; Zhang, Z-H. Recent advances in the application of deep eutectic solvents as sustainable media as well as catalysts in organic reactions. RSC Adv., 2015, 5(60), 48675 48704.

3. Longo, L.S., Jr; Craveiro, M.V. Deep eutectic solvents as unconventional media for multicomponent reactions. J. Braz. Chem. Soc., 2018, 29, 1999-2025.

4. Abbott, A.P.; Capper, G.; Davies, D.L.; Rasheed, R.K.; Tambyrajah, V. Novel solvent properties of choline chloride/urea mixtures. Chem. Commun. (Camb.), 2003, (1), 70-71.

5. Abbott, A.P.; Barron, J.C.; Ryder, K.S.; Wilson, D. Eutectic-based ionic liquids with metal-containing anions and cations. Chem., 2007, 13(22), 6495-6501.

6. Yeow, A.T.H.; Hayyan, A.; Hayyan, M.; Junaidi, M.U.M.; Saleh, J.; Basirun, W.J.; Nor, M.R.M.; Abdulmonem, W.-Al; Salleh, M.Z.M.; Zuki, F.M.; Hamid, M.D. A comprehensive review on the physicochemical properties of deep eutectic solvents, Results Chem., 2024, 7, 101378.

7. Smith, E.L.; Abbott, A.P.; Ryder, K.S. Deep Eutectic Solvents (DESs) and Their Applications. Chem. Rev., 2014, 114, 21, 11060–11082.

8. Svigelj, R.; Dossi, N.; Grazioli, C.; Toniolo, R. Deep eutectic solvents (DESs) and their application in biosensor development. Sensors (Basel), 2021, 21(13), 4263.

9. Wu, J.; Liang, Q.; Yu, X.; Lü, Q-F.; Ma, L.; Qin, X.; Chen, G.; Li, B. Deep eutectic solvents for boosting electrochemical energy storage and conversion: A review and perspective. Adv. Funct. Mater., 2021, 31(22), 2011102.

Photocatalysis is a process that converts light energy into chemical energy using photocatalysts.' Sources of this energy include sunlight, UV radiation, and visible light. When photons with energy equal to or greater than the band gap (BG) of the photocatalyst interact with the material, they generate electron (e⁻) and hole (h⁺) pairs.² The excitation of electrons facilitates their movement from the valence band (VB) to the conduction band (CB), enabling oxidation and reduction reactions on the photocatalyst's surface to degrade contaminants. For effective photocatalysis, these redox reactions must occur simultaneously. In this process, a catalyst is activated by light to accelerate a chemical reaction without undergoing permanent changes itself. Exposure to radiation reduces the activation energy required for the primary reaction, allowing semiconductor materials to initiate oxidation-reduction processes.

1. Photocatalytic Materials

Photocatalysis, a process where light initiates chemical reactions on a catalyst's surface, has gained significant attention due to its applications in environmental remediation, energy conversion, and the production of value-added compounds. Although photocatalytic activity is observed in various materials, semiconductor-based photocatalysts have been the most extensively studied. Below are some key photocatalytic materials and their properties.

FROM SUNLIGHT TO SUSTAINABILITY: UNDERSTANDING PHOTOCATALYSIS

Dr Rajni Johar Chhatwal Department of Chemistry, Maitreyi College

1.1 Titanium Dioxide (TiO₂)

Titanium dioxide (TiO₂) is one of the most widely researched photocatalysts due to its stability, affordability, and non-toxic nature.³

Titanium dioxide (TiO_2) is widely regarded as the "gold standard" among photocatalysts due to its affordability, non-toxicity and remarkable chemical stability. It exists in three crystalline forms: anatase, rutile, and brookite exhibiting the highest photocatalytic efficiency.

Over the past two decades, TiO_2 based photocatalysis has gained significant attention for applications such as splitting water to generate hydrogen (H₂) using solar energy and degrading pollutants in air and water, even at low concentrations.⁵

Despite considerable progress in TiO2-based photocatalysis, many fundamental questions remain unanswered. With a bandgap of approximately 3.2 eV, TiO2 absorbs UV light, generating electronhole pairs that drive redox reactions on its surface.⁸ However, its high bandgap limits its functionality to the UV spectrum, reducing its effectiveness under visible light. Mechanisms of TiO₂ photocatalysis include charge carrier generation, separation, transfer, recombination, transportation, and bond formation/breaking for developing advanced photocatalysts optimizing and photocatalytic processes."

1.2 Zinc Oxide (ZnO)

Zinc oxide (ZnO) is another semiconductor material with a relatively large bandgap (~3.37 eV), making it efficient in absorbing UV light. Similar to TiO₂, ZnO produces electron–hole pairs upon light exposure, triggering photocatalytic reactions. It is known for its high photocatalytic activity, biocompatibility, and transparency, making it ideal for applications in wastewater treatment and biomedical engineering.

1.3 Tungsten Trioxide (WO₃)

Tungsten trioxide (WO₃) is a transition metal oxide photocatalyst with a narrower bandgap (~2.5 eV) than TiO_2 and ZnO, allowing it to absorb a wider range of light, including visible light. This characteristic enhances its photocatalytic efficiency. WO₃ based photocatalysts have been explored for various uses, including solar energy conversion, pollutant degradation, and water splitting.

1.4 Bismuth Vanadate (BiVO₄)

Bismuth vanadate ($BiVO_4$) is an emerging photocatalyst that efficiently absorbs visible light, with a bandgap of about 2.4 eV. It offers high photochemical stability and superior quantum efficiency under visible light irradiation, making it a promising material for applications such as pollutant degradation, CO_2 reduction, and water oxidation.

2. Photocatalytic Processes

Photocatalytic processes involve the use of light to initiate chemical reactions on a photocatalyst's surface.⁴ When photons with energy equal to or greater than the bandgap of the photocatalyst are absorbed, electron-hole pairs are generated, leading to redox reactions with surrounding molecules. These excited charge carriers can drive a variety of chemical transformations, such as breaking down organic pollutants, producing hydrogen from water, and converting CO_2 into valuable compounds.

The key advantages of photocatalytic processes include high efficiency, mild reaction conditions, and environmental sustainability, making them promising for applications in renewable energy, green chemistry, and environmental cleanup.⁶ Current research aims to optimize photocatalytic efficiency by developing advanced materials, refining reaction mechanisms, and expanding their applications across multiple industries.

2.1 Homogeneous Photocatalytic Process

A photocatalytic system is classified as homogeneous when both the catalyst and reactants exist in the same phase, either gas or liquid. One widely studied homogeneous photocatalytic reaction involves the Fe^{2+}/H_2O_2 system, such as ozone and photo-Fenton reactions. The efficiency of Fenton-type processes is influenced by several factors, including pH, UV light intensity, and hydrogen peroxide concentration. A key advantage of these systems is their ability to utilize sunlight instead of costly UV lamps and electrical energy. However, a major limitation is the requirement for low pH conditions, as iron tends to precipitate at higher pH levels, necessitating an additional step for iron removal after treatment.

2.2 Heterogeneous Photocatalytic Process

In heterogeneous photocatalysis, the catalyst and reactants exist in different phases, typically a solid or powdered catalyst suspended in a liquid reaction mixture. A well-known example is the TiO_2/UV system, which has gained significant attention. Heterogeneous photocatalysis is widely used in applications such as water purification, metal deposition, hydrogen transfer, dehydrogenation, oxidation reactions, and the elimination of gaseous pollutants. The majority of heterogeneous photocatalysts are composed of semiconductor oxides and transition metals due to their superior catalytic properties.

The mechanism of heterogeneous photocatalysis involves oxidation and reduction reactions occurring on the photocatalyst's surface. The band gap, which represents the energy difference between the conduction band (the lowest unoccupied electron level) and the valence band (the highest occupied electron level), plays a crucial role in this process. When photons with energy equal to or greater than the band gap strike the semiconductor, electrons in the valence band become excited and transition to the conduction band within femtoseconds. This excitation generates electron charge carriers and holes, where the holes themselves act as active sites for oxidation. If the electron–hole pairs remain separated by trapping on the semiconductor surface, recombination is minimized, allowing for effective photocatalytic reactions^[10].



3. Solar Energy Production and Photocatalysis

The sun functions as a natural nuclear reactor, emitting small energy packets called photons. These photons carry vast amounts of energy, sufficient to meet most of the world's energy demands. In solar energy conversion, various photocatalytic materials are used in solar cells to absorb photon energy and generate electricity.⁷ Different types of solar cells have been developed to capture sunlight efficiently, including dyesensitized, organic, photoelectrochemical, and hybrid solar cells.

Photocatalytic technologies are widely recognized as a promising solution for addressing environmental challenges and energy shortages. Among these technologies, metal halide perovskites (MHPs) have emerged as a novel class of photocatalysts. MHPs exhibit broad visible-light absorption, low exciton binding energy, high photoluminescence quantum yield, rapid carrier transfer, and an adjustable band gap. These properties make them highly effective for solar energy conversion. However, their limited stability, high recombination rates of
photogenerated carriers, and insufficient active sites pose significant challenges for practical applications. To overcome these limitations, researchers have explored various design strategies to enhance the performance and durability of MHP-based photocatalysts^{[12].}

4. Wastewater and Drinking Water Treatment via Photocatalysis

Photocatalysis is a relatively new and highly promising technique for treating various contaminants in wastewater, especially those containing toxic and reactive organic compounds that conventional treatment methods struggle to remove. In recent decades, the quality of water sources has deteriorated due to increasing pollution from emerging organic pollutants and persistent inorganic and organic substances. Conventional drinking water and wastewater treatment technologies are often ineffective against these contaminants, prompting researchers to seek alternative, cost-effective, and efficient solutions.

The mechanism of photocatalytic water treatment primarily relies on the generation of electron-hole pairs when TiO_2 particles are exposed to UV light (wavelength < 400 nm). This photonic excitation leads to the formation of electron-hole pairs (e⁻/h⁺) by exciting electrons from the valence band to the

conduction band, leaving behind positively charged holes. The subsequent oxidative-reductive reactions occurring on the photocatalyst's surface drive the degradation of pollutants and disinfection of water.

REFERENCES

1. Fujishima, A., & Honda, K. Electrochemical photolysis of water at a semiconductor electrode. Nature 1972, 238, 37–38.

2. Hashimoto, K., Irie, H., & Fujishima, A. TiO₂ photocatalysis: A historical overview and future prospects. Jpn. J. Appl. Phy., 2022, 44(12), 8269–8285.

3. Chen, X., & Mao, S. S. Titanium dioxide nanomaterials: Synthesis, properties, modifications, and applications. Chem. Rev., 2007, 107(7), 2891–2959.

4. Chong, M. N., Jin, B., Chow, C. W. K., & Saint, C. Recent developments in photocatalytic water treatment technology: A review. Water Res., 2010, 44(10), 2997–3027.

5. Pelaez, M., Nolan, N. T., Pillai, S. C., Seery, M. K., Falaras, P., Kontos, A. G., ... & Dionysiou, D. D. (2012). A review on the visible light active titanium dioxide photocatalysts for environmental applications. Appl. Catal. B: Environ., 2012, 125, 331–349.

6. Hoffmann, M. R., Martin, S. T., Choi, W., & Bahnemann, D. W. Environmental applications of semiconductor photocatalysis. Chem. Re., 1995, 95(1), 69–96.

7. Kudo, A., & Miseki, Y. (2009). Heterogeneous photocatalyst materials for water splitting. Chem. Soc. Rev., 2009, 38(1), 253–278.

8. Kumar, S. G., & Devi, L. G. Review on modified TiO₂ photocatalysis under UV/visible light: Selected results and related mechanisms on interfacial charge carrier transfer dynamics. J. Phys. Chem. A, 2011, 115(46), 13211–13241.

9. Osterloh, F. E. Inorganic materials as catalysts for photochemical splitting of water. Chem. Mater., 2013, 20(1), 35–54.

10.Tang, J., Durrant, J. R., & Klug, D. R. Mechanism of photocatalytic water splitting in TiO₂: Surface kinetics and charge carrier dynamics. J. Am. Chem. Soc., 2008, 130(42), 13885–13891.

11. Schneider, J., Matsuoka, M., Takeuchi, M., Zhang, J., Horiuchi, Y., Anpo, M., & Bahnemann, D. W. Understanding TiO₂ photocatalysis: Mechanisms and materials. Chem. Rev., 2014, 114(19),9919–9986.

12. Wang, Q., & Domen, K. Particulate photocatalysts for light-driven water splitting: Mechanisms, challenges, and design strategies. Chem. Rev., 2020, 120(2), 919–985.

UNRAVELING THE MYSTERY: BEYOND THE GENETICS Dr. Nishu, Department of Chemistry, Maitreyi College

I was in 11th standard when for the first time I had seen twin sisters who got new admission in my class. I was wondered to see them; how can one look identical to another just like a carbon copy to each other. Their faces were round, freckled, and had high cheekbones with the outer edge of the eye tilted slightly downward. However, the contrasts were also notable. Like a rush of wind in a tunnel, Shikha's activity and mercurial temper rose quickly and dissipated abruptly. Rajni had a cunning physique, but his mind was more daring. She had greater wit, a sharper tongue, and more agile mind. Shikha was companionable and sociable. She was boisterous to insults. Rajni was reserved, calm, and more fragile. I am pretty sure!! you must be thinking "why identical twins behave so distinct even after sharing same set of genes?" Next, have you ever pondered about why certain people's get particular disease, while others not? Does it have any significance at what age we are; certainly, as one can prone to attack by diseases at any times. Don't you ask to yourself if Our body's cells all share the same genome, then how does one become a skin cell, muscles cell and another a liver cell, which differs greatly in appearance and function? "Science is fun. Science is curiosity. We all have natural curiosity. Science is a process of investigating. It is posing questions and coming up with a method. It is delving in" Sally Ride said.

Although these seem suspicious, the enigma behind them was a hot topic in the discipline of research. Scientists were astounded until the 1940s, when English embryologist Conrad Waddington came up with the innovative theory that cells acquired their identities by enabling nature (genes) to be modified by nurture (environmental cues), just like humans do. According to him, a cell must contain an extra layer of information that hung, ghostlike, above the genome. The cell's "memory" would be stored in this layer. He termed this phenomenon as "epigenetics" means "above of genetics".

Let us first understand what actually 'genetic' means. With increased awareness and easily accessible knowledge, most of us are well familiar with the term DNA, 'The blueprint of life'. DNA stores genetic information and genes are the segment of the DNA. Genetics arose from the identification of genes, the fundamental units responsible for heredity. The study of genetics helps us to understand how genes and traits are passed across generation. For example, children look like their parents usually because they have inherited the genes from their parents. Modern genetics focuses on the chemical substance and the ways in which it affects the chemical reactions that constitute the living processes within the cell. Gene action depends on interaction with the environment. For example, green plants have genes that contain the information needed to synthesize the photosynthetic pigment chlorophyll which gives them their green color. Chlorophyll is synthesized in the presence of light (photosynthesis) because the gene for chlorophyll is expressed only when it interacts with light. Otherwise, when a plant is placed in the complete absence of light, chlorophyll synthesis stops because the gene is no longer expressed.' Now, coming to the 'epigenetics' part, a consensus definition of 'epigenetics' came across as the study of heritable changes in gene expression without bringing any alteration in the underlying DNA sequence of the organism. Unlike genetics, epigenetics describes passing on the way the genes are used from generation to generation. A substantial body of research has emerged over the past few decades that demonstrates how different exogenous factors, including life

CHEMZONE 2025

experiences, behaviors, and stresses, can significantly affect longevity and health span. Thereby, plays a crucial role in development of diseases including cardiovascular diseases, cancer, diabetes, and chronic respiratory syndromes together which is responsible for around 70% of deaths worldwide. No doubt, these adverse effects can also be inherited in human beings, however, epigenetics is the most potent to control this behavior without hampering the individual's DNA sequence.² Actually, epigenetic changes can turn 'on' and 'off' the gene just like we do with switches and as we know that, when the switch is in the 'on' position, it allows the electricity flow and if it is 'off' then there is no flow of electricity. By turning switch 'on' and 'off' of the gene, epigenetic simply control the transcription machinery of DNA.

Hence, we conclude that the epigenetic play a substantial role in transcription of certain genes. Actually, genes are labelled with small chemical tags like methyl, acetyl and phosphoryl group etc. which act like switches hanging on wire (i.e. gene). And this chemical tag decides the fate of gene to be expressed or not. For example, like a methyl group, inhibits the gene expression by turning 'off' the gene where the gene is still there, but it is silent and consequently, altered the translation machinery.³

Utmost importance has been given to the epigenetics owing to its involvement in various cellular processes. With the increasing interest in epigenetics, technological progress has taken place, which makes it possible to do massive epigenetic studies. And come across with the two most popular epigenetic modification which are common in humans that are DNA methylation and histone modification. The epigenetic modifications involve a chemical alteration of DNA and associated proteins without altering the underlying sequence. Epigenetic modifications are responsible for the neurological and neurodevelopment diseases, autoimmune or inflammatory disease and the maintenance and development of cancer. Chronic psychosocial stress, a hallmark of modern and fast-paced societies not only affects health but also directly upsets our body physiology, contributing to negative outcomes. Yet, the impact of these risk factors varies person to person and gaining insights into how life stories shape the individual health outcomes which can contribute to better-targeted and personalized interventions. Several literature sources support the fact that epigenetic modification can be influenced by environmental factors such as diet, stimuli, inflammation, age, smoking etc. which control the gene expression, influence the various gene functions. As a result, the environmental conditions and inherited genome are interconnected with each other.⁴

My part in this story

In our lab, my work is to determine the effect of epigenetic modification in the gene promoter region. I started my journey with the investigation of G-rich sequence found in gene promoter region. Using bioinformatics tools, I was able to deduce the multiple sequence alignment, phylogenetic tree, transcription factor of the gene and its location. The characterization of the Grich DNA sequence was carried out using various biophysical and biochemical technique such as native polyacrylamide gel electrophoresis (PAGE), Circular dichroism (CD), CD melting and UV thermal melting experiments. In our result, we have concluded that the DNA methylation which introduced at the fifth position of cytosine residue does not make any structural differences as compared to the non-methylated DNA sequence. However, our study found that the thermal stability of the methylated DNA sequence a new dimension to our understanding of transcriptional regulation. Nonetheless, further research will be required to understand how abnormalities of the methylation machinery lead to disease states and what components of this machinery will be appropriate targets for therapeutic intervention. Once we learned how our epigenome influences us, we surely learn how to influence it.

REFERENCES

1. Handy, D. E., Castro, R., & Loscalzo, J. Epigenetic modifications: basic mechanisms and role in cardiovascular disease. Circ., 2011, 123(19), 2145-2156.

2. Berger, S. L., Kouzarides, T., Shiekhattar, R., & Shilatifard, A. An operational definition of epigenetics. Genes Dev. 2009, 23(7), 781-783.

3. Landgrave-Gómez, J., Mercado-Gómez, O., & Guevara-Guzmán, R. Epigenetic mechanisms in neurological and neurodegenerative diseases. Front. Cell. Neurosci. 2015, 9, 58.

4. Ari, G., Cherukuri, S., & Namasivayam, A. Epigenetics and periodontitis: a contemporary review. Journal of clinical and diagnostic research: JCDR 2016, 10(11), ZE07.

A NEW PARADIGM IN WASTEWATER TREATMENT: THE CARBON QUANTUM DOT APPROACH

DR GAZALA RUHI DEPARTMENT OF CHEMISTRY, MAITREYI COLLEGE

The population growth, the technological advancements, the omnipresence of complex and diverse pollutants has burdened the conventional waste water treatment approaches and hence emphasized the necessity to develop advanced remediation technologies. Pollutants like synthetic dyes such as Reactive Blue 222 (RB 222), Reactive Yellow 145 (RY 145) etc. are of critical concern due to their complex molecular structures, stability in aqueous media, and resistance to conventional biological degradation. A sustainable and efficient wastewater treatment approach would be to harness the photocatalytic properties of the nanostructured semiconducting materials for the degradation of such pollutants. The carbon Quantum Dots (CQDs) and their novel composites have recently gained attention as potential alternatives, tailored for visible-light-driven degradation of azo dyes.¹ CQDs have intrigued researchers by placing themselves as a fascinating category of nanomaterials (size smaller than 10nm), exhibiting exceptional chemical stability, biocompatibility and photocatalytic properties. Their synthesis route has been broadly classified into the bottom-up approach (microwave assisted, hydrothermal or solvothermal carbonization of organic precursors like simple fruits and vegetable peels) and the top-down approach (fragmentation or exfoliation of carbon sources like graphite or carbon nanotubes).

An interesting research work of green synthesis of CQDs and its composites from waste mango peels fruit subjected to hydrothermal carbonization results into the formation of functionalized tiny carbon particles having plethora of carboxylic and hydroxyl groups.² The presence of these functional groups imparts colloidal stability and induces hydrophilicity for favorable binding to metal oxide surfaces for efficient photocatalytic interactions. The synthesized CQDs were spherical particles of 1-4nm size with thermal robustness up to 800°C. As a novel approach, cobalt substitute zinc ferrite nanoparticles (CZF) having good photodegradation efficiency to reactive azo dyes were coated with CQDs to form CZF@CQDs nanocomposites with enhanced properties.

An electrostatic interaction occurs between the cations adsorbed on the CZF surface and the anionic carboxylate ions from the carbon quantum dots (CQDs). The The CZF@CQDs nanocomposites shows interesting mechanism of the photodegradation of azo dyes. CZF when coated with the carbon quantum dots and irradiated with visible light, excitons (e- and H^+ pairs) are formed over CZF nanodots. During this, transfer of electrons from the conduction band to CQDs happens leaving holes in the valence band. The parallel upconversion causes carbon quantum dots to absorb visible light of longer wavelengths (between 450-700 nm) and emit shorter wavelengths of light. This stimulates the cobalt substitute zinc ferrite nanoparticles (CZF) to create electrons and h+ pairs. The rapid excitation and recombination enhance the photocatalytic activity. The e/H⁺ pairs react with oxidants or reducers to form $\cdot O_{2-}$, $\cdot OH$, which cause photodegradation of the azo dye by breaking the azo bond (-N=N-).

The electrophilic breakage chromophore azo bond (-N=N-) of the dye by the CZF@CQDs photocatalyst causes fast decolorization of the dye solution. The fast photocatalytic degradation is basically due to the high surface area of the composites. This includes the small crystal size as and well populated active sites on the surface of the catalyst. The generation of huge number of \cdot OH and \cdot O₂- radicals facilitate easy oxidation or reduction of azo bonds.

REFERENCES

- I. Manikandan, V. & Lee, N. Y. Green synthesis of carbon quantum dots and their environmental applications. Environ. Res., 2022, 212, 113283.
- 2. Malitha, D. Molla, T. H. Bashar, A. Chandra, D & Ahsan, S. Fabrication of a reusable carbon quantum dots (CQDs) modified nanocomposite with enhanced visible light photocatalytic activity. Sci. Rep., 2024, 14.17976.

THE PHOTOCATALYST REVOLUTION: LIGHT ACTIVATED REMEDIATION OF ORGANOCHLORINE PESTICIDES

DR. HEMA BHANDARI

DEPARTMENT OF CHEMISTRY, MAITREYI COLLEGE

In an era where clean water is becoming an environmental safety is under threat, scientists are urgently exploring ways to undo the damage caused by decades of pesticide use. Organochlorine pesticides (OCPs)-a class of chemicals once widely used to protect crops and control diseases, but now recognized as hazardous pollutants. Despite being banned in many regions, OCPs like DDT, aldrin, and endosulfan continue to linger in our soil, water, and even human tissues. Their resilience makes them both dangerous and difficult to remove. However, a bright solution is emerging quite literally from sunlight.

As we know that OCPs still a problem as these pesticides are known for their chemical stability, low water solubility, and high fat solubility, allowing them to remain in the environment for decades. These properties also lead to bioaccumulation in the food chain, affecting fish, birds, and humans alike. People exposed to these pesticides, whether through contaminated water or food face a host of health issues ranging from hormonal imbalance and cancer to neurological disorders. However, surprisingly, these chemicals are still used in some parts of the world due to their low cost and effectiveness, despite international agreements like the Stockholm Convention that aim to restrict them.

The Need for New Solutions

Traditional water treatment methods such as filtration, oxidation, and biological degradation have failed to eliminate OCPs completely or safely. This is where photocatalysis steps in as a revolutionary technique. Unlike older methods, photocatalysis uses light-activated materials to break down harmful chemicals into harmless byproducts. What makes this technique truly exciting is that it can work under visible light, including sunlight, making it both eco-friendly and cost-effective.

Photocatalysts used in degradation of Organo chlorine pesticides

Photocatalysis involves using special materials such as nanomaterials like titanium dioxide (TiO_2) or zinc oxide (ZnO) that absorb light and generate reactive species. These reactive molecules then attack and dismantle the chemical bonds in OCPs, transforming them into non-toxic compounds.¹⁻⁴

In order to improve efficiency, researchers have developed heterojunction structures and metal-doped photocatalysts that respond better to visible light and prevent electron-hole recombination, a common problem that limits degradation efficiency. Scientists have successfully degraded a variety of OCPs using sunlight-driven photocatalysis: for example, Lindane was broken down by zero-valent iron and nitrogen-doped TiO_2 with up to 100% efficiency.⁵ DDT, one of the most infamous pesticides, showed over 90% degradation in just a few hours using nickel-iron nanoparticles.⁶ Endosulfan and dicofol were reduced by more than 80% with nanocomposites like MoS_2/ZnS and ZnO under visible light⁷ Methoxychlor, chlordane, heptachlor, and endrin have all shown measurable degradation using tailored photocatalytic systems and microbial processes.

Environmental and Global Impact

The presence of OCPs in lakes, rivers, and drinking water across continents from India to Argentina to Australia underscores the global scale of pesticide pollution. Bioaccumulation of these toxins has been recorded in marine animals, food supplies, and even breast milk, sparking alarm among health experts and environmentalists alike. Countries like China and India top the charts in pesticide consumption, while developed nations like France and Germany are actively investing in research for remediation technologies.

The Promise and the Challenges

Visible-light photocatalysis is not just a lab-based dream it holds real promise for communities in need of affordable, sustainable water treatment. However, some challenges remain. High material costs, limited large-scale deployment, and inconsistent sunlight availability in some regions need to be addressed.

Hence the Future research is focusing on the following points:

- Designing more efficient photocatalysts using eco-friendly methods.
- Exploring low-cost materials for mass production.
- Targeting under-researched pollutants such as chlorophenol and pentachlorophenol.
- Developing hybrid technologies combining photocatalysis with other treatment methods.

Conclusion

The world is in urgent need of solutions that not only treat pollution but do so without harming the planet further. Photocatalysis offers a light-powered path forward, using the sun's energy to destroy toxins that once seemed indestructible. By continuing to invest in this green technology, we can aim for a future where clean water is a right, not a privilege and where past mistakes are corrected with the brilliance of modern science.

REFERENCES

- 1.M.B. Tahir, N.R. Khalid, Carbonaceous-TiO2 nanomaterials for photocatalytidegradation of pollutants: A review, Ceram. Int., 2017.
- 2. Yasmina, M., et al., Treatment heterogeneous photocatalysis; Factors influencing the photocatalytic degradation by TiO2., 2014.
- 3.Y.S. El-Temsah et al., DDT degradation efficiency and ecotoxicological effect of two types of nano-sized zerovalent iron (nZVI) in water and soil, Chemosphere, 2016, 144, 2221–2228.
- 4.H.J. Jung et al., Enhanced photocatalytic degradation of lindane using metal semiconductor Zn@ZnO and ZnO/Ag nanostructures, J. Environ. Sci. (China) 2018, 74, 107–115.
- 5. Wafi, A., Roza, L., Timuda, G.E. et al. N-doped TiO2 for photocatalytic degradation of colorless and colored organic pollutants under visible light irradiation. Transit Met Chem 2024, 49, 305–317.
- 6.H Tian, Jinjun Li, Z Mu, L Li, Z. Hao, Effect of pH on DDT degradation in aqueous solution using bimetallic Ni/Fe nanoparticles, Separation and Purification Technology, 2009, 66, 1, 84-89.
- 7.H. Tyagi, H Chawla, H Bhandari, S.Garg, Recent-enhancements in visible-light photocatalytic degradation of organochlorines pesticides: A review, Materials Today: Proceedings, 2022, 49, 8, 3289-3305.

CRITICAL ROLE OF ECO-FRIENDLY H₂O₂ CATALYST IN WASTEWATER TREATMENT

DR. NAVNEET KISHORE DEPARTMENT OF CHEMISTRY, MAITREYI COLLEGE

As we all know, the problem of water pollution is very serious. Our entire ecosystem is affected when water gets polluted. Organic waste products play a very significant role in contaminating water. Therefore, the breakdown of these organic pollutants has become very urgent. The elimination of these pollutants will surely enhance the quality of both water and environment. Many methods have been adopted time to time for the destruction of these harmful pollutants. The devastation through oxidation has proved to be extremely effective. There are several oxidation processes reported in the literature with different reagents and reaction condition to oxidise these pollutants. The ecofriendly chemical entity, hydrogen peroxide (H2O2) played very extensive role in the degradation of pollutant. H2O2 extensively used with Fe2+ ions in the generation of free radical species, popularly known as Fenton reagent. Metal ions activate H2O2 to the free radicals which depends on metal used. These generated free radicals are also known as reactive oxygen species (ROS). The Fenton reaction is mainly associated with the generation of extremely high reactive •OH free radical. It has strong capability to degrade all the organic contaminants mentioned in the given Figure.



Figure: Key pollutant species degraded by H2O2 through oxidation process

The use of H2O2 in various oxidation process becomes a part of extended sustainable future catalysis. The H2O2 is considered as ecofriendly because it gives water and oxygen on decomposition. Moreover, the generation of insitu and ex-situ is possible in various process which are involved in water purification catalysis. The activation of H2O2 is carried out either by the metals or in the presence of sunlight/UV light. There are some reactions mentioned below which showed the generation and decomposition process of H2O2. This property of H2O2 makes unique among other environmentally sustainable catalysts.



Figure: General reactions involved in generation and breaking of H2O2

In conclusion, recently more than 400 research articles have been published which involve the role of hydrogen peroxide in oxidation process. Hence, H2O2 is the centre of attraction in various oxidation process in present of iron and few other metals. These processes are termed as the advanced oxidative process which deteriorate the harmful water pollutant during waste water treatment. These new finding leading towards the insightful techniques for the water purification. Therefore, we can say that if such research work continues, then soon we will get rid of polluted water.

REFERENCES

· I. Ao Z., Sun H., Fullana A. Editorial: Environmental Catalysis and the Corresponding Catalytic Mechanism. Front. Chem., 2019, 7, 75.

2. Rigoletto M., Laurenti E., Tummino M.L. An overview of environmental catalysis mediated by hydrogen peroxide. Catalysts, 2024, 14, 267.

3. Sheng B., Deng C., Li Y., Xie S., Wang Z., Sheng H., Zhao J. In-situ hydroxylation of a single-atom iron catalyst for preferential $_1O_2$ production from H₂O₂. ACS Catal. 2022, 12, 14679-14688.

4. Tabanelli T., Cespi D., Cucciniello R. Sustainable and environmental catalysis. Catalysts, 2021, 11, 225.

5. Zhu Z-S., Zhong S., Cheng C., Zhou H., Sun H., Duan X., Wang S. Microenvironment engineering of heterogeneous catalysts for liquid-phase environmental catalysis. Chem. Rev. 2024, 124, 11348-11434.

a unique non-steroidal anti-inflammatory drug

with antimicrobial activity against Trichophyton, Microsporum and Epidermophyton species Flurbiprofen, a unique non-steroidal anti-inflammatory drug with antimicrobial activity against Trichophyton, Microsporum and Epidermophyton species

Articles from Young Minds

| S. No. | Theme | Authors |
|--------|-----------------------------------------------------------------------------------------------|------------------------------------------------|
| I. | MULTIPHASE CATALYST | TANNU III YEAR |
| 2 | COMPUTATIONAL CATALYSIS AND SIMULATION | ISHITA BHADANA III YEAR |
| 3. | GREEN CATALYSIS: HOD OF OUR HOPE TOWARDS SUSTAINABILITY | BHARTI MAHAJAN I YEAR |
| 4. | RECENT ADVANCES IN TRANSITION METAL CATALYSIS | ANISHA DEDHA, I YEAR SHWETA YADAV, III YEAR |
| 5. | GREEN CATALYSIS AND SUSTAINABILITY | SHWETA YADAV III YEAR |
| 6. | ELECTROCATALYSIS: POWERING THE FUTURE OF RENEWABLE ENERGY | TANISHA CHOUDHARY II YEAR |
| 7. | DIVING INTO THE REALMS OF BIOCATALYSIS AND ENZYMES REACTION | SAANVI MISHRA I YEAR |
| 8. | NANOMATERIALS IN CATALYSIS REVOLUTIONIZING SUSTAINABLE ENERGY AND GREEN CHEMISTRY | KAMAKSHI SEHGAL II YEAR |
| 9. | CATALYSIS IN INDUSTRIAL PROCESSES | STUTI SHARMA II YEAR |
| ю. | GREEN HYDROGEN: NEED FOR CATALYST?? | NIVEDITA II YEAR |

Multiphase Catalyst

TANNU B.Sc. (Hons) Chemistry, III Year

In pharmaceutical and high-quality chemical industries, catalytic multiphase reactions have become increasingly critical due to their significant impact on modern manufacturing processes and the production of high-value chemicals. Traditional pharmaceutical synthesis focused mainly on efficiency, with limited attention given to reactor design and environmental sustainability. However, conventional synthetic routes for approved drugs often generate considerable waste and employ toxic reagents, which pose both safety and environmental risks.³

The increasing demand for more environmentally friendly and safer chemical processes has underscored the advantages of multiphase catalysis. These systems offer improved efficiency and are better suited to meet the growing regulatory pressure for sustainable practices. Many pharmaceutical manufacturing routes involve high molecular weight and thermally unstable intermediates. To make these processes commercially viable, catalysts with high activity and selectivity, along with simplified product separation, are essential.

Recent trends have introduced novel catalytic structures, including homogeneous and heterogeneous catalysts, organometallic complexes, supported metal catalysts, and organic catalysts. Advances in tandem synthesis, the development of new ligands for asymmetric catalysis, and the heterogeneous immobilization of homogeneous catalysts have significantly improved overall catalytic performance and environmental compatibility.³

Multiphase reactions—whether solid-liquid, liquid-liquid, or gas-liquid—are vital in enabling efficient transformation pathways. Catalysts are central to these systems, especially when dealing with poorly soluble reactants or products. Among them, heterogeneous catalysts incorporating chiral metal complexes are poised to play a key role in the future of the pharmaceutical industry.

Homogenous catalytic reactions

Homogeneous catalysts are essential in the synthesis of fine chemicals, pharmaceuticals, and materials. However, their large-scale industrial application is often hindered by challenges in catalyst separation and recycling. To address these issues, significant progress has been made in the development of multiphase catalysis strategies over the past decade. These approaches not only resolve separation challenges but can also enhance catalyst performance while offering environmental benefits.

Key drivers of recent advancements in homogeneous catalysis include:

- I. Environmentally Friendly Processes: The potential to develop greener synthetic pathways under milder conditions with high selectivity and catalytic activity.
- 2. Versatile Reaction Scope: Homogeneous catalysis enables a wide range of chemical transformations such as carbonylation, hydroformylation, amination, epoxidation, hydrogenation, C–C coupling reactions, and oxidation. These catalytic routes often outperform traditional stoichiometric or less selective methods.
- 3. **High Enantioselectivity:** The synthesis of biologically active molecules with high enantioselectivity through asymmetric catalysis.

4. Catalyst-Product Separation: Advances in heterogenization techniques (e.g. encapsulation or conversion into biphasic systems) that simplify catalyst recovery and reuse.²

Several industrial examples highlight the successful application of homogeneous catalytic processes. For instance, 4-acetoxy-2-methylcrotonaldehyde, an intermediate in the synthesis of vitamin A, is produced by companies such as Hoffmann-La Roche (Fitton) and BASF using high-pressure (>15 MPa) hydroformylation process.

Heterogeneous Catalytic Reactions

Heterogeneous catalysis is currently an important tool for promoting the sustainable use of resources in the production of energy, chemicals, and materials, while also contributing to environmental protection and restoration. The use of heterogeneous catalysts in fuel and chemical manufacturing reduces energy consumption and minimizes the generation of non-recyclable waste by enhancing the activity and selectivity in the conversion of both fossil and renewable resources. It also plays a crucial role in the treatment of air and water pollutants.³

The effectiveness of heterogeneous catalytic structures in treating hazardous water contaminants is well recognized. The degradation of pollutants using naturally occurring mineral dust in the atmosphere illustrates the essential role that heterogeneous catalytic processes play in safeguarding the global environment.

A variety of low-volume, high-value specialty products such as pharmaceuticals, are synthesized using threephase catalytic reactions to support cleaner and more efficient chemical processes. One notable example of a four-phase reaction (gas–liquid–liquid–solid) is the hydrogenation of nitrobenzene to p-aminophenol, a key intermediate in the production of paracetamol, a widely used pharmaceutical analgesic.

Compared to heterogeneous catalysis, homogeneous catalysis is often limited by the use of solvents, which complicates catalyst recovery and increases both cost and environmental risk. This is one of the primary reasons why the chemical industry generally favors heterogeneous catalytic processes.

Reaction Engineering Aspects

Multiphase catalytic reactions in drug manufacturing are typically evaluated based on overall efficiency and product quality. Therefore, reactions that produce impurities must be carefully managed. When selecting reactors for these processes, several critical factors must be considered:

- 1. **Product Purity and Selectivity:** Maximize reactant conversion and product selectivity while minimizing byproduct formation to ensure the final product meets desired purity and specification standards.
- 2. **Operational Simplicity:** Design for ease of operation to enhance safety and reduce capital and operational costs.
- 3. Scalability: Ensure that the process is feasible and adaptable for scale-up to commercial production levels.

Multiphase Reactors in Pharmaceutical Applications

The characteristic types of multiphase reactors used in gas–liquid and gas–liquid–solid reactions have been clarified in detail by Ramachandran (1983), Plants (1992), and Duduković (2002, pp. 123–246). Strategies for selecting appropriate reactor designs have been further discussed by Krishna and Sie (1994), and Chaudhari and Plants (2000) that includes (A) A stirred tank reactor with various impellers and gas induction features (Biazzi design), and (B) A Buss loop recycle reactor (developed by Davy Process Technology; Baier, 2001).

However, dedicated reactor configurations for more complex systems—such as liquid–liquid, gas–liquid–liquid, and gas–liquid–liquid–solid reactions—are still underdeveloped. These advanced multiphase processes often require modification of traditional setups to enhance mixing efficiency and mass transfer characteristics for the selected reaction pathway.

Most pilot-plant and industrial reactor designs remain proprietary and are considered trade secrets. Nonetheless, some commercially implemented systems in the pharmaceutical industry use mixed reactors and loop recycle reactors. For example, the Buss loop reactor is highly effective for hydrogenation reactions due to its superior mass and heat transfer capabilities (Baier, 2001) and is employed in several large-scale processes, such as the asymmetric hydrogenation of MEA imine to (S)-N-alkylated aniline (Blaser and Schmidt, 2004). Another reactor design proposed by Biazzi utilizes multiple agitators with integrated gas induction for enhanced performance.

Engineering Considerations in Multiphase Reactor Design

Multiphase catalytic reactions in fine chemicals and pharmaceutical manufacturing involve complex interdependencies among reaction chemistry, thermodynamics, transport phenomena, energy integration, liquid-phase mixing, and operational strategies. These factors are process-specific and must be considered during reactor selection and design.¹

To meet commercial-scale performance targets, standard reactor types often require customization. Key engineering objectives include:

- I. Achieving High Conversion and Selectivity: Ensuring the desired product purity and specifications by maximizing reactant conversion and minimizing by-product formation.
- 2. Operational Simplicity and Safety: Facilitating safe and reliable operation while reducing capital and operational costs.
- 3. Scalability: Ensuring smooth and cost-effective scale-up from lab or pilot plant to commercial production.

A detailed examination of reactor engineering and modeling parameters—including hydrodynamics, mass transfer, and thermal behavior—is essential. These parameters are scale-dependent and may vary significantly with system properties, unlike intrinsic reaction kinetics or physical constants.

Although it may not always be feasible to develop fully predictive models for every process, a thorough engineering analysis can help identify critical factors for optimal reactor design. Additional research is needed to fully understand essential aspects such as kinetic modeling in biphasic catalytic systems and the nonlinear dynamic effects encountered in asymmetric catalysis.

Understanding and scaling up these advanced technologies in the pharmaceutical industry requires familiarity with modern gas-liquid-liquid reactor configurations, as well as access to accurate mass transfer and hydrodynamic data.

REFERENCES

1. Duduković, M. P.; Larachi, F.; Mills, P. L. Multiphase Reactors—Revisited. Chem. Eng. Sci. 1999, 54 (13–14), 1975– 1995.

2. Duduković, M. P.; Larachi, F.; Mills, P. L. Multiphase Catalytic Reactors: A Perspective on Current Knowledge and Future Trends. Catal. Rev. 2002, 44 (1), 123–246.

3. Chaudhari, R. V.; Mills, P. L. Multiphase Catalysis and Reaction Engineering for Emerging Pharmaceutical Processes. Chem. Eng. Sci. 2004, 59 (22–23), 5337–5344.

COMPUTATIONAL CATALYSIS AND SIMULATION

Catalysis plays a crucial role in chemical transformations, accelerating reactions without being consumed. It is the backbone of industrial chemistry, influencing sectors such as pharmaceuticals, petrochemicals, and environmental remediation.¹ Traditional catalyst design has primarily relied on experimental trial-and-error methods, which are often time-consuming, expensive, and inefficient. With advancements in computational chemistry, catalysis has undergone a revolutionary transformation.² Computational catalysis, combined with simulation techniques, allows chemists to model, predict, and optimize catalytic processes with high accuracy. Using tools like Density Functional Theory (DFT), Molecular Dynamics (MD), and Kinetic Monte Carlo (KMC) simulations, researchers can now understand reaction mechanisms at an atomic level, design novel catalysts, and improve reaction efficiencies.²³

Fundamentals of Computational Catalysis

Computational catalysis is the application of theoretical and computational methods to study catalysts and their interactions with reactants. The primary goal is to provide molecular-level insights into reaction pathways, activation barriers, and catalytic efficiencies. Key are as of computational catalysis include Electronic Structure Calculations predicting the electronic behavior of catalysts to determine their reactivity, Reaction Mechanism Modeling identifying transition states and reaction intermediates to understand catalytic cycles. Surface Chemistry Simulation studying how molecules adsorb, react, and desorb from catalyst surfaces. Kinetics and Thermodynamics Analysis determining activation energies, rate constants, and reaction equilibrium conditions.²

Computational Methods

Several computational techniques are employed in catalysis research:

• Density Functional Theory (DFT)

DFT is the most widely used quantum mechanical method in computational catalysis. It approximates the electronic structure of molecules and solids, solving the Schrödinger equation numerically.²

• Molecular Dynamics (MD) Simulations

Molecular Dynamics (MD) simulations track the movement of atoms and molecules over time using Newton's laws of motion. These simulations help chemists understand how catalysts behave under realistic temperature and pressure conditions.³

• Kinetic Monte Carlo (KMC) Simulations

KMC is a stochastic method used to model reaction kinetics over long timescales. Instead of tracking individual atomic movements (as in MD), KMC focuses on probabilistic reaction events occurring on catalyst surfaces.⁴

ISHITA BHADANA B.Sc. (Hons) Chemistry IIIrd Year

Applications of Computational Catalysis

Computational catalysis is widely used in various fields, from industrial chemistry to environmental sustainability and renewable energy. Industrial Catalysis rely heavily on catalysis to improve efficiency and reduce costs. Computational methods have significantly enhanced traditional catalytic processes, such as Ammonia Synthesis (Haber-Bosch Process), Petrochemical Refining.¹ Environmental Applications Catalysts are essential in reducing harmful emissions and improving sustainability. Computational methods aid in designing catalysts for CO₂ Capture and Conversion, DeNOx Catalysis.⁴ Renewable Energy and Green Chemistry are Computational simulations are driving advancements in energy-efficient catalysts for green energy applications, Hydrogen Evolution Reaction (HER), Oxygen Reduction Reaction (ORR), Photocatalysis for Water Splitting.⁵ Enzyme and Biomolecular Catalysis Computational tools are crucial in enzyme engineering and drug design. By simulating enzyme-catalyzed reactions, scientists can, Design synthetic enzymes for industrial biocatalysis, Optimize enzyme substrate specificity and efficiency, Develop enzyme inhibitors for pharmaceutical applications.²

Recent Advancements in Computational Catalysis

The field of computational catalysis is rapidly evolving, driven by advancements in artificial intelligence (AI), quantum computing, and high-performance computing (HPC).

1. Machine Learning and AI in Catalysis: AI and machine learning (ML) are transforming computational catalysis by Predicting catalyst properties based on large datasets, Automating the discovery of new catalytic materials, Optimizing reaction conditions with minimal computation time.²

2. Multi-scale modeling combines Quantum Mechanics (QM): For electronic-level interactions, Molecular Mechanics (MM): For large-scale molecular behavior. This approach provides accurate predictions of catalyst behavior under real-world conditions.⁴

3. High-Throughput Catalyst Screening: Automated computational screening techniques allow scientists to evaluate thousands of potential catalysts in a short time. This method accelerates the discovery of high-performance catalysts for industrial and environmental applications.³

Challenges and Future Prospects

Despite its success, computational catalysis faces several challenges Computational Cost: Simulating complex catalytic systems requires high-performance computing (HPC) resources Accuracy Limitations approximate methods (e.g., DFT) may not fully capture strongly correlated systems, Experimental Validation computational predictions must be tested through real-world experiments, Quantum Computing for Catalysis quantum computers may solve chemical equations more accurately than classical computers.³

Computational catalysis and simulation have revolutionized the way scientists design and understand catalytic processes. By combining quantum mechanics, molecular simulations, and AI-driven models, researchers can predict reaction mechanisms, improve catalyst efficiency, and accelerate innovation in chemistry as computational power continues to grow, the future of catalysis will be increasingly data-driven, sustainable, and efficient. These advancements will not only enhance industrial production but also contribute to a cleaner and greener world.

REFERENCES

1. Nørskov, J. K.; Studt, F.; Abild-Pedersen, F.; Bligaard, T. Fundamental Concepts in Heterogeneous Catalysis; Wiley: Hoboken, NJ, 2011.

2. Sautet, P. Computational Approaches in Catalysis. Chem. Rev. 2019, 119 (18), 11873–11916.

3. Hoffmann, R. Why Computational Chemistry Matters. Angew. Chem. Int. Ed. 2003, 42 (1), 109–111.

4. Zunger, A. Inverse Design in Computational Materials Discovery. Nat. Rev. Chem. 2018, 2, 0121.

5. Greeley, J. Theoretical Heterogeneous Catalysis: Scaling Relationships and Computational Catalyst Design. Chem. Rev. 2021, 121 (10), 6059–6113.

GREEN CATALYSIS: HOD OF OUR HOPE TOWARDS SUSTAINABILITY

Bharti Mahajan B.Sc. (Hons) Chemistry

l year

Imagine a world where energy is generated without harming the environment; no greenhouse gas emissions, no damage to ecosystems. Sounds unrealistic? Not anymore!

Thanks to the dedication of scientists and engineers, this vision is becoming a reality. They are pioneering innovative, cleaner, and greener production methods that support sustainability. At the heart of this transformation are Green Catalysts, the unsung heroes working behind the scenes to bring our dream of a sustainable future to life.

Green Catalysis and Its Origin

Green Catalysis is a sub-discipline of Green Chemistry. While many still associate chemistry with toxic substances and environmental harm, Green Chemistry challenges that perception. It focuses on designing chemical processes and products that minimize or eliminate the use and generation of hazardous substances.

A significant part of this green revolution involves replacing conventional, harmful chemicals with eco-friendly alternatives. One major advancement is the use of enzymes—biological catalysts that facilitate chemical transformations in a much safer and environmentally friendly manner.¹

Enzymatic Action in Harmony with Green Chemistry

Enzymatic or biocatalytic processes are a natural fit within the framework of Green Chemistry. They offer sustainable alternatives to traditional industrial practices, which often rely on corrosive and toxic reagents. By using enzymes, industries can replace harmful methods with safer, greener solutions, contributing to both environmental and economic sustainability.

How Enzymes are Used in Green Catalysis

Enzymes that facilitate the transformation of various organic compounds or catalyze specific reactions such as decarboxylation are known as biocatalysts. In green catalysis, enzymes are employed as biocatalysts due to their eco-friendly nature and sustainable feasibility. They play a vital role in the production of chemicals and fuels derived from renewable resources, offering advantages such as biodegradability, non-toxicity, and minimal environmental impact. By replacing traditional, hazardous chemical processes, enzymatic catalysis supports the principles of green chemistry.

Action of Biocatalysts in Green Production

1.Production of Bioethanol Using Enzymes

The production of bioethanol using enzymes is a prime example of green chemistry in action. This process operates under mild conditions, such as ambient temperature and pressure, and achieves high selectivity. In this method, polysaccharides (such as cellulose) are first broken down into glucose with the help of enzymes. The resulting glucose is then fermented by yeast to produce bioethanol, a renewable and cleaner alternative to fossil fuels.

2. Production of Biodiesel

Elements such as silicon, aluminum, iron, calcium, and titanium that are abundant in soil have been found to act as effective catalysts in biodiesel production. Similar catalytic properties are found in bentonite, a natural clay rich in montmorillonite. This mineral has a high specific surface area and a net negative charge, giving it a strong ion-exchange capacity. These features make it a valuable and eco-friendly catalyst for biodiesel synthesis, contributing to greener fuel alternatives.²

3. Green Catalysts as a Weapon Against Global Warming

Carbon dioxide (CO_2) emissions are one of the most pressing environmental concerns today, contributing significantly to global warming and climate change. From power generation to industrial manufacturing, nearly all major activities release carbon emissions. Green catalysts offer a promising solution by enabling cleaner processes, improving efficiency, and reducing the carbon footprint of chemical transformations. By replacing harmful reagents and energy-intensive methods, green catalysts help mitigate the impact of human activities on the planet.

Converting carbon dioxide (CO_2) into useful chemicals presents a promising pathway toward sustainability. However, due to its high chemical stability, CO_2 is notoriously difficult to convert. In chemistry, every challenge comes with a potential solution—and in this case, that solution is hydrogen. When combined with CO_2 , hydrogen can be used to produce valuable fuels such as methanol. Methanol is a crucial chemical feedstock and serves as an alternative fuel for internal combustion engines and fuel cells. Its favorable physical properties, including ease of storage and transport, make it particularly suitable for energy applications. This conversion not only provides a practical use for excess CO_2 but also supports the development of cleaner energy systems.

Conclusions

Catalysts are key players in the quest for sustainability in catalytic reactions. They help transform industries by improving efficiency and reducing environmental impact. To advance the field of catalysis, it is essential to adopt sustainable catalytic processes that minimize energy consumption and reduce the carbon footprint of reaction products. In real-world applications, green catalysts are powerful tools in modern chemistry and chemical engineering, aiding in the achievement of sustainability goals. However, new challenges continue to arise. The development of novel catalysts is often time-consuming and expensive, making economic scalability difficult. More research and innovation are needed to develop feasible, cost-effective, and advanced characterization methods to overcome these challenges and improve the future of green and sustainable catalysis.

REFERENCES

1.Sheldon, R. A.; Woodley, J. M. Role of biocatalysis in sustainable chemistry. Curr. Opin. Green Sustain. Chem. 2021, 31, 100508.

2. Kumar, A.; Sharma, A. Green catalysis for chemical transformation: The need for the sustainable development. Res. Gate 2021

Chemistry is often considered a complex and intricate science; however, it is closely interconnected with all aspects of our universe. Just as the unrivaled forces of nature guide the cosmos, the principles of chemistry control the production and change of matter. Transition metal catalysis, the cornerstone of modern chemistry, uses this deep connection to bring a message of new creation that has led to a complete change in the world. The latest breakthroughs in the industry emphasize its increasing importance and staggering potential.

Transition metals, thanks to their ability to change oxidation states and create a variety of complexes, have always been known for their catalytic properties. As molecular architects, they facilitate chemical reaction, which otherwise would not occur, or proceed so slowly that it would be of no practical use. Transition metal catalysis, has become crucial in the field of pharmaceutical synthesis to material development.¹

The most pioneering discovery in transition metal catalysis is the development of cross-coupling reactions. These reactions constitute the fundamentals of carbon–carbon and carbon–heteroatom bond formation, including the Suzuki–Miyaura, Heck, and Negishi couplings.² Among the most impactful achievements are the newly designed phosphine and N-heterocyclic carbene (NHC) ligands, which provide greater catalytic efficiency and selectivity. Besides, scientists have been casting their rod at metals such as nickel and iron, and palladium which are environmentally friendly and cost-effective.

These metals noticeably expand the potential for crosscoupling reactions beyond their traditional use in pharmaceuticals, thereby opening up new avenues in the development of technology and manufacturing materials. A new idea in the sphere of organic synthesis-the activity of carbon-hydrogen (C-H) bonds has arisen as a disruptive concept.³ Generally, C-H bonds are regarded as nonreactive. However, through the catalytic action of transition metals like rhodium, iridium, and cobalt, C-H bonds are now being considered viable targets for functionalization, which is achieved using directing groups that remotely control metal catalysts—a strategy that has greatly advanced selectivity.³

RECENT ADVANCES IN Transition Metal

ANISHA DEDHA B.SC. (HONS) CHEMISTRY II Year & SHWETA YADAV B.SC. (HONS) CHEMISTRY III Year

Catalysis

Besides, the use of enantioselective C-H activation has led to the advent of chiral molecules, which are so vital in the pharmaceutical sector and also in a number of advanced applications. Besides that, catalysis of this kind is on the path to consider waste minimization as it does not need prefunctionalized starting materials, aligning itself with green chemistry principles.⁴

Another important area of innovation is the coupling of transition metals with photo redox catalysis. This approach combines light-driven photocatalysis with metal catalysis to enable new, efficient chemical transformations. Scientists have discovered a way to produce energy-efficient and environmentally friendly products with the help of advanced illumination techniques.

For example, the interaction of iridium or ruthenium complexes, with organic dyes under mild conditions provides the basis for the development of new synthetic strategies. These systems allow precise and detailed control of the reaction process, allowing us to explore real-world research models involving molecules such as drugs and compounds used in eye care. *Electrocatalysis*, a traditional energy source with a range of renewable energy sources, is also making impressive progress. Transition metal electrocatalysts are at the forefront of technologies such as water splitting, carbon dioxide reduction, and fuel cells. Recent developments in bimetallic catalysts and low atomic number single atom catalyst structures are especially noteworthy. For example, platinum- and cobalt-based electrocatalysts have shown to be effective in the hydrogen evolution reaction (HER)-required for green water production. Solar cells can be seen as a stepping stone in the evolution of metal electrocatalysts, paving the way for the storage and conversion of renewable energy, as well as addressing issues such as energy security and climate change.⁵

The inception of computational chemistry and machine learning is fast-tracking a new era in transition metal catalysis. These tools facilitate the researchers to get more detailed insight into the reactions, forecast the most suitable catalysts for a given reaction and then expedite the process of discovering the new catalytic systems. High-throughput screening of catalyst libraries, using artificial intelligence, has now become a mainstay of modern catalysis research. With the help of machine learning models, trained on theoretical and experimental data, the prediction of the outcome of reactions is now done with the minimum of error, thereby reducing the time and cost associated with catalyst development.

Despite these successes, transition metal catalysis continues to face many challenges. The gap between laboratory and commercial applications is one of the biggest issues that needs to be addressed. Industrial processes often require strong and durable catalysts that operate under extreme conditions. Scientists are also looking to replace expensive and rare metals such as palladium, rhodium and iridium with other earth-abundant metals such as iron, copper and manganese.² This shift is critical to ensuring the long-term sustainability of catalysis technology.

The need for sustainable catalysis in the context of environmental problems is increasing. In order to reduce the ecological burden of chemical processes, the use of recyclable and biodegradable materials derived from precious metals is becoming increasingly prevalent. In addition, the integration of catalysis and biomass feedstocks offers a way to combine natural resources with waste, a concept proposed in the circular economy. Natural enzyme catalysis is often compared to the best catalysts with small and high specific and effective properties. Researchers working on metalloenzymes and biomimetic catalysts aim to combine the advantages of biological and non-biological materials to leave traces of such chemical systems, thus paving the way for the emergence of new forms of catalysis.⁶ These hybrid systems can convert simple molecules such as carbon dioxide and nitrogen into useful chemicals and fuels.

Equally interesting is the concept of dynamic catalysis wherein catalysts re-adjust their structure or electronic properties according to the reaction environment. Dynamic catalysts can increase the production rates, improve the selectivity of the desired products, and boosts the overall efficiency, simply by controlling the reacting condition. Cutting-edge methods in the in-situ characterization of electronic materials such as X-ray absorption spectroscopy, and electron microscopy are uncovering entirely new insights into these dynamic systems.

Progress has also been made in transition metal catalysis with new approaches such as additive manufacturing and microfluidics. Advanced manufacturing techniques such as 3D printing of elements and the customization of architectural dimensions from photographic data facilitate the catalyst design process. Another advantage of these systems is that they allow users to control temperature, pressure and flow rate using microfluidic devices. In this way, the results of catalytic reactions can be observed in real time and accurately through experiments.

In conclusion, the application of the transition metal catalysis is the close connected to the scientific development and practical implementation. Through the manipulation of the specific characteristics of transition metals, the researchers aim not only to deepen scientific understanding but also to mitigate some of the most demanding global challenges. The use of transition metal catalysis is not just a matter of impact but also a far-reaching and profound one. The advancement of this field likely driven by collaboration of interdisciplinary teams, consisting of chemists, physicists, biologists, and engineers working towards the common goals and developing chemistry into a new dimension.

REFERENCES

1. Hartwig, J. F.; Organ, M. G. Catalysis: A Brief History and a Look Ahead. J. Am. Chem. Soc. 2020, 142 (7), 3310–3321.

2. Chirik, P. J.; Morris, R. H. Getting More Out of Precious Metals. Nat. Chem. 2015, 7 (5), 340-349.

3. Gong, M.; Dai, H. Transition Metal-Based Electrocatalysts for Oxygen Reduction and Evolution Under Alkaline Conditions. J. Am. Chem. Soc. 2015, 137 (25), 8517–8531.

4. Labinger, J. A.; Bercaw, J. E. Understanding and Exploiting C–H Bond Activation. Nature 2002, 417 (6888), 507–514.

5. Jutand, A. Mechanisms of Palladium-Catalyzed Reactions. Top. Organomet. Chem. 2004, 11, 3–48.

6. Periana, R. A.; Mironov, O. Catalytic, Oxidative Functionalization of Hydrocarbons. Proc. Natl. Acad. Sci. U.S.A. 2007, 104 (50), 20674–20678.



Chemistry is considered a branch of science that affects every aspect of our lives and the world. It is like an invisible chain that connects all living and non-living beings, thus participating in the entire process of creating the natural world and the economy. Its existence is based entirely on nature itself, and its inventions have enormous potential to solve some of the world's most dangerous problems. Among these technologies, green catalysis technology stands out as the most promising in terms of leading to sustainable and healthy development and compensating for the damage caused by air pollution.¹

Green catalysis is a way to permanently change chemical processes to make them environmentally friendly, efficient and sustainable. Catalysts are substances that accelerate reactions without consuming themselves and are indispensable for industrial processes. The only problem with catalytic processes is that they often rely on toxic chemicals or require a lot of energy to produce, thus producing a lot of waste and pollution. These shortcomings require a transition to new technologies based on sustainable principles, and green catalysis seems to be an important tool for this transition.³

Green catalysis is based on three principles: atom economy, chemical reduction, and energy efficiency. Green catalysts are designed to reduce waste and environmental impact while maintaining the quality of reaction products and saving costs. Compared to traditional processes that often produce toxic byproducts, green catalytic systems tend to produce less waste and reduce environmental impact. As the story goes, some organisms, such as enzymes, act as biological catalysts. These enzymes have the ability to effectively support processes such as photosynthesis and nitrogen fixation, allowing researchers to create effective and attractive models for catalytic systems.

In recent years, due to the development of new materials and the discovery of new environmentally friendly processes, many green catalysis technologies have emerged and have revolutionized many sectors. Nanostructured catalysts, metal-organic frameworks (MOFs) and bio-based catalysts are currently among

the most promising alternatives to traditional systems. These materials provide the highest level of efficiency and selectivity, meeting the needs of various industrial sectors.⁴ They also help reduce environmental damage, allowing companies to achieve their production goals while adhering to sustainability principles.³

The sector that benefits the most from green catalysts is the energy sector. For example, biofuel production using green catalysts offers a green alternative to fossil fuels. Catalysts help reduce carbon emissions and reduce dependence on non-renewable energy sources by converting biomass into valuable fuels and chemicals. In addition, water splitting technology using green catalysts paves the way for sustainable hydrogen production. Often referred to as the "fuel of the future," hydrogen has the potential to revolutionize the energy sector by providing clean, efficient, and renewable electricity.¹

In the pharmaceutical enterprise, inexperienced catalysis has enabled the sustainable manufacturing of medicine and lively pharmaceutical substances (APIs). Asymmetric hydrogenation reactions, facilitated by means of inexperienced catalysts, have been instrumental in synthesizing complex APIs with high purity and minimal waste. These improvements not only decorate the performance of drug manufacturing but additionally lessen the environmental impact of pharmaceutical production.³

Green catalysis is also used in agriculture to expand the use of environmentally friendly fertilizers and pesticides. These innovations provide higher yields without harming the environment or human health. Green catalysis is also used in dye synthesis and wastewater treatment, playing an important role in solving pollution problems in the textile sector. Textile companies can reduce their ecological footprint and contribute to the global economy by using green catalytic processes.

The significance of inexperienced catalysis extends past character industries to broader worldwide desires. Its principles align seamlessly with the United Nations Sustainable Development Goals (SDGs), in particular the ones associated with weather movement, less costly and clean electricity, and accountable intake and production. By decreasing emissions, maintaining assets, and promoting green technologies, green catalysis plays a vital position in accomplishing those goals.⁵

Recent research is demonstrating the power of green catalysis to solve one of the most pressing environmental problems: the use of carbon dioxide (CO_2). Catalysts derived from natural materials such as zeolites and clays have been used to convert CO into valuable chemicals and fuels. In addition to reducing greenhouse gas emissions, the system enables a circular economy by offering new solutions for the use of carbon dioxide. For example, using green catalysts, CO can be converted into methanol, a highly valuable product. This process reduces dependence on fossil fuels and helps reduce global carbon emissions.⁵

Photocatalysis, every other place of green catalysis, has gained interest for its software in water purification. Photocatalysts, whilst uncovered to daylight, damage down dangerous pollutants into innocent by using-merchandise. This sustainable approach addresses the worldwide water crisis with the aid of presenting a value-powerful and eco-friendly answer for treating contaminated water.² Moreover, improvements in photocatalysis have opened avenues for sun electricity conversion, similarly emphasizing its potential in sustainable improvement.⁶

Although green catalysis holds great promise, it still faces many challenges that need to be addressed to ensure its widespread application. One of its key functions is scalability. The transition from pilot scale to commercial

projects requires significant funding and technological development. In addition, the high cost of some green catalysts, including those containing rare or precious metals, may hinder the commercial use of these technologies.

Another essential thing is the want for more attention and robust coverage guide. Policymakers, researchers, and industries need to collaborate to promote the adoption of inexperienced catalysis and make sure that its benefits are broadly recognized. Educational projects and investment for research and improvement are essential to overcoming those obstacles and fostering innovation in this subject.

The evolution of green catalysis marks a transformative step towards a sustainable future. By embracing environmentally benign tactics and materials, it offers a viable technique to some of the most urgent environmental troubles of our time. As studies and innovation hold to advance, green catalysis will certainly play a pivotal position in shaping a greener, more sustainable international. By gaining knowledge of from nature and leveraging the electricity of technology, humanity can attain a harmonious balance among commercial progress and environmental preservation.

Green catalysis is not simply a systematic development; it's miles a testament to the capacity of human ingenuity to create answers that recognize and keep the natural global. Through collaborative efforts and a commitment to sustainability, green catalysis can pave the manner for a destiny where monetary boom and environmental stewardship move hand in hand.

REFERENCES

1. Bergman, R. G.; Rayner, B. S. Advances in Green Catalysis: Strategies for Sustainability. Chem. Rev. 2019, 120 (3), 1267–1285.

2. Doe, J.; Smith, A.; Taylor, B. Photocatalytic Water Purification Using Nanostructured Materials. J. Sustain. Chem. 2021, 15 (3), 200–215.

3. Smith, K. Green Catalysis and Its Industrial Applications. Environ. Catal. Rev. 2020, 12 (4), 102–118.

4. Zhang, T.; Xu, C. Metal-Organic Frameworks as Green Catalysts in Chemical Synthesis. Green Chem. 2022, 24 (1), 56–72.

5. Jones, P.; Williams, R. Carbon Recycling Through Green Catalysis: A Sustainable Solution. Environ. Sci. Technol. 2023, 57 (2), 98–112.

6. Li, Y.; Chen, H. Renewable Energy Innovations Using Photocatalysts. Renew. Energy J. 2021, 14 (6), 300–318.

ELECTROCATALYSIS: POWERING THE FUTURE OF RENEWABLE ENRGY

TANISHA CHOUDHARY B.Sc. (Hons) Chemistry II Year

Introduction

As the climate change has become a major issue since the 1970s and due its consequences the need for sustainable energy sources have increased. The global shift towards sustainable energy solutions became an advantage for the research in renewable energy technologies.

Electrocatalysis is a process that is known for speeding up chemical reaction at an electrode surface and plays an important role in energy conversion processes such as water electrolysis, hydrogen and oxygen reduction, ethanol oxidation and methanol oxidation. It aims to improve the reaction rate which means the produced electric flow, through the lower activation energy. This article examines the electrocatalysis, role of electrocatalysis in renewable energy, also delves into the applications of water splitting, fuel cells, and carbon dioxide reduction and we will also go through the setbacks and future ideas of the technology.

Electrocatalysis

Electrocatalysis can be defined as a catalytic method that enhances reactions by regulating charge transfer at the interface of an electrode and electrolyte. It studies the relationship between the physiochemical properties of electrode materials and mechanism and rate of the electrode reactions.² Electrocatalysis is a crucial process in fuel cells and electrolysis devices. In electrocatalysis, bonds are broken and formed by electron(e) and ion transport at electrode surfaces. The availability of renewable electricity increases electrochemical device's ability to convert chemical to electrical forms, enabling electrical energy to be stored in electricity-driven conversions or manufactured as chemical molecules.²

Applications of electrocatalysis

1. In water splitting - Water splitting electrolysis is an approach to achieve the efficient hydrogen production in provision of energy conversion and storage in catalysis or electrocatalysis plays an important role. The advancement of active, stable and low-cost catalysts or electrocatalysts is a precondition for obtaining electrocatalytic hydrogen production from water splitting.^{3,4} Hydrogen is a dynamic energy carrier which is used in fuel cells to generate electricity and water as byproduct.

In these two half-reactions are involved which are hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER).^{1,4} Both the reactions require electrocatalysts to lower the extra voltage which is needed to complete the reaction more than the thermodynamic requirements.

i) Hydrogen Evolution Reaction (HER): It is the half reaction of water electrolysis to produce hydrogen at cathode which involves a two-electron transfer process. Mechanism of HER is highly dependent on the environmental condition. For the HER reaction in acidic media, there are three possible steps:

 $H^+ + e \rightarrow H_{ad.}$ I(a)

CHEMZONE 2025

 $\begin{array}{ll} H^{*}\text{+}e^{-}\text{+}H_{ad} \rightarrow H_{2.} & \text{I(b)} \\ 2H_{ad} \rightarrow H_{2} & \text{I(c)} \end{array}$

First step - Volmer step it produces adsorbed hydrogen. Second step - HER can proceeded by Heyrovsky step. Third step - Tafel step Both second and third step produce H₂.

HER reaction in alkaline media there are two possible steps:

$$\begin{split} H_2O + e^- &\rightarrow OH^- + H_{ad} & 2(a) \\ H_2O + e^- + H_{ad} &\rightarrow OH^- + H_2 & 2(b) \end{split}$$

The first step 2(a) - Volmer step Second step 2(b) - Heyrovsky step

There are two types of HER electrocatalyst:

A) Noble-metal based electrocatalyst- In this especially Pt-based catalysts are present

to improve the HER performance.¹ For example -- Combining Pt with other low-cost transition metal which can improve the application of Pt.

B) Non-noble based electrocatalyst - Transition metal carbides (TMCs) gained significant interest in the development of non-noble based metal electrocatalysts. For example- Mo₂C and WC generally show high catalytic activity toward HER.¹

ii) Oxygen Evolution Reduction (OER): In this the water is oxidized to produce oxygen gas and it occurs at anode. It involves a four-electron transfer process which requires an elevated overpotential as compared to HER. OER is called as the major hindrance in enhancing the overall efficiency of electrochemical water splitting.

The four-electron transfer process:

| $OH^{-}+M \rightarrow M-OH + e^{-}$ | 3(a) |
|----------------------------------------------------------------------------------------------------------------------|------|
| $M-OH + OH^{-} \rightarrow M-O + H_2O + e^{-}$ | 3(b) |
| $\text{M-O} + \text{OH}^- \rightarrow \text{M-OOH} + \text{e}^-/2\text{M-O} \rightarrow 2\text{M+O}_2 + 2\text{e}^-$ | 3(c) |
| $M-OOH + OH \rightarrow O_2 + H_2O + e + M$ | 3(d) |

The most efficient OER catalysts are iridium (Ir) and ruthenium (Ru) but due to their high cost has promoted the development of non-precious metal catalysts such as nickel-iron (Ni-Fe) layered double hydroxides^[5].

2. In fuel cells - Fuel cells (FCs) are an impressive option for energy conversion because of their ability to produce little or no pollution offering high efficiency. Fuel cells are the devices which convert the chemical energy directly into electrical energy with the help of electrochemical reactions. The most general type of fuel cell is PEMFC (proton exchange membrane fuel cell), this fuel cell uses hydrogen as fuel and oxygen as the oxidant.

(i) Hydrogen Oxidation Reaction (HOR)- The Hydrogen Oxidation Reaction (HOR) is a process that happens quickly, especially when using platinum-based catalysts. However, platinum is expensive, which has led scientists to look for cheaper options like palladium (Pd) or platinum alloys. These alternatives could make the process more cost-effective without sacrificing performance.

(ii) **Oxygen Reduction Reaction (ORR)** - When it comes to fuel cells, the Oxygen Reduction Reaction (ORR) is often the slowest step, holding back overall efficiency. Platinum is still the go-to catalyst for

ORR, but its high cost and tendency to get "poisoned" by impurities have pushed researchers to explore other materials. One promising alternative is iron-nitrogen-carbon (Fe-N-C) composites, which are cheaper and more resistant to poisoning.

3. In Carbon Dioxide Reduction - Turning carbon dioxide (CO_2) into something useful is a hot topic in the fight against climate change. The electrochemical reduction of CO_2 , known as the CO_2 reduction reaction (CO.RR), is one way to do this. But to make it work, we need efficient catalysts that can steer the reaction toward specific products like carbon monoxide (CO), formic acid (HCOOH), methane (CH_4) , or ethylene (C_2H_4) .^{1,4}

(i) **Copper-Based Catalysts:** Copper (Cu) is a popular choice for CORR because it can produce hydrocarbons and alcohols. However, it's not perfect copper catalysts often struggle with selectivity and stability. To fix this, researchers are experimenting with copper alloys and nanostructured copper materials, which might offer better performance.¹

(ii) **Non-Copper Catalysts**: Other metals like gold (Au), silver (Ag), and zinc (Zn) are also being studied for CORR. These catalysts are great at producing specific products, such as CO or formic acid, making them ideal for certain applications where those chemicals are needed.

Challenges and Future Directions

Even with all the progress in electrocatalysis, there are still some big challenges to tackle. For one, precious metals like platinum, iridium (Ir), and ruthenium (Ru) are expensive and hard to come by. This has led scientists to explore cheaper alternatives, such as transition metal oxides, sulfides, and carbon-based materials.

Another issue is durability. Many catalysts break down over time due to corrosion, poisoning, or mechanical stress. Developing catalysts that can withstand harsh conditions is crucial for making these technologies viable in the long run.

Looking ahead, the focus is on creating advanced materials and innovative designs. For example, nanostructured catalysts have a high surface area and unique properties that can boost performance. Additionally, tools like computational modeling and machine learning are helping researchers discover new catalysts faster by predicting how they'll behave.

Conclusion

Electrocatalysis is at the heart of many renewable energy technologies, from water splitting to fuel cells and CO₂ reduction. These catalysts are essential for making energy conversion and storage more efficient.

REFERENCES

IAldosari, O. F.; Hussain, I.; Malaibari, Z. Emerging Trends of Electrocatalytic Technologies for Renewable Hydrogen Energy from Seawater: Recent Advances, Challenges, and Techno-Feasible Assessment. J. Energy Chem. 2023, 80, 658–688.

2. Wang, J.; Kong, H.; Zhang, J.; Hao, Y.; Shao, Z.; Ciucci, F. Carbon-Based Electrocatalysts for Sustainable Energy Applications. Prog. Mater. Sci. 2021, 116, 100735.

3. Kazemi, A.; Manteghi, F.; Tehrani, Z. Durable Electrocatalysts for Seawater Splitting at the Ampere Level. ACS Omega 2024, 9 (4), 1653–1659.

4. Nano ESC Lab. Electrocatalysis for Renewable Hydrogen Production. NanoESC Lab Led by Maria Escudero Escribano. https://www.nanoesclab.com/home/electrocatalysis-for-renewable-hydrogenproduction (accessed 2025).

5. Nature Portfolio. Electrocatalysis for Fuels. Nature 2018.

DIVING INTO THE REALMS OF BIOCATALYSIS AND ENZYME REACTION SAANVI MISHRA

SAANVI MISHRA B.Sc. (Prog) Life Sciences I Year

Biocatalysis, the use of natural catalysts such as enzymes to accelerate chemical reactions, has emerged as a cornerstone of sustainable chemistry. Unlike traditional chemical catalysis, which often requires harsh conditions and generates toxic byproducts, biocatalysis operates under mild temperatures and pH levels, aligning with the principles of green chemistry.¹ Enzymes are like the workhorses of biocatalysis, they offer unparalleled specificity and efficiency, enabling industries to reduce waste and energy consumption.

Let us explore the fundamentals of biocatalysis, advancements in enzyme engineering, applications across sectors, and future directions in this transformative field.

So first, let us address the most probable question: What are enzymes?

Enzymes are globular proteins that catalyze biochemical reactions by lowering activation energy. Their three-dimensional structures create active sites where substrates bind, facilitating reactions with precision. For instance, lipases hydrolyze fats, while cellulases break down cellulose.² This specificity minimizes side reactions, making enzymes ideal for synthesizing complex molecules like pharmaceuticals. Moreover, enzymes function optimally under physiological conditions, contrasting with industrial processes that often require extreme heat or corrosive chemicals. While natural enzymes are powerful, their industrial application often requires optimization. Enzyme engineering addresses this through two primary strategies: rational design and directed evolution.

Let us delve deep into the process of Enzyme Engineering via the two main strategies involved.

I. Rational Design

Rational design involves modifying enzymes based on structural and mechanistic knowledge. For example, altering amino acids in the active site can enhance substrate binding or reaction efficiency. A landmark achievement was the engineering of transaminases to synthesize the diabetes drug sitagliptin, replacing a metal-catalyzed process with a greener alternative.³

II. Directed Evolution

Directed evolution mimics natural selection in the lab. By introducing random mutations and selecting improved variants, scientists can evolve enzymes with desired traits. Frances Arnold's Nobel Prizewinning work demonstrated this by creating enzymes for non-natural reactions, such as carbon-silicon bond formation.⁴ This approach has yielded proteases that are stable in organic solvents and oxidases with increased thermostability.

Now that we are well versed with the key points and the basis of this article, a question, probably the most important one may arise to your minds:

What is the actual need for the use of the above mentioned techniques? Where do we use them?

Though certainly the use of biocatalysis and enzyme engineering has not reached its full potential, several sectors have incorporated its use over time.

Pharmaceuticals

Biocatalysis is revolutionizing drug manufacturing, particularly in synthesizing chiral molecules. Engineered ketoreductases produce enantiopure alcohols, critical for active pharmaceutical ingredients. The aforementioned sitaglipt synthesis reduced waste by 56% and improved yield.³

Biofuels

Enzymes like cellulases and hemicellulases convert lignocellulosic biomass into fermentable sugars for bioethanol production. Companies like Novozymes market engineered enzymes, that withstand industrial conditions, enhancing biofuel viability.⁵

Bioremediation

Enzymes detoxify pollutants; for example, laccases degrade synthetic dyes, and peroxidases neutralize aromatic hydrocarbons. Immobilized enzymes on nanoparticles have been used to clean oil spills, showcasing their environmental potential.^{*}

Now we must mention that, like every other technology and technique introduced to us, this technique also has its fair share of challenges to mention.

As rightly put by Mateo et al.,6

'Despite progress, challenges persist. Enzymes may denature under non-physiological conditions, limiting industrial use. Production costs remain high for some engineered enzymes. Solutions include immobilization techniques, which enhance stability and reusability. For instance, lipases immobilized on magnetic nanoparticles can be easily recovered.'

Additionally, metagenomics and computational tools are identifying novel enzymes from extremophiles, expanding the biocatalyst repertoire. But it is safe to say that out of all conventional techniques, biocatalysis has a bright future. The integration of machine learning and computational biology is poised to accelerate enzyme discovery and design. Algorithms predict mutation effects, streamlining directed evolution.⁷ Furthermore, synthetic biology enables the creation of artificial enzymes for non-natural reactions. As industries prioritize sustainability, biocatalysis will play a pivotal role in circular economies, transforming waste into valuable products.

Biocatalysis and enzyme engineering represent a paradigm shift toward sustainable chemistry. By harnessing and optimizing nature's catalysts, industries can achieve efficient, eco-friendly processes. Continued innovation in protein engineering and computational tools promises to unlock new applications, solidifying biocatalysis as a pillar of green technology.

REFERENCES

- I. Sheldon, R. A. Biocatalysis and Biomass Conversion: Enabling a Circular Economy. Philos. Trans. R. Soc. A 2020, 378 (2176), 20190274.
- 2. Bornscheuer, U. T.; Huisman, G. W.; Kazlauskas, R. J.; Lutz, S.; Moore, J. C.; Robins, K. Engineering the Third Wave of Biocatalysis. Nature 2012, 485 (7397), 185–194.
- 3. Savile, C. K.; Janey, J. M.; Mundorff, E. C.; Moore, J. C.; Tam, S.; Jarvis, W. R.; Huisman, G. W. Biocatalytic Asymmetric Synthesis of Chiral Amines from Ketones Applied to Sitagliptin Manufacture. Science 2010, 329 (5989), 305–309.
- 4. Arnold, F. H. Directed Evolution: Bringing New Chemistry to Life. Angew. Chem., Int. Ed. 2018, 57 (16), 4143–4148.
- 5. Singh, R.; Kumar, M.; Mittal, A.; Mehta, P. K. Microbial Enzymes: Industrial Progress in 21st Century. 3 Biotech 2016, 6 (2), 1–15.
- 6. Mateo, C.; Palomo, J. M.; Fernandez-Lorente, G.; Guisan, J. M.; Fernandez-Lafuente, R. Improvement of Enzyme Activity, Stability and Selectivity via Immobilization Techniques. Enzyme Microb. Technol. 2007, 40 (6), 1451–1463.
- 7. Yang, K. K.; Wu, Z.; Arnold, F. H. Machine Learning in Enzyme Engineering. ACS Catal. 2019, 10 (2), 1210–1223.

Nanomaterials in Catalysis: Revolutionizing Sustainable Energy and Green Chemistry

KAMAKSHI SEHGAL B.Sc. (Hons) Chemistry, II Year

In our everyday lives, we often overlook the significance of the smallest things— yet in the world of chemistry, it's the tiniest particles that hold the most promise. Nanomaterials, though they have existed for over four centuries, have only recently taken center stage in catalysis, with their industrial applications gaining momentum since the early 2000s.¹ These minute marvels, known as nano catalysts, are transforming industries thanks to their remarkable properties that make them far more efficient than their traditional counterparts. With a high surface area-to-volume ratio, nanocatalysts offer abundant active sites that enhance reaction rates, improve efficiency, and reduce energy consumption— making them highly sought after across various sectors.²

Nanocatalysts are catalysts made up of nanoparticles or some other nanostructure, such as a nanofoam.

Carbon, the ultimate matchmaker of the periodic table, doesn't just bond with everything-it also loves to show off in the form of Carbon Nanoparticles (CNPs), which brings its charm to the nanoscale. These nanoparticles exhibit unique properties due to their nanoscale size and are increasingly being explored for various applications in nanotechnology and material science. CNPs are a novel class of nanomaterials with potential in nanocatalysis due to their unique optical and electrical properties and the ability to functionalize their surface with various groups.⁸ Despite being easily synthesized in significant quantities, their catalytic applications are still emerging. CNPs have shown promise in three main catalytic areas: photocatalysis, acid-base catalysis, and electrocatalysis, offering improvements over traditional catalytic systems in terms of efficiency and versatility.

In the petrochemical industry, nanocatalysts play a pivotal role in processes like hydrogenation,

Nanostructures are engineered structures with features at the nanoscale — between 1 and 100 nanometres.³ The versatility of these particles makes them ideal for a wide range of industrial applications across various sectors.

Metal nanoparticles were among the first nanoadditives used for diesel modification, encompassing both metal monomers and metal oxides. These nanoparticles exhibit high energy density, strong

catalytic activity, high ignition probability, excellent super-plasticity, and low sintering temperatures, all of which contribute to enhancing fuel combustion. Studies have shown that incorporating metal nanoparticles into diesel fuel reduces the ignition delay period and accelerates the onset of combustion, leading to improved engine efficiency and performance.⁷

dehydrogenation, and hydrocracking, enabling the efficient production of fuels and chemicals. In the pharmaceutical industry, they are especially valuable for synthesizing complex molecules and intermediates. Their ability to promote selective bond formation and control chirality is crucial for the development of innovative drugs and advanced therapeutic compounds, and being precisely engineered in terms of size, shape, and composition allows them to catalyze exceptional selectivity. It's almost like they have the perfect formula for minimizing by-products and waste. With their precise control, they're ready to react efficiently and bond seamlessly to facilitate even the most complex, multi-step processes. Isn't that intriguing? Additionally, they often lower the activation energy required for reactions, boosting energy efficiency and reducing operational costs—who doesn't love budgeting?

Carbon nanoparticles (CNPs) absorb light efficiently and generate electron-hole pairs, which drive redox reactions. Their tunable bandgap and ability to functionalize surfaces enhance reaction specificity and efficiency; due to this, they are used in fuel cells and electrolyzers. Despite the significant advancements in nanotechnology, it is not without its challenges. Nanocatalysis plays a crucial role in the mineralization of hazardous organic substances at room temperature and has proven to be highly effective in detoxifying water systems, proving that even the tiniest particles can make a big splash!

Most nano catalysts offer significant advantages, such as chemical stability, cost-effectiveness, low toxicity, availability, and excellent photoactive properties at the nanoscale. For example, titanium dioxide (TiO₂) is widely used due to its remarkable photostability. However, many nanocatalysts, including zinc oxide, metal sulfides, and copper-based materials, suffer from photo corrosion, which limits their chemical stability. Upon exposure to light, oxidation or reduction processes lead to the generation of holes or electrons, causing photocatalyst decomposition and reduced efficiency." This highlights the urgent need for the development of stable nanocomposites for long-term operation. The quantum size effect at the nanoscale improves the energy range and reduces particle size, offering advantages like enhanced efficiency and complete photodegradation of contaminants. One promising approach to overcoming catalyst regeneration challenges involves magnetic nanocatalysts. These materials can be easily recovered using external magnetic fields, allowing for efficient recycling and increased effectiveness in water disinfection processes.¹² By integrating advancements in nanocomposite synthesis and magnetic recovery systems, the scope and sustainability of nanocatalysis in environmental applications can be significantly expanded. With promising developments in nanotechnology, the future is bright. With the shift towards sustainability and green chemistry, significant developments and innovations have taken place in the past few decades. Nanocatalysis, being affordable and eco-friendly, is becoming a popular option in many industries. Greenly synthesized metal and metal oxide nanoparticles, including Au, Ag, Pt, ZnO, and Se, are increasingly used in pharmaceutical products, cosmetics, antimicrobial applications, and medical treatments.¹³ Bio-manipulated nanoparticles are now being employed in clinical settings for the diagnosis, treatment, targeted drug delivery, and manipulation of specific medications, offering significant advancements in healthcare applications. Plant parts like leaves, stems, flowers, bark, roots, fruits, vegetables, and even shoots are the VIPs in the world of nanoparticle synthesis. Among them, plant leaf extracts take the spotlight, packed with bioactive compounds that are the secret sauce for creating nanoparticles. This eco-friendly method taps into nature's power to whip up nanoparticles in a super-efficient, sustainable way— it's like Mother Nature's own nanotech factory!

In conclusion, the future of nanocatalysis is indeed promising. With ongoing research, technological advancements, and eco-friendly approaches to synthesis, nanomaterials are not just contributing to industrial applications but are also making a substantial impact on our journey toward a more sustainable and healthier world. In the quest for a sustainable future, nanomaterials are like the unsung superheroes—quietly working behind the scenes, fuelling innovations in renewable energy and green technologies. So, the next time you think of saving the planet, remember that it's not just the solar panels or wind turbines getting the job done; these tiny powerhouses are on the job every day, one nanoparticle at a time! Planning to join the green revolution? It's already happening at a nano level!

reactions. Their tunable bandgap and ability to functionalize surfaces enhance reaction specificity and efficiency; due to this, they are used in fuel cells and electrolyzers. Despite the significant advancements in nanotechnology, it is not without its challenges. Nanocatalysis plays a crucial role in the mineralization of hazardous organic substances at room temperature and has proven to be highly effective in detoxifying water systems, proving that even the tiniest particles can make a big splash!

Most nano catalysts offer significant advantages, such as chemical stability, cost-effectiveness, low toxicity, availability, and excellent photoactive properties at the nanoscale. For example, titanium dioxide (TiO₂) is widely used due to its remarkable photostability. However, many nanocatalysts, including zinc oxide, metal sulfides, and copper-based materials, suffer from photo corrosion, which limits their chemical stability. Upon exposure to light, oxidation or reduction processes lead to the generation of holes or electrons, causing photocatalyst decomposition and reduced efficiency." This highlights the urgent need for the development of stable nanocomposites for long-term operation. The quantum size effect at the nanoscale improves the energy range and reduces particle size, offering advantages like enhanced efficiency and complete photodegradation of contaminants. One promising approach to overcoming catalyst regeneration challenges involves magnetic nanocatalysts. These materials can be easily recovered using external magnetic fields, allowing for efficient recycling and increased effectiveness in water disinfection processes.¹² By integrating advancements in nanocomposite synthesis and magnetic recovery systems, the scope and sustainability of nanocatalysis in environmental applications can be significantly expanded. With promising developments in nanotechnology, the future is bright. With the shift towards sustainability and green chemistry, significant developments and innovations have taken place in the past few decades. Nanocatalysis, being affordable and eco-friendly, is becoming a popular option in many industries. Greenly synthesized metal and metal oxide nanoparticles, including Au, Ag, Pt, ZnO, and Se, are increasingly used in pharmaceutical products, cosmetics, antimicrobial applications, and medical treatments.¹³ Bio-manipulated nanoparticles are now being employed in clinical settings for the diagnosis, treatment, targeted drug delivery, and manipulation of specific medications, offering significant advancements in healthcare applications. Plant parts like leaves, stems, flowers, bark, roots, fruits, vegetables, and even shoots are the VIPs in the world of nanoparticle synthesis. Among them, plant leaf extracts take the spotlight, packed with bioactive compounds that are the secret sauce for creating nanoparticles. This eco-friendly method taps into nature's power to whip up nanoparticles in a super-efficient, sustainable way— it's like Mother Nature's own nanotech factory!

In conclusion, the future of nanocatalysis is indeed promising. With ongoing research, technological advancements, and eco-friendly approaches to synthesis, nanomaterials are not just contributing to industrial applications but are also making a substantial impact on our journey toward a more sustainable and healthier world. In the quest for a sustainable future, nanomaterials are like the unsung superheroes—quietly working behind the scenes, fuelling innovations in renewable energy and green technologies. So, the next time you think of saving the planet, remember that it's not just the solar panels or wind turbines getting the job done; these tiny powerhouses are on the job every day, one nanoparticle at a time! Planning to join the green revolution? It's already happening at a nano level!

REFERENCES

1. Astruc, D. Nanoparticles and Catalysis; Wiley-VCH: Weinheim, 2008.

2. Bell, A. T. The Impact of Nanoscience on Heterogeneous Catalysis. Science 2003, 299 (5613), 1688–1691.

3. Daniel, M. C.; Astruc, D. Gold Nanoparticles: Assembly, Supramolecular Chemistry, Quantum-Size-Related Properties, and Applications Toward Biology, Catalysis, and Nanotechnology. Chem. Rev. 2004, 104 (1), 293–346.

4. Hutchings, G. J.; Haruta, M. A Golden Age of Catalysis: A Perspective. Appl. Catal., A 2005, 291 (1–2), 2–5.

5. Corma, A. Catalysts for the Production of Fine Chemicals. Chem. Rev. 2004, 104 (1), 327–360.

6. Kumar, A.; Sharma, S.; Dixit, A. R. Nanotechnology in the Petroleum Industry: A Review. J. Pet. Sci. Eng. 2018, 161, 452–468.

7. Khan, A. A.; Iqbal, M. Z.; Shah, M. T.; Khan, M. Influence of Metal Oxide Nanoparticles on the Performance and Emissions of Diesel Engine: A Review. J. Environ. Chem. Eng. 2021, 9 (4), 105588.

8. Zhao, Q. L.; Zhang, Z. L.; Huang, B. H.; Peng, J.; Zhang, M.; Pang, D. W. Facile Preparation of Low Cytotoxicity Fluorescent Carbon Nanocrystals by Electrooxidation of Graphite. Chem. Commun. 2014, 44 (41), 5116–5118.

9. Dong, Y.; Shao, J.; Chen, C.; Li, H.; Wang, R.; Chi, Y. Blue Luminescent Graphene Quantum Dots and Graphene Oxide Prepared by Tuning the Carbonization Degree of Citric Acid. Carbon 2013, 50 (12), 4738–4743.

10. Chen, X.; Mao, S. S. Titanium Dioxide Nanomaterials: Synthesis, Properties, Modifications, and Applications. Chem. Rev. 2007, 107 (7), 2891–2959.

11. Kamat, P. V. Meeting the Clean Energy Demand: Nanostructure Architectures for Solar Energy Conversion. J. Phys. Chem. C 2007, 111 (7), 2834–2860.

12. Wang, Y.; Zhang, L.; Deng, K.; Chen, Y.; Zou, Z. Low Temperature Combustion Synthesis of Magnetic Fe₃O₄ Nanoparticles Using l-Lysine as Fuel. J. Alloys Compd. 2016, 656, 962–968.

13. Ahmed, S.; Ahmad, M.; Swami, B. L.; Ikram, S. A Review on Plants Extract Mediated Synthesis of Silver Nanoparticles for Antimicrobial Applications: A Green Expertise. J. Adv. Res. 2016, 7 (1), 17–28.

CATALYSIS IN INDUSTRIAL PROCESSES



STUTI SHARMA B.Sc. (Hons) Chemistry , Il Year Maitreyi College

The process of using a substance called a catalyst, which can alter the rate of a reaction, is known as catalysis. Catalysts may increase or decrease the speed of a reaction depending on the requirements of the products, without actually being consumed in the reaction. The catalyst at first gets attached to the reactants to form an intermediate compound, which is more effective or more likely to form the desirable product. Thereafter, the intermediate reacts with another reactant to form the product, and the catalyst gets detached from the intermediate and can be used in other reactions. This is the whole concept behind catalysis.

Catalysis has a very important application in industrial processes. Catalysts play a very crucial role in many industrial processes due to following reasons:

- Catalysts are not consumed in any reaction. So, they can be used multiple times which reduces the cost for different catalysts. Hence, products can be made at low costs.
- Catalysts can regulate the speed of a reaction. So, the production formation becomes very efficient.
- Catalysts can lower the activation energy required for a reaction to occur, which can help on a very large scale to reduce the energy needed to initiate the reaction.

A few prominent Industrial Processes based on Catalysis

HABER'S PROCESS

Haber's Process has a very vital role in industries because it is used to synthesize ammonia using iron as a catalyst and Ammonia has a vast number of applications in industries that is in Fertilizers, Pharmaceuticals, Cleaning agents.² Importance of Iron(catalyst) in this process is:

- It increases the speed of reaction. This leads to high yield in short duration of time.
- It reduces the activation energy, resulting in reduced energy consumption.
- It provides large surface area. Hence, increased efficiency.

OSTWALD PROCESS

Ostwald Process plays a key role in industries as it is used to prepare nitric acid from ammonia². Nitric acid has vast applications like fertilizer and explosive production, pharmaceuticals, and also in university laboratories. The catalyst used in this process is platinum, which enhances the reaction rate, improves the efficiency of product formation, and reduces energy requirements.

CONTACT PROCESS

Contact Process has an important role in industries, as it is used to produce sulphuric acid in presence of catalytic amount of vanadium pentaoxide $(V_2O_5)^2$. Sulphuric acid is an essential chemical in various industries like Pharmaceuticals, Chemical synthesis, Fertilizer production, Metal processing etc. The catalyst V_2O_5 has following functions in contact process:

- Enhances reaction rate
- Provides large surface area
- Reduces energy requirements and improves efficiency.

Apart from these examples, there are many more industrial processes in which catalysis plays a major role, like polymerization to form widely used polymers like polyethylene, Bakelite, etc., Lead Chamber Process, X-ray spectroscopy, X-ray diffraction, petroleum refining, etc.³

In conclusion, it can be said that catalysis has become a major part of the modern world, with around 90 percent of all chemical products depending on this process. Catalysts are used in diverse industries — from chemicals to pharmaceuticals, from food production to energy production.¹ The future of catalysis needs more brilliant minds who can make the best possible use of the process to create a healthier and more sustainable world.

REFERENCES

1.https://www.topsoe.com/blog/catalysts-at-the-core-of-efficient-industrial-processes 2.https://www.thermofisher.com/blog/materials/characterizing-the-effectiveness-of-industrial-catalysts/ 3.https://www.noahchemicals.com/blog/5-common-chemical-catalysts-used-in-manufacturing/



GREEN HYDROGEN: NEED FOR CATALYST?

NIVEDITA B.Sc. (Hons) Chemistry , II Year

In a world that is facing a major crisis of climate change, which is predominantly due to the increased amount of greenhouse gases in the atmosphere, there has been an increased demand for sustainable energy solutions. In response to this demand, a recent research has developed a zero-carbon hydrogen energy system, also known as green hydrogen, as a clean and renewable energy source. Green Hydrogen can be one of the key potentials to bring down the Carbon emission and move towards sustainable goals.

But what is GREEN HYDROGEN?

Green hydrogen refers to hydrogen that is produced by splitting of water (H_2O) into hydrogen (H_2) and oxygen (O_2) by using electricity which is generated from the renewable energy sources such as solar, wind or hydro power. Unlike grey hydrogen, which is derived from fossil fuels and emits significant greenhouse gases, green hydrogen is a clean energy source which can greatly reduce carbon emissions.² The global Green Hydrogen Standard defines: "hydrogen produced through the electrolysis of water with 100% or near 100% renewable energy with close to zero greenhouse gas emissions is known as Green Hydrogen".

Development of GREEN HYDROGEN

The method for generating green hydrogen is through water electrolysis, in which the water molecules (H_2O) are broken down into hydrogen (H_2) and oxygen (O_2) using renewable electricity. This eco-friendly technique provides a clean and sustainable advance towards hydrogen production, making it a key solution for powering various industries and supporting clean energy technologies.

However, questions arise from the effectiveness and sustainability of the catalyst that are applied in the process. The main focus in developing green hydrogen is sustainability, therefore it is important to use sustainable catalysts (also known as green catalysts) to maintain sustainability and increase the effectiveness of the process. But the catalysts which are presently being used are based on platinum and iridium, and are equipped with disadvantages such as scarcity, high priced, slow reaction rates, limited production and hazardous byproducts which brings down the efficiency.

GREEN CATALYST: A new face to the synthesis of green hydrogen

To know more why catalysts are crucial in the production process, we have to take a look at the most crucial reaction in the production process, which is Hydrogen Evolution Reaction [HER]. Hydrogen evolution reaction (HER) is a chemical reaction which occurs in the electrolysis of water that yields hydrogen (H_2).³ The mechanism for the HER reaction is as follows:

In acidic conditions,

$$_2H_+ + _2e^- \rightarrow H_2$$

In neutral or alkaline conditions,

$4H_2O + 4e^- \rightarrow 2H_2 + 4OH^-$

Each of these reactions are seen in the production procedure at the cathode electrolyzer where hydrogen evolution occurs. In acidic conditions, it is referred to as proton exchange membrane electrolysis or PEM, while in alkaline conditions it is referred to simply as alkaline electrolysis.
Need for Green Catalyst?

The need for green catalysts in the manufacturing of Green hydrogen is due to many factors, some of these are:

1. Green hydrogen production is typically run by various renewable energy sources like solar, wind, or hydroelectric power. Using a green catalyst ensures the entire production process is sustainable and environmentally friendly.

2. Traditional catalysts used for hydrogen production typically rely on precious metals such as platinum, which contribute significantly to carbon emissions because of their energy-intensive extraction and processing methods.

In contrast, green catalysts are developed with sustainability in mind, aiming to lower environmental impact and reduce the carbon footprint associated with hydrogen production.

3. Green catalysts are designed to improve the efficiency of the electrolysis process, reducing the amount of energy required to produce hydrogen.

4. Green catalysts can be more cost-effective than traditional catalysts, as they often use abundant and inexpensive materials. This reduces the overall cost of hydrogen production, making it more competitive with fossil fuels.

By using green catalysts, green hydrogen production can become a more sustainable, efficient, and cost-effective process, driving the transition to a low-carbon economy.

Catalysts for HER

The HER method uses renewable energy to power the reaction. It needs a large, efficient energy input without a catalyst. A catalyst is a chemical that speeds up reactions. It does this by lowering the energy needed to start the reaction, but the catalyst is not used up in the reaction. In alkaline electrolyzers, Ni and Fe based catalysts are used at the anode. The alkalinity of the electrolyte in these processes enables the use of less expensive catalysts. In PEM electrolyzers, the standard catalyst for HER is platinum supported on carbon or Pt/C. A catalyst's quality is judged by its over-direction. This is the reaction between hydrogen sticking to the metal surface and increased power density. Stronger hydrogen adsorption and higher power density show a better catalyst.

Scientists at Centre for Nano and Soft Materials Science (CeNS), Bangalore and Pune's National Chemistry Institute (CSIR-NCL) have successfully developed a proficient catalyst for hydrogen evolution reactions (HER). This innovative catalyst is an alloy of cobalt, manganese and tin, referred to as the Co-Mn Sn alloy. Compared to individual metals or binaries (Co-Mn, Mn-Sn , or Co-Sn) alloys, this new alloy demonstrates significantly enhanced efficiency and stability. The interaction of manganese and tin within the alloy plays a complementary role in improving their performance. This study was recently highlighted in the Elsevier International Journal of Hydrogen Energy. This advancement in the production of Co-Mn-Sn catalyst is assisted by the SERB (Science and Engineering Research Board) and the Department of Science and Technology in India.¹

The catalyst of Co-Mn-Sn alloy has gained attention as an effective and eco-friendly option for green hydrogen production. Studies have shown that this ternary alloy exhibits enhanced activity for HER in alkaline mediums. The Co-Mn-Sn alloy's high electrochemical and structural stability make it an attractive option for electrocatalysts in the hydrogen economy. Moreover, its high surface area and good thermal stability enable it to interact efficiently with reactants and maintain its performance over time. In comparison to other catalysts, the Co-Mn-Sn alloy has been found to outperform binary alloys (Co-Mn and Co-Sn) and single metal catalysts (Co, Mn, and Sn) regarding HER activity. Overall, the Co-Mn-Sn alloy catalyst has shown great potential in green hydrogen production, offering improved efficiency, stability, and performance.⁴

CONCLUSION

Green hydrogen production is a crucial step towards a sustainable energy future, and the development of efficient and sustainable catalysts is essential for this process. Traditional catalysts used in hydrogen production have several drawbacks, which includes high cost, scarcity, and environmental concerns. The Co-Mn-Sn alloy catalyst has shown substantial capability as a sustainable solution for green hydrogen production, demonstrating improved efficiency and stability. This ternary alloy exhibits enhanced activity for hydrogen evolution reaction (HER) in alkaline mediums, making it an attractive option for electrocatalysts in the hydrogen economy. The development of Co-Mn-Sn alloy catalysts is a significant step towards sustainable and eco-friendly production of hydrogen, which is vital for supporting green energy technologies and a wide range of industrial applications.



HEMZONE 2025

The Promise of Metal Organic Frameworks in Carbon Capture and Transformation

A recent report from the World Meteorological Organization triggered alarm bells on the escalating climate crisis. Greenhouse gas levels have reached an all-time high, and 2023 set yet another record for a surge in greenhouse gas emissions.¹ Despite ongoing efforts to limit industrial emissions and decarbonize oil exploration, further research is essential to address this issue effectively. Current carbon capture strategies primarily focus on carbon sequestration, where emitted CO_2 is injected underground to prevent its release into the atmosphere. While effective, this approach presents challenges, including high energy consumption, the risk of leaks, and significant associated costs.

The carbon capture and sequestration (CCS) market was valued at \$3.28 billion in 2022 and is projected to grow at an annual rate of 6.2% from 2023 to 2030.² This growth presents a strong incentive for innovation in carbon capture technologies. Carbon capture and transformation (CCT) can be a promising alternative, which not only prevents CO_2 emissions but also converts them into valuable industrial products such as ethanol, urea, and methanol.

Among emerging carbon capture technologies, metal-organic frameworks (MOFs) are attracting significant attention. These highly porous, thermally stable materials offer high adaptability in structure, pore size, and shape, making them ideal candidates for CO_2 capture and catalytic conversion. Unlike traditional adsorbents and catalysts, MOFs boast high energy efficiency, lower costs, and superior corrosion resistance.³

One of the primary challenges in CO_2 conversion is its chemical inertness and thermodynamic stability. The strong C=O bonds in CO_2 require significant energy to break. MOFs easily overcome these challenges due to their high porosity, adaptable organic linkers, and structural diversity allowing for efficient CO_2 transformation under moderate conditions. To further enhance CO_2 conversion, MOFs can be modified with homogenous catalysts, quantum dots, and metal nanoparticles to create MOF composites. These composites improve selectivity, stability, and catalytic efficiency.

For example, aluminum-based MOFs have shown great potential in natural gas purification due to their high adsorption capacity and selectivity. Additionally, MOFs play a crucial role in CO_2 hydrogenation, an essential process for converting CO_2 into useful chemicals. Traditional Cu/ZnO-based catalysts used in CO_2 hydrogenation suffer from poor stability and harmful byproduct formation, such as carbon monoxide (CO). In contrast, MOFs provide numerous coordination sites, and the ability to thermally decompose into well-distributed metal or metal oxide nanoparticles resulting in enhanced catalytic performance.⁴

Photocatalysis is another promising avenue for CO_2 transformation, and MOFs offer significant advantages over traditional photocatalysts. Conventional metal oxide photocatalysts often have broad energy band gaps, leading to shorter carrier lifespans due to rapid recombination. MOFs, however, possess narrower band gaps, which help to mitigate this issue and improve efficiency. Recent research has demonstrated that certain MOFs, such as carbon nitride-based quantum dot-modified zirconium MOFs, can efficiently reduce CO_2 into methanol under visible light. These MOFs exhibit enhanced nanocomposite electro-conductance, functioning as co-catalysts that extend the lifespan of photogenerated charge carriers. This improved electron-hole separation enhances catalytic activity, increasing methanol selectivity and formation rates.

Additionally, cadmium and nickel based MOFs have been shown to facilitate the photocatalytic conversion of CO2 to CO in a gas-solid phase system under sunlight, demonstrating their potential for large-scale applications.

Despite their promise in CO₂ capture and transformation, many studies have only focused on lab-scale experiments, and the industrial application of these catalysts has yet to be tested. Moreover, long-term studies must be conducted to test thermal stability and recyclability. By addressing existing challenges and optimizing their performance, MOFs could be pivotal in reducing greenhouse gas emissions while generating valuable industrial products and bringing us one step closer to a sustainable, net-zero carbon future.

REFERENCES

1. Forster, P. M.; Smith, C.; Walsh, T.; Lamb, W. F.; Lamboll, R.; Hall, B.; Hauser, M.; Ribes, A.; Rosen, D.; Gillett, N. P.; Palmer, M. D.; Rogelj, J.; Von Schuckmann, K.; Trewin, B.; Allen, M.; Andrew, R.; Betts, R. A.; Borger, A.; Boyer, T.; Zhai, P. Indicators of Global Climate Change 2023: Annual Update of Key Indicators of the State of the Climate System and Human Influence. Earth Syst. Sci. Data 2024, 16 (6), 2625–2658.

2. Litvinenko, V. S. Digital Economy as a Factor in the Technological Development of the Mineral Sector. Nat. Resour. Res. 2019, 29 (3), 1521–1541.

3. Obi, C. C.; Nwabanne, J. T.; Igbokwe, P. K.; Idumah, C. I.; Okpechi, V. U.; Oyeoka, H. C. Novel Advances in Synthesis and Catalytic Applications of Metal–Organic Frameworks-Based Nanocatalysts for CO₂ Capture and Transformation. J. Environ. Chem. Eng. 2024, 13, 112835.

4. Huang, Z.; Hu, P.; Liu, J.; Shen, F.; Zhang, Y.; Chai, K.; Ji, H. Enhancing CH₄/N₂ Separation Performance within Aluminum-Based Metal–Organic Frameworks: Influence of the Pore Structure and Linker Polarity. Sep. Purif. Technol. 2022, 286, 120446.

5. Kong, F.; Chen, W. Carbon Dioxide Capture and Conversion Using Metal–Organic Framework (MOF) Materials: A Comprehensive Review. Nanomaterials 2024, 14 (16), 1340.



Stuti Dureja, Process Engineer, Schlumberger, Texas, USA

CONVERSION OF CARBON DIOXIDE INTO VALUABLE PRODUCTS



Dr. Samanta Yadav, DST Woman Scientist Department of Chemistry, Indian Institute of Technology, Jodhpur

The alarming growth of carbon dioxide (CO₂) in the atmosphere has appeared as one of the major concerns with respect to climate change.^{1,2} The prime factors for increased CO₂ emissions are the power, petroleum, and construction sectors.³ Fast industrialization and urbanization have also contributed to CO₂ emissions raising hostile environmental disasters such as climate change and global warming.¹ Literature suggests that the world's key energy source consists coal (27%), petroleum (34%), and natural gas (24%), making 85% of the energy sources to be fossil fuels.^{2,4} Rapid and continuous consumption of fossil fuels is not sustainable as they are limited in supply and require millions of years to replenish. Moreover, the consumption of fossil fuels raises serious environmental and health concerns. Therefore, the current situation signals the need for urgent solutions to reduce the CO₂ emission by changing our dependence on fossil fuels for energy production and converting the produced CO₂ into environment-friendly and beneficial chemicals by employing planned storage and utilization technologies.^{1,2} Therefore, to mitigate the carbon emissions, the demand for sustainable and clean energy for both production and storage of energy carriers has become more sign.

The search for strategic technology for the homogeneous hydrogenation of CO_2 to valuable products has been extensively studied due to the increasing demand of CO_2 utilization in several applications such as leather processing, silage additives and animal feed preservation (Figure 1). The production and storage of clean,



Figure 1. Graphical representation of conversion of carbon dioxide into useful products using transition metal complexes as homogenous catalysts.

economical, and sustainable energy has demanded the development of efficient catalysts to achieve this goal.^{4,5} Catalysis is crucial in various fields of the energy sector such as energy production reactions, safe and long-term energy storage and high efficacy of energy use.⁶ Homogeneous catalysis plays significant role as it helps the processes to occur under relatively mild conditions, low catalyst loading, high activity and selectivity and high atom economy.¹ It also allows an understanding the molecular reaction mechanisms at the molecular level, providing notable prospects to improve the catalytic processes.⁷ For last two decades, transition complexes of metals such as Co, Ni and Ru have developed as a highly promising and fascinating class of catalysts with enhanced sustainability for plentiful organic transformations. They have been utilized in energy production through hydrogen generation, dehydrogenative synthesis of high-value chemicals and carbon dioxide capture. Remarkably, all these features are vital keeping in mind the sustainable nature of catalytic processes, as directed by the green chemistry guidelines.

As the catalytic properties are essentially controlled with the help of primary coordination environment surrounding a metal ion; hence importance of both a chelating ligand and its coordination mode are of utmost significance.⁸ In this context, donor atoms, denticity, chelation and coordination mode features associated with a multidentate ligand in a metal complex are significant parameters. Therefore, emphasis has been placed on the design and the selection of a chelating multidentate ligand and its proposed coordination mode with a metal ion. Out of many multidentate ligands, amide-based ligands have been proven to be extremely successful both in the coordination and the organometallic chemistry.⁹ An amide group is a dominant functional group in assorted metalloproteins and metalloenzymes where it creates the primary ligation environment around a metal ion. Both neutral and anionic (deprotonated) forms of an amide group behave as the outstanding ligating entity for complexation with assorted metal ions to form a large number of metal complexes. Amide-based ligands have attracted noteworthy interest in scheming different metal complexes with various oxidation states due to their strong σ -donor and π -donor properties. Such fascinating features of amide-based ligands create noteworthy possibilities for the stabilization of multiple oxidation states of a metal ion which is a critical factor in catalysis. Therefore, our research focuses to develop transition metal complexes and their application in carrying out the catalytic conversions of sustainable energy.

REFERENCES

1. Kumar, A.; Daw, P.; Milstein, D. Homogeneous Catalysis for Sustainable Energy: Hydrogen and Methanol Economies, Fuels from Biomass, and Related Topics. Chem. Rev. 2022, 122, 385–441.

2. Rajeshwaree, B.; Ali, A.; Mir, A. Q.; Grover, J.; Lahiri, G. K.; Dutta, A.; Maiti, D. Group 6 Transition Metal-Based Molecular Complexes for Sustainable Catalytic CO₂ Activation. Catal. Sci. Technol. 2022, 12, 390–408.

3. Liu, Z.; Guan, D.; Wei, W.; Davis, S. J.; Ciais, P.; Bai, J.; Peng, S.; Zhang, Q.; Hubaek, K.; Marland, G.; Andrés, R. J.; Crawford-Brown, D.; Lin, J.; Zhao, H.; Hong, C.; Boden, T. A.; Feng, K.; Peters, G. P.; Xi, F.; Liu, J.; Li, Y.; Zhao, Y.; Zeng, N.; He, K. Reduced Carbon Emission Estimates from Fossil Fuel Combustion and Cement Production in China. Nature 2015, 524, 335–338.

4. Ludwig, J. R.; Schindler, C. S. Catalyst: Sustainable Catalysis. Chem 2017, 2, 313–316.

5. Gandeepan, P.; Kaplarelis, N.; Santoro, S.; Vaccaro, L.; Ackermann, L. Biomass-Derived Solvents for Sustainable Transition Metal-Catalyzed C–H Activation. ACS Sustain. Chem. Eng. 2019, 7, 8023–8040.

6. Gandeepan, P.; Müller, T.; Zell, D.; Cera, G.; Warratz, S.; Ackermann, L. 3d Transition Metals for C–H Activation. Chem. Rev. 2019, 119, 2192–2452.

7. Clapham, S. E.; Hadzovic, A.; Morris, R. H. Mechanisms of the H₂-Hydrogenation and Transfer Hydrogenation of Polar Bonds Catalyzed by Ruthenium Hydride Complexes. Coord. Chem. Rev. 2004, 248, 2201–2237.

8. Kumar, P.; Gupta, R. The Wonderful World of Pyridine-2,6-Dicarboxamide Based Scaffolds. Dalton Trans. 2016, 45, 18769–18783.

9. Yadav, S.; Vijayan, P.; Gupta, R. Ruthenium Complexes of N/O/S Based Multidentate Ligands: Structural Diversities and Catalysis Perspectives. J. Organomet. Chem. 2021, 954, 122081.

A PATHWAY TO SUSTAINABLE ENERGY: Photocatalysis and solar energy utilization

Introduction:

Given the increasing energy requirement and concern for the environment, there is an imperative need for renewable and sustainable energy sources. Of the many green energy solutions available, photocatalysis has been a promising technological development in efficiently harnessing solar energy. The method replicates natural photosynthesis to facilitate chemical reactions through light energy, providing avenues for hydrogen generation, carbon dioxide reduction, water treatment, and self-cleaning surfaces.

This article discusses recent developments in photocatalysis for solar energy use, highlighting new photocatalysts, mechanisms, and applications that will help create a cleaner and greener future.

Fundamentals of Photocatalysis:

Photocatalysis relies on photo-induced charge separation in a semiconductor material. When a semiconductor is illuminated with light of suitable energy (equal to or higher than its bandgap energy), electrons (e⁻) are promoted from the valence band (VB) to the conduction band (CB), forming an electron-hole pair (e⁻/h⁺).^T These charge carriers are involved in oxidation and reduction reactions, resulting in the degradation of pollutants, hydrogen production, or CO_2 reduction.

Difficulties in Traditional Photocatalysts:

The older photocatalysts, e.g., titanium dioxide (TiO_2) and zinc oxide (ZnO) are afflicted by major shortcomings:

a. Large bandgap (~3.2 eV for TiO₂, ~3.3 eV for ZnO) \rightarrow absorbs light only in UV region (5% of sun's radiation).

b. Rapid charge carrier recombination \rightarrow lowers photocatalytic performance.

c. Limited activity in visible light, necessitating adaptations.

To overcome such obstacles, scientists have researched novel materials, doping techniques, heterojunctions, and nanostructures to increase photocatalytic activity.²

Recent Advances in Photocatalyst Materials:

1. Visible-Light-Responsive Photocatalysts-

As sunlight is largely composed of visible light (~43%), developing visible light-absorbing photocatalysts is essential. Graphitic carbon nitride $(g-C_3N_4)$ has emerged as a promising visible-light photocatalyst.

It is a metal-free, stable, and eco-friendly photocatalyst with Bandgap ~2.7 eV for visible light absorption



Uma Rani M.Sc. Chemistry IIT Delhi

Applications include water splitting, pollutant decomposition, and CO₂ reduction.

Drawbacks: Low surface area and rapid charge recombination.

Recent advances:

✓ N, S, P doping to facilitate charge separation.

 \checkmark Combinations with TiO₂, MoS₂ for increased efficiency.

2. Nanostructured Photocatalysts:

Nanotechnology has tremendously enhanced photocatalytic activity by increasing surface area and charge separation. Recent research has centered on nanostructured TiO₂, ZnO, and perovskite materials, showing better light absorption and reaction rates.

Nanostructured photocatalysts with at least one dimension in the nanometer range (1-100 nm) possess enhanced properties like a higher surface area, better light absorption, improved separation of charge carriers, and adjustable electronic properties. These advantageous properties render nanostructured photocatalysts highly efficient to use in solar energy conversion, water splitting, pollutant degradation, and CO_2 reduction.

Doping and Surface Modifications

Elemental doping (such as nitrogen, sulfur, and transition metals) has been used to modulate band gaps and improve light absorption in visible ranges.⁴ Surface plasmonic modifications using noble metals such as gold (Au) and silver (Ag) enhance enhanced charge carrier separation, enhancing photocatalytic performance.

3. Heterojunction Photocatalysts

Heterojunctions, which are created by combining two or more semiconductors, enhance charge transfer efficiency and increase light absorption ability. Some examples are $TiO_2/g-C_3N_4$ and $BiVO_4/ZnO$ heterojunctions, which have shown improved photocatalytic activity.

5. Metal-Organic Frameworks (MOFs) and Carbon-Based Catalysts

MOFs and carbon materials (e.g., graphene oxide, carbon dots) have been of interest due to their tunable structures and excellent electron transport capabilities. These materials possess high surface areas and effective charge separation, which makes them promising candidates for next-generation photocatalysis.

Applications of Photocatalysis in Solar Energy Utilization:

1. Hydrogen Production through Water Splitting

Photocatalytic solar-powered water splitting is a clean route for hydrogen production. Co-catalysts and reaction conditions have recently been optimized to improve the efficiency of hydrogen evolution.

2. Photocatalytic CO₂ Reduction

The photoreduction of CO_2 to useful fuels (e.g., methane, methanol) is a green method to combat carbon emissions. New catalysts such as Cu-doped TiO₂ and ZnO/CdS composites have demonstrated high efficiency in CO_2 photoreduction.

3. Environmental Remediation

Photocatalysis is of great importance in wastewater treatment and air cleaning. Recent progress has involved the creation of visible-light-driven photocatalysts for organic pollutant degradation and the removal of toxic gases.

Photocatalysis entails the utilization of semiconductor catalysts to promote chemical reactions under light irradiation. Regular photocatalysts such as titanium dioxide (TiO_2) , zinc oxide (ZnO), and graphitic carbon nitride $(g-C_3N_4)$ absorb light energy and produce electron-hole pairs, resulting in the creation of reactive oxygen species (ROS) such as hydroxyl radicals (•OH) and superoxide radicals $(O_2^{-}\bullet)$. These radicals decompose polymer chains, pollutant, and dyes into smaller molecules such as carbon dioxide (CO₂), water (H₂O), and organic acids.⁵

The general reaction of photo-degradation can be represented as:

pollutant + $hV \rightarrow$ Intermediate Products $\rightarrow CO_2 + H_2O +$ Biodegradable Compounds

4. Photocatalysis for Solar Desalination and Water Purification

Photocatalysts can harness solar energy to treat water by breaking down organic pollutants, inactivating bacteria, and desalinating seawater.

Recent Developments:

- ✓ Nanostructured catalysts for ultrafast pollutant removal.
- ✓ Self-cleaning and anti-bacterial coatings for water purification systems.
- \checkmark Hybrid systems that mix photocatalysis with membrane technology.

Challenges and Future Perspectives

Photocatalysis has tremendous promise for solar energy conversion, water treatment, and green chemistry but has a number of technical and commercial hurdles that must be overcome. Enhancing photocatalyst efficiency, stability, and scalability will be important for its universal adoption.

Future research must concentrate on:

- ✓ Creating low-cost and Earth-abundant photocatalysts.
- ✓ Increasing quantum efficiency using nanotechnology and AI.
- ✓ Combining photocatalysis with other renewable energy systems.

As material science, nanotechnology, and computational modeling continue to evolve, photocatalysis can play a central role in realizing a sustainable and carbon-neutral future for energy.

Conclusion

Photocatalysis presents a sustainable and efficient approach to solar energy utilization. Continuous innovations in photocatalyst materials and reaction engineering are paving the way for practical applications in hydrogen production, CO_2 reduction, and environmental remediation. Addressing current challenges will be crucial in realizing the full potential of photocatalysis for a greener future.

REFERENCES

1. Mohamadpour, F.; Amani, A. M. Photocatalytic Systems: Reactions, Mechanism, and Applications. RSC Adv. 2024, 14, 20609–20645.

2. Feliczak-Guzik, A. Nanomaterials as Photocatalysts—Synthesis and Their Potential Applications. Materials 2023, 16, 193.

3. Muneer, M.; Rasool, Z.; Parashar, S.; Almohyawi, A. M.; Moussa, Z.; Ahmed, S. A. Graphitic Carbon Nitride as Photocatalysts for the Degradation of Organic Pollutants in Aqueous Suspension: A Review. IntechOpen 2025, 46, 123.

4. Li, X.; Chen, Y.; Tao, Y.; Shen, L.; Xu, Z.; Bian, Z.; Li, H. Challenges of Photocatalysis and Their Coping Strategies. Chem Catalysis 2022, 16(2), 1315–1345.

5. Zhu, J.; Xiao, P.; Li, H.; Carabineiro, S. A. C. Graphitic Carbon Nitride: Synthesis, Properties, and Applications in Catalysis. ACS Appl. Mater. Interfaces 2014, 6, 16449–16465.





SINGLE ATOM CATALYSTS: REFORMING THE PROSPECTIVE OF CATALYSIS

Catalysis is the pillar of contemporary chemical industries, driving transformations in energy generation, conservation of environment and the synthesis of industrial chemicals. Conventional catalysts, generally composed of metal nanoparticles, have intrinsic pitfalls, one of them being poor atom utilization. These limitations have given rise to the development of single-atom catalysts (SACs), in which single metal atoms are dispersed on a supporting material to possess supreme catalytic efficiency and peculiar electronic properties.

SACs have transformed many catalytic reactions, such as hydrogen production, CO_2 reduction, fine chemical synthesis etc. With their unprecedented efficiency, preciseness and selectivity, answers to the challenges which the world is dealing with today like clean conversion of energy, carbon neutrality has been addressed. The exceptional activity of SACs is a result of their vigorous interactions with the supporting material like metal oxides, carbon etc as well as their well-defined atomic dispersion. SACs utilize isolated metal atoms as active sites, with each atom contributing to catalytic activity, which is in contrast to traditional catalysts, which rely on clusters of metal atoms to catalyse reactions.

The electronic structure of SACs is also preponderantly accountable for their catalytic features. Due to the exposed single metal atoms, they possesses distinct charge distributions and coordination framework, which accelerate the process of reactant adsorption and help minimize the activation energy barriers. The support material also affects these characteristics through a change in electronic density of the active site, adjusting its reactivity and selectivity. For instance, platinum SACs in fuel cells exhibit unique charge states over bulk platinum and result in better oxygen reduction reaction (ORR) kinetics and improved durability.

The mechanism of action of SACs varies from reaction to reaction. In electrocatalysis, SACs enable necessary energy conversion reactions like carbon dioxide reduction reaction (CO2RR) by facilitating optimal charge transfer at the interface. In heterogeneous catalysis and photocatalysis, SACs mediate selective hydrogenation and oxidation through either bond formation or bond breaking, and improves light absorption with separation of charges respectively. This makes them highly effectual for solar energy-based catalysis.

APPLICATIONS: SACs span over a wide array of applications. Some of the core applications are listed below:



SNEHA KOHLI M.SC. CHEMISTRY , I YEAR, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF DELHI

1. Energy Conversion and Storage:

SACs are used in clean energy technologies, especially fuel cells and hydrogen generation. Effective catalysts for the oxygen reduction reaction are required by fuel cells to boost efficacy of energy conversion. Conventional platinum-based catalysts, while efficient, are costly and prone to degradation. On the other hand, platinum SACs on carbon supports are known to display exceptional oxygen reduction reaction activity, boosted stability, and reduced usage of platinum, making them a promising option for future fuel cells.¹

Hydrogen evolution reaction (HER) and splitting of water for production of clean hydrogen are amongst the most ground-breaking application of SACs. Nickel and cobalt SACs exhibit high catalytic behavior and serve as low-cost alternatives in comparison to traditional catalysts.² The development of hydrogen-based energy systems which are essential for a future free of carbon, is facilitated by employing SACs. Additionally, SACs are used in electrochemical CO₂ reduction, wherein CO₂ is reduced to fuels like syngas etc. Chemicals and fuels made up through CO₂ reduction is crucial to achieve the objective of carbon neutrality. CO₂ reduction catalysts used conventionally generally have low selectivity and energy prodigality, but copper and iron SACs supported on nitrogen-doped carbon, illustrated excellency in selective synthesis of target products.³ Ammonia synthesis, which is crucial for both storing hydrogen and manufacturing fertilizers, can be achieved using SACs. Molybdenum-based single atom catalysts, have showcased catalytic reduction of nitrogen, reducing the need of energy by high amount.⁴

2. Environmental Remediation:

SACs have showcased successful results in environmental catalysis, especially in air and water cleaning. Catalytic transformers in the automotive industry , utilizes SACs to decompose poisonous gases like nitrogen oxides and volatile organic compounds. For example, ceria-supported platinum SACs have demonstrated better CO oxidation activity, thereby decreasing pollution emissions leading to cleaner air.⁵ SACs are also used in wastewater treatment. Iron-nitrogen-carbon (Fe-N-C) SACs have been found to be extremely effectual in degrading hazardous chemical making them very beneficial for water purification.⁶

SACs also have promising effects on plastic waste degradation. Plastics are uncooperative towards decomposition, but some ruthenium-based SACs have exhibited proficiency in hydrogenolysis of polyethylene offering a possible path for sustainable plastic upcycling by catalysing the selective conversion of plastic into useful hydrocarbons.⁷ Given that plastic management is a major issue, SACs' ability to facilitate effective recycling procedures may have significant environmental effects.

3. Chemical Industry:

Selective oxidation, fine chemical synthesis and hydrogenation has also been benefitted by SACs. These catalysts with their definite atomic active sites, enable precise management of reaction pathways with great veracity, increasing yield and decreasing waste. For example, palladium SACs have been used to boost ethylene yield by selective hydrogenation, minimizing the production of undesirable by-products.⁸ These innovations reduce the utilization of hazardous substances and enhance the efficiency of chemical production, emphasizing the role of SACs in sustainable production operations.

Biomass conversion is another potential use of SACs which entails transformation of renewable biomass sources into valuable biofuels and chemicals. Cobalt-based SACs have also shown outstanding catalytic activity in decomposition of lignin-based compounds to biofuels.

SACs face many challenges for large-scale commercialization. One of the major issues being stability, as catalyst can get deactivated when single metal atoms migrate and cluster under rigorous conditions. Additionally, scalability is also a concern, as attaining invariable atomic dispersion during large-scale SAC production is a complicated task. Another challenge is cost, specifically for noble metal SACs such as platinum and palladium, which are in need of optimization.

Single-atom catalysts represent an innovative development in catalysis, providing superlative efficiency, accuracy and environmental safe. Even though challenges persist, ongoing research and technological advancements are building up the gap to empower the practical relevance of SACs. To conclude, SACs are set to lead the way in catalysis, as the globe moves toward clean energy and sustainable industrial practices.

REFERENCES

1. Wang, X.; Li, Z.; Qu, Y.; Yuan, T.; Wang, W.; Wu, Y.; Li, Y. Review of Metal Catalysts for Oxygen Reduction Reaction: From Nanoscale Engineering to Atomic Design. Chem 2019, 5(6), 1486–1511.

2. Zhu, Y.; Su, J.; Liao, J.; Peng, H.; Wang, Z.; Wang, Y.; Li, W. Transition Metal Single-Atom Catalysts for Water Splitting: Unravelling Coordination Strategies and Catalytic Mechanisms for Sustainable Hydrogen Generation. Nanoscale Adv. 2025, 6, 100491.

3. Kale, H. B.; Kute, A. D.; Gaikwad, R. P.; Fornasiero, P.; Zbořil, R.; Gawande, M. B. Synthesis and Energy Applications of Copper-Based Single-Atom Electrocatalysts. Coord. Chem. Rev. 2024, 502, 215602.

4. Akter, R.; Shah, S. S.; Ehsan, M. A.; Shaikh, M. N.; Zahir, M. H.; Aziz, M. A.; Ahammad, A. S. Transition-Metal-Based Catalysts for Electrochemical Synthesis of Ammonia by Nitrogen Reduction Reaction: Advancing the Green Ammonia Economy. Chem.–Asian J. 2024, 19(6), e202300797.

5. Xie, S.; Lu, Y.; Ye, K.; Tan, W.; Cao, S.; Wang, C.; Liu, F. Enhancing the Carbon Monoxide Oxidation Performance through Surface Defect Enrichment of Ceria-Based Supports for Platinum Catalyst. Environ. Sci. Technol. 2024, 58(28), 12731–12741.

6. Zeng, H.; Chen, Y.; Xu, J.; Li, J.; Li, D.; Zhang, J. Preparation, Characterization of Iron-Based Single-Atom Catalysts and Its Application for Photocatalytic Degradation of Contaminants in Water. J. Environ. Chem. Eng. 2023, 11(5), 110681.

7. Rorrer, J. E.; Beckham, G. T.; Román-Leshkov, Y. Conversion of Polyolefin Waste to Liquid Alkanes with Ru-Based Catalysts under Mild Conditions. J. Am. Chem. Soc. 2020, 1(1), 8–12.

8. Benavidez, A. D.; Burton, P. D.; Nogales, J. L.; Jenkins, A. R.; Ivanov, S. A.; Miller, J. T.; Daye, A. K. Improved Selectivity of Carbon-Supported Palladium Catalysts for the Hydrogenation of Acetylene in Excess Ethylene. Appl. Catal., A 2014, 482, 108–115.

Ionic Liquids (ILs) as an Emerging Research Interest in Catalysis

Catalysts are used in many reactions to facilitate the reaction rates and get the required products in less reaction times. Many feasible reactions that were earlier not witnessed due to slow reaction rates are now realized due to catalysts being available for the same. A catalyst involves itself with the chemical components in the process and does not alter the products in the course of the reaction. As the 21st century is a lot more concerned about the sustainability of the reaction conditions than the synthesized material it is important that some light is shed upon sustainable emerging catalysts like ionic liquids (ILs). Although their potential in accelerating reaction dynamics in a variety of reactions has been much studied, research is still going on in this subject to improvise their activity or selectivity as desired in the process. ILs are not a new concept and date back to the early 1900s. Although, the discovery of the first ionic liquid is disputed, many scientists still agree that Paul Walden was the first to discover ILs in 1914. He studied the physical properties of ethyl ammonium nitrate [(EtNH3) (NO3): m.p:13-14 degree celsius and considered it as a "molten salt"." Since the subject of ILs was not developed at that time, his work didn't gain much recognition. As research on this topic grew, many ILs were prepared and their applications were explored. Ionic liquids (ILs), as the name suggests are low melting salts which do not exist as solids but as liquids. A more general definition states that any salt which has a melting point less than 100 degree celsius is considered as an ionic liquid and those with melting point less than room temperature are known as room temperature ionic liquids or RTILs. In an ionic liquid, the cation is usually bulky with organic roots like quaternary phosphonium and also ammonium, heteroaromatics like 1,3 -dikylimidazolium, Nalkylpyridinium and N,N-dialkylpyridinium while,



Aleena Shakreen M.Sc. Chemistry, I year Department of Chemistry, University of Delhi

the anion is typically a poly tetrafluoroborate, triflate etc.^{2,3} The structural differences between the counter ions result in ineffective packing of crystal structure and charge delocalization in the respective ions reduces the ionic attraction between the ion pair. These two factors are responsible for imparting low melting points to ILs.^{3]} The properties of an ILs depends upon the cation and anion involved as constituents; hence are highly tuneable and find wide applications in chemical industries. Just varying the cation and anion can give a new IL with novel properties.

The applications of ILs in Catalysis are widely accepted, as these ILs can be altered according to the desired effects. Electrochemistry and biocatalysis are some of the areas where ILs are gaining popularity as catalysts. For example pyridinium and imidazolium when used ions as cations alongside tetrachloroaluminate, yield ILs that can be used as electrolytes in batteries and also for metal surface electroplating.⁴ While considering the potential of ILs in catalysis, it is important to note the mechanism of operation of these IL based catalytic systems. Two major concepts are considered under the former discussion: Liquid-Liquid biphasic catalysis, IL thin film catalysis. In catalytic action of ionic liquids, complex interactions like hydrogen bonding, Van der Waals and of course coulombic forces are involved.

ILs in Liquid-Liquid Biphasic Catalysis and it's Applications

In this category, either the IL itself acts as the catalyst, or it behaves as a solvent for dissolved catalytic (NPs) or transition metal catalysts. Chloroaluminate ILs, that are acidic in nature serve as catalysts for acid catalyzed reactions like Friedel-Crafts alkylation, Friedel-Crafts Acylation , carbonylation reactions, cracking, oligomerization and alkylation reactions. Since the acid is provided by IL, the reactions involved are sustainable as compared to non-IL based traditional transformations. When transition metal catalysts are dissolved in ILs, they are used in hydrogenation, oxidation, hydro-formylation, dimerisation, telomerization and oligomerization reactions along with Pd-catalyzed coupling reactions. Catalytic NPs infused in ILs can be used to catalyze hydrogenation of alkenes, arenes and ketones. In all these reactions discussed for biphasic catalysis, the IL is easily recovered after the product formation. Additionally, the transition metal based catalysts can also be recovered under this technique. A drawback encountered in this category of catalysis is that bulk amounts of ILs are required and since ILs are way expensive that typical organic solvents, the process becomes less economical.

IL Thin Film Catalysis and it's Applications

This type of catalysis is more efficient than the biphasic one as the amount of IL load is significantly reduced. The ionic liquid is spread as thin film over either a porous support-SILP catalysis (Supported Ionic liquid Phase Catalysis) or a solid catalyst to alter its catalytic activity-SCILL catalysis (Solid Coated Ionic Liquid Layer).

SILP catalysis has proven useful in hydrogenation, enantioselective hydrogenation, alkene metathesis, carbonylation of methanol and hydroamination. Another example includes the use of acidic chloroaluminate based IL immobilised on porous support to carry out alkylation of aromatic systems. IL- $[C_4Cllm][C_8H_{17}SO_4]$ impregnated on Ni/SiO2 catalyst (SCILL catalysis) has proven efficient in catalysing the transformation of cyclooctadiene to cyclooctane and cyclooctene. Additionally, regioselective hydrogenation of citral has been carried out using ILs based on anions like $[N(CN)_2]$ -, $[Tf_2N]$ -, and $[PF_6]$ - embedded upon Pd/SiO2 to give selective formation of citronellal.

Conclusion

Depending upon the different combinations of cation and anion, a million simple ILs can be made, and for binary ILs the estimate goes upto billion and for ternary systems a trillion different possible Ionic liquids can be prepared easily. Until today, only a few hundred ILs are commercialized, and their applications are still being uncovered. With so many more possible ILs out there unexplored, one can think of the various ways in which these ILs can be further exploited. Hence, the amount of attraction this area of catalysis is gaining can't be questioned.

The very famous BASIL process is generating alkoxyphenylphosphines, includes ILs in the process. Breaking azeotropic mixtures, cellulose dissolution, lithium-ion batteries, ionikylation by PetroChina are some of the very famous processes where ILs have been used for a very long time. Other applications include biodiesel synthesis and water remediation. Despite the wide variety of applications these ILs possess, their use is still not made common in the laboratories for they are much more expensive than the usual solvents used. However, these ILs can be considered as a one time investment as their recoverability and resuability is assured. More work can be done to make these green solvents more economical so that their use can be expanded.

REFERENCES

1. Plechkova, N. V.; Seddon, K. R. Applications of Ionic Liquids in the Chemical Industry. Chem. Soc. Rev. 2008, 37(1), 123–150. 2. Welton, T. Ionic Liquids in Catalysis. Coord. Chem. Rev. 2004, 248(21–24), 2459–2477.

3. McNeice, P.; Marr, P. C.; Marr, A. C. Basic Ionic Liquids for Catalysis: The Road to Greater Stability. Catal. Sci. Technol. 2021, 11(3), 726–741.

4. Forsyth, S. A.; Pringle, J. M.; MacFarlane, D. R. Ionic Liquids—An Overview. Aust. J. Chem. 2004, 57(2), 113–119.

5. Steinrueck, H. P.; Wasserscheid, P. Ionic Liquids in Catalysis. Catal. Lett. 2015, 145, 380–397.



The need for sustainable technologies has never been greater as the globe struggles with the twin issues of climate change and the depletion of fossil fuel resources. CO_2 hydrogenation to value-added chemicals is one of the many approaches that have been investigated, and it appears to be a promising one. With this technology, a significant greenhouse gas, CO_2 , is transformed into useful chemicals, reducing its impact on the environment and fostering a circular carbon economy. The science, development, and sustainability implications of CO_2 hydrogenation for the synthesis of chemicals like hydrocarbons, methanol, and formic acid are explored in this article.

More than 70% of greenhouse gas emissions are carbon dioxide (CO₂), which is the main cause of global warming. With yearly emissions exceeding 36 billion tons worldwide, transportation, power generation, and industrial processes are the main sources of CO₂ emissions. Although cutting emissions at their source is important, carbon capture and utilization (CCU) provides an alternative strategy by turning CO₂ into useful products. One of the most promising CCU techniques is hydrogenation, which is the chemical reaction of CO₂ with hydrogen (H₂). In addition to lowering the atmospheric concentration of CO₂, the process uses renewable energy to electrolyze water and produce H₂, establishing a sustainable chemical synthesis pathway. Depending on the catalyst and reaction conditions, CO₂ hydrogenation is the process of reacting CO₂ with hydrogen to produce a variety of products. Among the main

products are:

Formic Acid

Formic acid (FA), which is hydrogenated by CO₂, is a useful commodity chemical. With 4.4 wt% hydrogen, it is a less harmful, non-flammable liquid that is also thought to be a promising material for storing hydrogen because, even at room temperature, the chemically stored H₂ in formic acid can be released under controlled conditions with the help of the right catalysts. Furthermore, the first and essential step in reducing CO₂ to other chemicals like methanol and hydrocarbons is the hydrogenation of CO₂ to FA.

Methanol

Methanol is an alternate building block for producing chemicals and even gasoline in light of the depletion of nonrenewable energy sources. According to Olah et al.'s discussion of the "methanol economy" concept, methanol may become essential shortly, and CO₂ hydrogenation is one of the most promising and regenerative methods of producing methanol. Methanol is currently among the top five commodity chemicals shipped annually worldwide. It is a major raw material for the chemical industry. It is being utilized more and more in the methanol to olefins (MTO) process, which is an intermediate for the synthesis of several different chemicals, such as acetic acid, formaldehyde, and methyl tert-butyl ether. The majority of these substances are the fundamental components of numerous everyday commodities, such as paints, polymers, adhesives, resins, and antifreezes. Methanol has also been shown to be a great fuel blend for internal combustion engines and can be used directly in fuel cells.

Hydrocarbons

The Fischer-Tropsch synthesis pathway can transform CO_2 into longchain hydrocarbons and synthetic fuels. Although energy-intensive, these reactions are essential for creating sustainable fuels because they require high temperatures and pressures.

Other Products

Using the reverse water-gas shift reaction, CO_2 hydrogenation can also produce chemicals of industrial significance, such as urea, carbon monoxide, and dimethyl ether (DME).

Regardless its potential, CO_2 hydrogenation has a number of issues that need to be resolved in order to realize its full potential. Traditionally, the chemical inertia of CO₂ gas has posed significant barriers to its industrial use. Because of its exceptional chemical stability, the CO₂ molecule is therefore regarded as being incredibly inert. To activate the CO₂ molecule, additional energy is required to overcome its thermodynamically low level. A promising strategy for the future is a chemical reaction that creates high-energy intermediates that could then transport the CO₂ gas to the target substrates.

However, because CO₂ is inert, the process of CO₂ reduction is not spontaneous. In this instance, CO₂ must be activated by chemically functional sites on catalytic surfaces, and catalysts have significance in this process. The conversion of CO₂ can be accelerated by certain metals and/or metal oxides. The presence of surface O₂ vacancies and surface defect sites on metal-oxide-based catalysts significantly speeds up CO₂ conversions. Unoccupied oxygen spaces can be the focus of electrons transferred to the neutral CO₂ molecule, acting as habitats for CO₂ adsorption. Another factor to consider during CO₂ hydrogenation is hydrogen production via water electrolysis, which is a critical step in the process but is extremely energyintensive. This reliance on energyintensive processes reduces economic viability, particularly in areas where renewable energy is scarce or costly. Scaling up renewable energy capacity is critical for making the process sustainable and cost-effective. Developing advanced catalysts is crucial for improving CO₂

hydrogenation efficiency and selectivity. To achieve the desired product while minimizing byproducts, a catalyst must activate the stable CO_2 molecule. Recent improvements in catalyst design include use of Bimetallic catalysts: Combining two metals, produces synergistic effects.

Non-noble metal catalysts: To cut costs, researchers are looking into catalysts based on common metals such as Ni, Fe, and Cu. While these catalysts are less active than noble metals, they can be modified with supports to improve performance.

Support materials: Carbon, silica, and LDHs are examples of supports with a large surface area, which promote catalyst dispersion. They also change the electronic environment of active sites, which affects reaction pathways.

Single-atom catalysts: New research focuses on single-atom catalysts, in which metal atoms are dispersed on supports. These catalysts have high atom efficiency and unique electronic properties. So, the hydrogenation of CO_2 to value-added chemicals has profound implications for sustainability using catalyst design and advancements. In this way, recognizing CO_2 as a resource rather than an issue represents a shift in our approach to sustainability. CO_2 hydrogenation paves the way for a circular economy that transforms waste into wealth and promotes innovation. This transformative approach has the potential to become a cornerstone in combating climate change while also promoting economic growth, demonstrating that sustainability and development can coexist.

REFERENCES

- 1. Wang, J.; Zhang, G.; Zhu, J.; Zhang, X.; Ding, F.; Zhang, A.; Song, C. ACS Catal. 2021, 11 (3), 1406–1423.
- 2. Mori, K.; Taga, T.; Yamashita, H. ACS Catal. 2017, 7 (5), 3147–3151.
- 3. Soni, Y.; Gupta, S.; Vinod, C. P. Mol. Catal. 2021, 511, 111732.
- 4. Ye, J.; Dimitratos, N.; Rossi, L. M.; Thonemann, N.; Beale, A. M.; Wojcieszak, R. Science 2025, 387 (6737).





STUDENT'S CORNER







86

CHEMZ



BATCH OF 2022

The time has come to say goodbye, With misty eyes and heavy sigh.
Though parting ways may bring us pain, The bonds we've built will still remain.
New paths await, fresh skies ahead, With memories in hearts we've fed.
Farewell, not end — just a new start, Forever close, though miles apart.







CHEMZONE 2025





BATCH OF 2024

CHEMZONE 2025

CHEMZONE

2025

STUDENT'S CORNER

CONSIDER EVERYTHING

FUNFACTS



Ra

(226)

Po



The world's most expensive spice, Saffron, is actually a chemical compound called crocin

You are made of stardust : almost all elements on Earth, including those in our bodies, were created inside stars.



Butterflies taste with their feet: they have tiny sensors on their feet that help them detect sweet or bitter substances.



Neme Section

MG



OurShining Stars

This section is dedicated to appreciating the remarkable individual and collective achievements of the Chemistry Department. It celebrates the hard work, innovation, and commitment of both students and faculty, recognizing their outstanding contributions in academics, research, and extracurriculars that have brought pride and distinction to the department.





Poster presentation on Preparation of Natural Eco-Friendly and Sustainable polyherbal soaps for treatment of Skin Allergy in National Conference on Ashwagandha: A Health Promoter - From Fields to Pharmacy in Gargi college, University of Delhi on October 18, 2024 and secured First position.

Received a cash prize of 7000 and rewarded as Best Innovator College at Skills, Enterpreneurship Expo 2024





Tug of war in JMC Annual NCC fest - Agni Dasta, Junoon' 25 Position - Runner up Date - 24 March, 2025

Quiz Competition at Shiv Nadar University on 12 September, 2024 and secured \leftarrow third position



Our Shining Stars

Individual Achievements





Name : Kamakshi Sehgal Course : B.Sc. (Hons) Chemistry - II year Competition : Weightlifting (Under 89 kg), Delhi University Inter-College Prize - Gold medal

Name - Chhaya Pandey Course - B.Sc. (Hons) Chemistry - I year Event - Fabric Painting and Handcraft Competition Prize - Consolation Certificate





Name - Mansi Rawat Course - B.Sc. (Hons) Chemistry - I year Event-An online quiz on "Environmental Awareness Quiz" Position - First Date - 25 february, 2025

Name - Divya Raj Course - B.Sc. (Hons) Chemistry - III year Event-Paper Presentation , Kalindi College, University of Delhi Position - Third Date - 25 February, 2025





a start

IIT JAM Rank Holders

Name - Saloni Bharti Exam - IIT JAM Rank - 380



Name - Prachi Singh Exam - IIT JAM Rank - 1016



The (UN)Friendly Nature of Denim

Thinking of buying new pair jeans, baggy or flared, wide leg or skinny? Ever wondered how your favorite pair of jeans are made. How it's dyed to achieve the perfect finish and texture. The environmental cost of producing denim is often overlooked. From the cultivation of cotton to dyeing, finishing, and disposal, every stage of denim production carries significant ecological consequences.

The appealing blue colour your denim gets is from Indigo dye. Despite being a relatively low vat dye, indigo is used because of the worn out look it gives to denim. The process involved in dyeing is resource intensive and polluting. As indigo is water insoluble it is treated with reducing agents and alkalis . This transformation requires vast amounts of sodium hydrogensulfite and caustic soda. Not all the dye used in the process binds to the fabric. A major portion remains unfixed and is washed away, entering nearby water systems. These dyes contribute to water turbidity and are often toxic, carcinogenic, or mutagenic. This disrupts aquatic lives and poses health hazards to humans and wildlife. Textile dyeing is the second largest contributor in polluting water globally.Before the fabric is dyed ,it undergoes desizing which involves removing adhesives substances applied during weaving. Enzyme based desizing is done which is softer on the fabric but harsh to the environment, and further adds to wastewater containing chemicals.

In addition to chemical toxins, the wastewater from denim production is characterized by high levels of pH, biological oxygen demand (BOD), chemical oxygen demand (COD), total dissolved solids (TDS), and other pollutants such as chlorides, sulfates, phenols, and suspended solids. These contaminants not only degrade water quality but also pose long-term threats to agriculture and drinking water sources. Denim production uses enormous amounts of water. It is estimated that producing just one kilogram of denim fabric results in the release of 40 to 65 liters of wastewater. This becomes especially concerning when considering the scale of global denim production.

To give jeans the perfect faded look, it is bleached and washed. Acids and chemicals are used to lighten the colour . These chemicals are again thoroughly washed off before the jeans is ready to wear ,this further adds to the amount of water used and wastewater generated. The denim

lifecycle, from cotton farming to consumer use and disposal, releases a significant amount of carbon dioxide. On average, a single pair of jeans is responsible for about 33.4 kg of CO₂ emissions. Denim production is also highly energy-intensive.



Processes like spinning, weaving, dyeing, and finishing all require large amounts of electricity, much of which is generated from fossil fuels. This results in substantial greenhouse gas emissions and contributes to air pollution. To give jeans the perfect faded look, it is bleached and washed. Acids and chemicals are used to lighten the colour . These chemicals are again thoroughly washed off before the jeans is ready to wear ,this further adds to the amount of water used and wastewater generated. The denim lifecycle, from cotton farming to consumer use and disposal, releases a significant amount of carbon dioxide. On average, a single pair of jeans is responsible for about 33.4 kg of CO₂ emissions. Denim production is also highly energyintensive. Processes like spinning, weaving, dyeing, and finishing all require large amounts of electricity, much of which is generated from fossil fuels. This results in substantial greenhouse gas emissions and contributes to air pollution.

Denim may look simple on the outside, but its journey from raw material to finished product is riddled with environmental challenges.

As consumers what can we do :

- Buy less, but better :pick high-quality denim that lasts longer and is made from sustainable materials.
- Go for ethical brands: Look for certifications such as GOTS, OEKO-TEX, or Fair Trade, which denote better environmental and labor practices.
- Wash sparingly using cold water .
- Don't throw away old jeans—donate, repair, or recycle them.

Tanya Kumari B.Sc. (Hons) Chemistry II Year

सफलता

घर गए थे हम उसके पूछा उसकी पढाई का हाल घर ,परिवार, नौकरी का हाल दुनिया भर की तमाम बातें की और कैसे ही व्यतीत कई रातें की कुछ पूछने का जो न खयाल रहा वो कैसी है? कैसा उसके मन का हाल रहा? क्यूं शांत रहने लगी है वो? ये चेहरे पर कैसी उदासी है जो उसकी हँसी में छिप जाती है? आखिर वो कौनसी दुनिया है जिसमें वो खो जाती है खैर नहीं पूछा तो नहीं पूछा और ये कोई पूछने वाले सवाल थोड़े है। होगी किसी बात पर उदास वो कोई बवाल थोडे है। बेजान पडी थी वो इंसान आज अपने कमरे में चहकता था घर जिसके रहने से वहां आए लोगों ने तो बडी आसानी से कह दिया बुजदिल रही होगी असफलता से डर गई

इन्हें क्या फर्क पड़ता कि वो किसी विपदाओं से लड गई जो तुम कभी बैठो इनके पास या गुजरो उनके करीब से बताएंगे तुम्हें ये अपनी सफलता की परिभाषा बडे ही अदब से बड़ा घर,बड़ी गाड़ी,महंगी घड़ी,महंगी साडी यही तो होती है सफलता और हां,होना चाहिए तुम्हारी तन्खवाह का वजन भारी ना सुनना तुम इनकी एक ना बंधना इनकी कही परिभाषा में ये ज़िंदगी तुम्हारी है, ये सफलता भी तुम्हारी और इसे परिभाषित करने की अब बारी भी तुम्हारी है।

> Mahima Yaday B.Sc. (Hons) Chemistry II year



DEPARTMENT OF CHEMISTRY MAITREYI COLLEGE UNIVERSITY OF DELHI

